

# OAK RIDGE NATIONAL LABORATORY

MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

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March 3, 2006

Dr. Anjuli Bamzai  
U.S. Department of Energy  
Germantown Building  
1000 Independence Ave., SW  
Washington, DC 20585

**Subject: Program Announcement LAB 06-04 Scientific Discovery through Advanced Computing (SciDAC): Scientific Application Partnership**

Dear Dr. Bamzai:

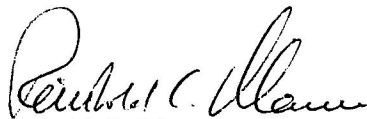
Enclosed please find the proposal entitled, "A Scalable and Extensible Earth System Model for Climate Change Science," for your consideration.

This work proposes the creation of a first-generation Earth system model based on the Community Climate System Model, which treats the coupling between the physical, chemical and biogeochemical processes in the climate system. The model will include comprehensive treatments of the processes governing well-mixed greenhouse gases, natural and anthropogenic aerosols, the aerosol indirect effect, and tropospheric ozone for climate change studies.

The total request is \$31M over 5 years.

Questions regarding this proposal should be directed to John B. Drake at (865) 574-8670 or drakejb@ornl.gov.

Sincerely,



Reinhold C. Mann  
Associate Laboratory Director  
Biological and Environmental Sciences

RM/cs

c: J. B. Drake  
J. A. Nichols  
File

United States Government

Department of Energy

Oak Ridge Office

# memorandum

DATE: March 3, 2006

REPLY TO  
ATTN OF: SE-31:Buhaly

SUBJECT: **NEW FIELD WORK PROPOSAL (FWP) SUBMITTED IN RESPONSE TO  
PROGRAM ANNOUNCEMENT LAB 06-04**

TO: Jerry W. Elwood, Climate Change Research Division, SC-23.3, HQ/GTN

Attached is a FWP entitled, "A Scalable and Extensible Earth System Model for Climate Change" prepared by Oak Ridge National Laboratory (ORNL) in response to the Program Announcement LAB 06-04, Scientific Discovery through Advanced Computing (SciDAC).

If this proposal is selected for funding, please let me know as soon as practical. Upon receipt of the Work Authorization and funding in the Approved Funding Program Plan, we would authorize ORNL to begin work.

If there are any questions, please contact me at (865) 576-1954 or [buhalydl@ornl.gov](mailto:buhalydl@ornl.gov). The ORNL Principal Investigators may be reached at the telephone number and address shown on the attached table.



David L. Buhaly  
Program Coordinator  
Laboratory Support Team

#### Attachments

1. Proposal

cc w/attachments 1:

J. Y. Hackett, FM-72, ORO

R. K. Bain, ORNL

J. A. Nichols

R. C. Mann, ORNL

J. Wadsworth, ORNL – RC



# Face Page

TITLE OF PROPOSED RESEARCH:  
A Scalable and Extensible Earth System Model for Climate Change Science

1. CATALOG OF FEDERAL DOMESTIC ASSISTANCE #  
81,049

2. CONGRESSIONAL DISTRICT:  
Applicant Organization's District: 2nd & 3rd Districts  
Project Site's District: 2nd & 3rd Districts

3A. I.R.S. ENTITY IDENTIFICATION OR SSN:  
621788235

3B. DUNS Number:  
\_\_\_\_\_

4. AREA OF RESEARCH OR ANNOUNCEMENT TITLE/#:  
LAB-06-04

5. HAS THIS RESEARCH PROPOSAL BEEN SUBMITTED TO ANY OTHER FEDERAL AGENCY?  
 YES  NO

PLEASE LIST \_\_\_\_\_

6. DOE/OER PROGRAM STAFF CONTACT (if known):  
Dr. Anjuli Bamzai

7. TYPE OF APPLICATION:  
 New  Renewal  
 Continuation  Revision  
 Supplement

8. ORGANIZATION TYPE:  
 Local Govt.  State Govt.  
 Non-Profit  Hospital  
 Indian Tribal Govt.  Individual  
 Other  Inst. of Higher Educ.  
 For-Profit  
 Small Business  Disadvan. Business  
 Women-Owned  8(a)

9. CURRENT DOE AWARD # (IF APPLICABLE):  
None

10. WILL THIS RESEARCH INVOLVE:  
10A. Human Subjects  No  If yes  
Exemption No. \_\_\_\_\_ or  
IRB Approval Date \_\_\_\_\_  
Assurance of Compliance No: \_\_\_\_\_  
10B. Vertebrate Animals  No  If yes  
IACUC Approval Date \_\_\_\_\_ or  
Animal Welfare Assurance No: \_\_\_\_\_

11. AMOUNT REQUESTED FROM DOE FOR ENTIRE PROJECT PERIOD \$ 30,750,000.00

12. DURATION OF ENTIRE PROJECT PERIOD:  
07/01/06 to 09/30/11  
MM/DD/YY MM/DD/YY

13. REQUESTED AWARD START DATE  
07/01/06  
MM/DD/YY

14. IS APPLICANT DELINQUENT ON ANY FEDERAL DEBT?  
 Yes (attach an explanation)  No

15. PRINCIPAL INVESTIGATOR/PROGRAM DIRECTOR  
NAME John B. Drake  
TITLE Group Leader  
ADDRESS Cimate Dynamics  
Oak Ridge National Laboratory  
P.O. Box 2008, MS 6016  
Oak Ridge, TN 37830  
PHONE NUMBER 865-574-8670

16. ORGANIZATION'S NAME Oak Ridge National Laboratory  
ADDRESS P.O. Box 2008  
Oak Ridge, TN 37831-6163

CERTIFYING REPRESENTATIVE'S  
NAME Reinhold C. Mann  
TITLE Associate Laboratory Director  
PHONE NUMBER (865) 574-4333

SIGNATURE OF PRINCIPAL INVESTIGATOR/ PROGRAM DIRECTOR  
(please type in full name if electronically submitted)  
Date 03-03-2006

SIGNATURE OF ORGANIZATION'S CERTIFYING REPRESENTATIVE  
(please type in full name if electronically submitted)  
Date 3/3/06

PI/PD ASSURANCE: I agree to accept responsibility for the scientific conduct of the project and to provide the required progress reports if an award is made as a result of this submission. Willful provision of false information is a criminal offense. (U.S. Code, Title 18, Section 1001).

CERTIFICATION and ACCEPTANCE: I certify that the statements herein are true and complete to the best of my knowledge, and accept the obligation to comply with DOE terms and conditions if an award is made as the result of this submission. A willfully false certification is a criminal offense. (U.S. Code, Title 18, Section 1001).

NOTICE FOR HANDLING PROPOSALS  
This submission is to be used only for DOE evaluation purposes and this notice shall be affixed to any reproduction or abstract thereof. All Government and non-Government personnel handling this submission shall exercise extreme care to ensure that the information contained herein is not duplicated, used, or disclosed in whole or in part for any purpose other than evaluation without written permission except that if an award is made based on this submission, the terms of the award shall control disclosure and use. This notice does not limit the Government's right to use information contained in the submission if it is obtainable from another source without restriction. This is a Government notice, and shall not itself be construed to impose any liability upon the Government or Government personnel for any disclosure or use of data contained in this submission.

PRIVACY ACT STATEMENT  
If applicable, you are requested, in accordance with 5 U.S.C., Sec. 562A, to voluntarily provide your Social Security Number (SSN). However, you will not be denied any right, benefit, or privilege provided by law because of a refusal to disclose your SSN. We request your SSN to aid in accurate identification, referral and review of applications for research/training support for efficient management of Office of Science grant/contract programs.

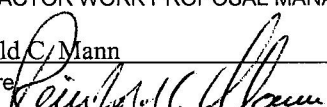
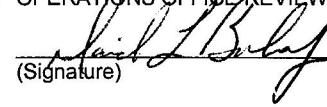
**PROGRAM: KP Biological and Environmental Research**

1. WORK PROPOSAL NO. ERKP576	2. REVISION NO. 0	3. DATE PREPARED 03-03-2006	12
4. WORK PROPOSAL TITLE: A Scalable and Extensible Earth System Model for Climate Change		5. BUDGET AND REPORTING CODE KP 12 01 01 0	
6. WORK PROPOSAL TERM  BEGIN: 07-01-2006    END: 09-30-2011		PATENT STATUS This proposal is being transmitted in advance of patent review for evaluation purposes only. No further dissemination or publication shall be made without prior approval of the Assistant General Counsel for Patents, DOE.	7. Is This Work Proposal Included in the Institutional Plan?  <input checked="" type="checkbox"/> Yes <input type="checkbox"/> No
NAME: (Last, First, MI) (Phone Number) 8. HEADQUARTERS/OPERATIONS OFFICE PROGRAM MANAGER: Elwood, Jerry W.    (301)903-3281		11. HEADQUARTERS ORGANIZATIONS: <b>Office of Science</b>	14. DOE ORGANIZATION CODE: <b>SC</b>
9. OPERATIONS OFFICE WORK PROPOSAL REVIEWER: Buhaly, David L.    (865)576-1954		12. FIELD OFFICE: <b>Oak Ridge Operations</b>	15. DOE ORGANIZATION CODE: <b>ON</b>
10. CONTRACTOR WORK PROPOSAL PRINCIPAL INVESTIGATOR(S)/MANAGER:  Drake, John B.    (865)574-8670		13. CONTRACTOR NAME: <b>Oak Ridge National Laboratory Managed by UT-Battelle, LLC For the U.S. Department of Energy Post Office Box 2008 Oak Ridge, TN 37831</b>	16. DOE CONTRACTOR CODE: <b>41</b>

17. WORK PROPOSAL DESCRIPTION (Approach, anticipated benefits in 200 words or less)

Our challenge is to create a first generation Earth system model based on the Community Climate System Model (CCSM) that treats the coupling between the physical, chemical, and biogeochemical processes in the climate system. The model will include comprehensive treatments of the processes governing well-mixed greenhouse gases, natural and anthropogenic aerosols, the aerosol indirect effect, and tropospheric ozone for climate change studies. We will improve the representation of carbon and chemical processes, particularly for treatment of greenhouse gas emissions and aerosol feedbacks in collaboration with the U.S. Department of Energy (DOE) Aerosol Science program and the DOE Carbon Cycle Research program.

Integration of new numerical methods or model improvements requires substantial software expertise and knowledge of the component models for the rapid evaluation of these new methods. In the near term, CCSM will require improved scalability to thousands of processors. Future computational architectures will require much greater scalability. Consequently, there is urgency to continue our leading role in the development of more scalable dynamical formulations and in promoting the elements of model design, flexible data structures and software infrastructure. Over the next five years, the evolution of CCSM and the supporting computational infrastructure will require consideration of alternative dynamical formulations. We will modify the simulation framework to accommodate new methods and enable scalable parallel science applications of the new CCSM as an Earth system model. This will open the path for innovative approaches and accelerate climate model development.

18. CONTRACTOR WORK PROPOSAL MANAGER: (Name and Phone No.)  <u>Reinhold C. Mann</u> (865)574-4333 Signature:  Date: 03-03-2006	19. OPERATIONS OFFICE REVIEW OFFICIAL   3/3/06 (Signature)    (Date)
--	---

20. DETAIL ATTACHMENTS: (See instructions for page 3)

<input checked="" type="checkbox"/> a. Facility Requirements	<input checked="" type="checkbox"/> e. Approach	<input type="checkbox"/> i. NEPA Requirements	<input checked="" type="checkbox"/> m. ES&H Considerations
<input checked="" type="checkbox"/> b. Publications	<input checked="" type="checkbox"/> f. Technical Progress	<input checked="" type="checkbox"/> j. Milestones	<input checked="" type="checkbox"/> n. Human/Animal Subjects
<input checked="" type="checkbox"/> c. Purpose	<input checked="" type="checkbox"/> g. Future Accomplishments	<input type="checkbox"/> k. Deliverables	<input checked="" type="checkbox"/> o. Other (Specify)
<input checked="" type="checkbox"/> d. Background	<input checked="" type="checkbox"/> h. Relationships To Other Projects	<input type="checkbox"/> l. Perform Measures/Expectations	

**WORK PROPOSAL REQUIREMENTS FOR OPERATING/EQUIPMENT  
OBLIGATIONS AND COSTS**

**PROGRAM: KP Biological and Environmental Research**

<b>CONTRACTOR NAME:</b> <b>UT-BATTELLE, LLC</b>	<b>WORK PROPOSAL TITLE:</b> A Scalable and Extensible Earth System Model for Climate Change Science		
	<b>WORK PROPOSAL NO.</b> ERKP576	<b>REVISION NO.</b> 0	<b>DATE PREPARED</b> 04-15-2006

20. DETAIL ATTACHMENT CONTINUED:

21. STAFFING (in staff years)	FY 2006	FY 2007	FY 2008		FY 2009	FY 2010	TOTAL TO COMPLETE
			REQUEST	AUTHOR.			
a. SCIENTIFIC / OTHER DIRECT - ORNL	0.4	2.1	2.0		2.0	2.0	
b. OTHER DIRECT - OTHER SITES							
c. TOTAL DIRECT	0.4	2.1	2.0		2.0	2.0	

22. OPERATING EXPENSE (in Thousands)	FY 2006	FY 2007	FY 2008	FY 2009	FY 2010	TOTAL TO COMPLETE
a. TOTAL OBLIGATIONS COSTS:						
1) WAGE POOL AND ORG. BURDEN	101	522	528	545	560	
2) MATERIALS AND SERVICES	6	26	26	26	28	
3) SUBCONTRACTS AND CONSULTANTS						
4) INDIRECT COSTS	44	224	241	248	256	
b. TOTAL COSTS	151	772	795	819	844	

23. EQUIPMENT (in Thousands)						
a. EQUIPMENT OBLIGATIONS						
b. EQUIPMENT COSTS						

24. MILESTONE SCHEDULE (TASKS:)	DOLLARS (in Thousands)		SCHEDULE (DATE)	
	PROPOSED	AUTHORIZED	PROPOSED	AUTHORIZED
Phase 0 control simulations of biogeochemical intercomparison.			09/06	
Coupled chemical-climate model simulations and investigation of feedbacks			09/07	
Scalability of chemical atmosphere model.			09/08	
Generalized grid interfaces to support scalable dynamical methods for atmosphere			09/09	

25. REPORTING REQUIREMENTS (DESCRIPTION:)

Results will be reported in periodic highlights to DOE, in six-month progress reports, and in journals and conference proceedings.

m. ES&H Considerations

Paper studies only.

n. Human/Animal Subjects

No human or animal subjects involved.

**WORK PROPOSAL REQUIREMENTS FOR OPERATING/EQUIPMENT  
OBLIGATIONS AND COSTS**

**PROGRAM: KP Biological and Environmental Research**

CONTRACTOR NAME: <b>UT-BATTELLE, LLC</b>	WORK PROPOSAL TITLE: A Scalable and Extensible Earth System Model for Climate Change Science		
	WORK PROPOSAL NO. ERKP576	REVISION NO. 0	DATE PREPARED 04-15-2006

20. DETAIL ATTACHMENT CONTINUED:

o. Other

(1) OBLIGATIONS FOR OPERATING EXPENSES-Budget Authority (B/A)

	Obligation Estimates		
	FY 2006	FY 2007	FY 2008
Cost (B/O) Estimates	151	772	795
Less: Uncosted Balance (--) at 10/01		36	36
Plus: Commitments for Continued Operations	4	4	4
Outstanding Commitment Balance 10/08	32	32	32
<b>TOTAL OBLIGATIONS--CHANGE</b>	<b>187</b>	<b>772</b>	<b>795</b>

(2) CAPITAL EQUIPMENT OBLIGATIONS AND COSTS - None

# **A Scalable and Extensible Earth System Model for Climate Change Science**

## **A Proposal Submitted to the DOE Office of Science**

Program Announcement: LAB 06-04  
Program Area: Scientific Application: Climate Modeling and Simulation  
Program Office: Office of Biological and Environmental Research  
Technical Contact: Dr. Anjuli Bamzai

### **Applicant**

<i>Institution</i>	<i>Principal Investigator</i>
OakRidge National Laboratory PO Box 2008, MS 6016 Oak Ridge, TN 37831-6016	John B. Drake (865)574-8670 drakejb@ornl.gov
Field Work Proposal ERKP576	

### **Participating Institutions/Senior Personnel**

**Lead PI: John B. Drake, Oak Ridge National Laboratory**

**Co-Lead PI: Phil Jones, Los Alamos National Laboratory**

#### *Institution*

Argonne National Laboratory (ANL)  
Brookhaven National Laboratory (BNL)  
Lawrence Berkeley National Laboratory (LBNL)  
Lawrence Livermore National Laboratory (LLNL)  
Los Alamos National Laboratory (LANL)  
  
National Center for Atmospheric Research (NCAR)  
  
Oak Ridge National Laboratory (ORNL)  
  
Pacific Northwest National Laboratory (PNNL)  
Sandia National Laboratories (SNL)

#### *Senior Personnel*

Robert Jacob  
Robert McGraw  
Inez Fung, Michael Wehner  
Phillip Cameron-Smith, Arthur Mirin  
Scott Elliot, Philip Jones, William Lipscomb,  
Mat Maltrud  
Peter Gent, William Collins, Tony Craig,  
Jean-Francois Lamarque,  
Mariana Vertenstein, Warren Washington  
John B. Drake, David Erickson, W. M. Post,  
Patrick Worley  
Steven Ghan  
Mark Taylor

### **Scientific Application Partnerships**

#### *Institution*

Brookhaven National Laboratory  
Lawrence Berkeley National Laboratory  
Lawrence Livermore National Laboratory  
Oak Ridge National Laboratory  
University of Maryland

#### *Principal Investigators*

Robert McGraw  
Philip Colella,  
Dean Williams  
Patrick Worley  
Eugenia Kalnay

**Projected Funding Request:** \$6.6M per year for five years. This includes \$4.3M U.S. Department of Energy Office of Biological and Environmental Research portion of collaborations with \$2.3M in SciDAC SAP projects.

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## ABSTRACT

Our challenge for SciDAC is to transform an existing, state-of-the-science third generation global climate model, the Community Climate System Model (CCSM), to create a first generation Earth system model that fully simulates the coupling between the physical, chemical, and biogeochemical processes in the climate system. The model will incorporate new processes necessary to predict future climates based on the specification of greenhouse gas *emissions* rather than specification of atmospheric *concentrations*, as is done in present models that make assumptions about the carbon cycle that are likely not valid. We will include comprehensive treatments of the processes governing well-mixed greenhouse gases, natural and anthropogenic aerosols, the aerosol indirect effect and tropospheric ozone for climate change studies. We will improve the representation of carbon and chemical processes, particularly for treatment of greenhouse gas emissions and aerosol feedbacks in collaboration with the DOE Atmospheric Science Program, DOE Atmospheric Radiation Measurement Program, and DOE Terrestrial Carbon Programs.

These additions are not possible unless we also improve the software and testing framework of the CCSM to enable the rapid integration and evaluation of new components. To focus these efforts, specific integration tasks are proposed: inclusion of a new ice sheet model, more flexible horizontal and vertical grids and advanced dynamical formulations. Integration and evaluation work will rely on collaboration with other SciDAC Centers for Enabling Technologies and Scientific Application Partnerships.

During the integration of new methods and new chemical and biogeochemical processes, we will ensure that the model continues to perform well on DOE computational platforms. Methods that improve scalability to thousands of processors will be introduced maximizing the length and number of simulations that can be performed, and facilitating the aggressive schedule of simulations required for scheduled National and international climate change assessments to which the CCSM is committed as part of the national Climate Change Science Program strategy.

# 1 NARRATIVE

## 1.1 BACKGROUND

The Grand Challenge for climate modeling is to *predict future climates based on scenarios of anthropogenic emissions and other changes resulting from options in energy policies*. This challenge has been restated in the mission of the DOE Climate Change Prediction Program (CCPP), including the SciDAC Climate Modeling and Simulation Science Application, which is:

*To determine the range of possible climate changes over the 21<sup>st</sup> century and beyond through simulations using a more accurate climate system model that includes the full range of human and natural climate feedbacks with increased realism and spatial resolution.*

Over the next five years, we propose to support this goal through four integrated areas:

1. Extend the capabilities of the Community Climate System Model (CCSM) to include representations of biological, ecological, chemical, and aerosol processes that will allow scientists and policy-makers to simulate climate and climate change using a comprehensive Earth system model,
2. Provide the necessary software and modeling expertise to rapidly integrate new methods and model improvements,
3. Pursue the development and evaluation of innovative methods in the coupled context of the CCSM, and
4. Improve the performance, portability and scalability of the CCSM on available and future computing architectures for use in national and international assessments of climate change.

The primary goal of this proposal is to develop, test, and exploit first generation of Earth system models based upon the CCSM. We will bring to the community a new well-validated version of CCSM that will run efficiently on thousands of processors and include a significantly better representation of (1) atmospheric aerosols (including the first and second indirect effects), (2) ocean biogeochemistry and the associated emissions and (3) land biogeochemistry (including feedbacks between atmospheric composition and biogenic emissions) within a dynamic vegetation model.

Fluxes of CO<sub>2</sub> to the atmosphere resulting from fossil fuel burning and changes in land use are altering the CO<sub>2</sub> concentration of the atmosphere. These fluxes interact with large reservoirs and exchanges of carbon dioxide governed by natural ecological and biogeochemical processes. Assessment of simulations to date with coupled carbon cycle-climate models (such as the recent coupled climate carbon cycle intercomparison project, C<sup>4</sup>MIP) show that carbon cycle feedbacks to climate change could significantly alter the rate of atmospheric CO<sub>2</sub> concentration increase and climate change over the next century. Similarly, changes to biogeochemical cycles are responsible for the atmospheric abundance of other greenhouse gases as well as sulfate aerosols that represent the radiative forcing of the climate system.

DOE's scientific objectives related to the interaction of carbon emissions and climate change requires accelerated development of a new generation of climate models. While continued research on correction of biases in the physical climate system is essential, the major challenges and uncertainties are in the climate-carbon feedbacks. The specific objectives include carbon sequestration analyses, carbon management, and integration of terrestrial and oceanic observations for model testing. Other agency goals that would benefit from new capabilities are research to assess the efficacy of adaptation and mitigation strategies and studies to assess the efficacy of carbon management practices in a changing climate. Current models used for climate assessment, including the CCSM, have only limited capability to simulate the uptake of carbon by ocean and terrestrial ecosystems and the full range of aerosol feedbacks. In response to these challenges, the DOE SciDAC

LAB 06-04 request for Science Application proposals calls for a new class of climate model that can predict the evolution and interaction of anthropogenic forcing agents with the rest of the climate system. The requisite processes include the aerosol indirect effect, dynamic vegetation, ocean biogeochemistry and atmospheric chemistry. The proper inclusion of these new capabilities will dramatically increase the accuracy of model-based projections of future climate responses to greenhouse gas forcings. Our proposal's focus on biogeochemical and atmospheric chemical simulation in area 1 is in response to this theme of the call. We will develop and test advanced global carbon cycle models so that climate change simulations can be performed requiring only specification of actual anthropogenic emissions. The new CCSM will also include comprehensive treatments of short-lived radiatively active agents, particularly aerosols, tropospheric ozone, and stratospheric ozone. The natural and anthropogenic species of aerosols will include sulfates, black and organic carbon, soil dust, sea salt, and nitrates. These aerosols will be linked to cloud processes to enable climate simulations with the indirect effects of anthropogenic aerosols on cloud shortwave forcing.

The CCSM is one example of an effort to combine the broad expertise from across the climate science community into a working model for use in climate change prediction and assessment. The major assessments by the Intergovernmental Panel on Climate Change (IPCC) occur roughly every six years, and simulations from CCSM have been extensively used in the third and fourth IPCC reports. For the fifth assessment (AR5), we plan to use the Earth-system version of CCSM that predicts the co-evolution of the physical and chemical climate. However, the six-year assessment timescale and the complex interactions between physical processes make it difficult to rapidly integrate and test new algorithms and mechanisms required to improve our prediction of climate change. Our proposed areas 2 and 3 address these needs. We will improve the software infrastructure of the model to enable more rapid integration of new algorithms and new physical parameterizations. To drive the software infrastructure requirements, we will concentrate on specific integration tasks that are needed by the model, including the earth system model integration above, integration of new components like land ice and integration of new horizontal grids and dynamical cores. Any integration of new ideas requires extensive testing. Work performed under area 3 will develop a more robust testing framework by identifying suites of unit and system tests for all components and improving the software infrastructure for automating and performing such tests. In addition, we will be investigating new methods, including assimilation and statistical analysis techniques, for providing a more quantitative evaluation of the model to more objectively evaluate the effectiveness of new improvements or additions to the model.

New capabilities and improvements in climate models are adding more computational complexity and increasing the number of prognostic fields required by the models. In addition, a more quantitative evaluation of uncertainty in climate projections and assessments is requiring a larger number of scenarios and ensembles of simulations for each scenario. However, the timescales for these simulations remain constant and processor speed is not keeping up with the computational demands. Improvement of the formulations and algorithms for the component models to increase the simulation throughput and portability of the CCSM is the focus of work under area 4. A scalable and optimized simulation code on existing and new computer architectures capable of utilizing five thousand processors in the near term and ten to fifty thousand processors by the end of the project is the stated goal. The adaptation to new computer architectures will be accomplished by improving performance through scalability to allow more resolved simulations with more comprehensive treatment of processes and feedbacks. The success of efforts in area 1 (see section 1.2.1) is closely linked with the success in area 4 (section 1.2.3). The two are facilitated and integrated in the proposal by new developments in areas 2 and 3 (described in section 1.2.2).

Scientific Application Partnerships (SAPs) are proposed for those tasks that are intensively mathematical, algorithmic or require significant computer science expertise. Since we are, by necessity, already a well-integrated, cross-disciplinary team, these partnerships overlap personnel with the scientific staff of the proposal. The proposed SAPs also go outside the lab framework to engage exemplary expertise in the universities. In each case, the SAP proposed is a strongly integrated team organized around a significant task of critical importance to the development of advanced coupled carbon-climate models using highly scalable parallel computers. More

than twenty SAP teams offered to collaborate on this proposal. The proposed partnerships represent only the most important and best-integrated efforts with proven track records.

### *1.1.1 The Community Climate System Model*

Leading research institutions including the National Center for Atmospheric Research (NCAR) and several government research laboratories operated by DOE, NASA, and NOAA have collaborated in the development of the Community Climate System Model. The CCSM3 development is based at the National Center for Atmospheric Research (NCAR) with major and essential contributions from the DOE National Laboratory System and academic institutions. The latest release in June 2004 follows three decades of climate modeling at NCAR [Williamson, 1983, Boville, 1998] and fifteen years of partnership between NCAR and the DOE laboratories [Drake, 1995]. With each release, a more comprehensive system is modeled and the scope of science applications of the model expands. The application of the CCSM to decadal and century long climate change is of particular interest to the Department of Energy science mission. The latest model, CCSM3, is described in an upcoming issue of the *Journal of Climate* [Collins2006] and computational aspects are described in a special issue on climate modeling of *The International Journal of High Performance Computing and Applications* [Drake2005]. The CCSM is an identified element of the U.S. national effort in the CCSP Strategic Plan and will be called upon in the future to help guide policy just as it has been extensively used in previous assessment activities.

### *1.1.2 Collaboration and Past Accomplishments*

The Department of Energy Laboratories have an impressive and long, fifty year history of climate research associated with the production of energy and understanding the role of the carbon cycle in the environment. The partnership described in this proposal overlaps the research portfolios of the DOE and National Science Foundation (NSF) to address climate model development and to complement the science missions of both agencies. The agency level cooperation in model building with the CCSM, in particular, has a long record of success that predates SciDAC and sets the example of collaboration for other SciDAC efforts.

To achieve the goals of this proposal, we are building on an already successful collaboration between the DOE national laboratories and NCAR that first produced the highly successful Parallel Climate Model [Washington, 2000] under the predecessor to the CCM3 program and the CCSM3. For the present IPCC assessment (AR4), the CCSM team has produced the largest ensemble of simulations of any modeling group in the world. For all the climate-change scenarios, CCSM3 performed over 10,000 years of simulation. These simulations were performed at relatively high-resolution (approximately 150 km for the atmospheric model), leading to the creation of over 110 Terabytes of climate model results distributed via the DOE Earth System Grid (ESG), making the data available quickly to hundreds of researchers worldwide. Building on the experience of building the PCM, the latest versions of CCSM code, executed efficiently on a wide variety of platforms (both scalar and vector processors), with a particular emphasis on the systems available at NCAR and at DOE laboratories. This accomplishment was possible because of the critical software engineering work performed by the SciDAC team members on all the components of CCSM.

Though the CCSM3 and other climate models are internationally recognized as state-of-the-art, they still require the specification of time-dependent atmospheric concentrations of carbon-dioxide and other gases that are produced by both anthropogenic and natural processes. The future concentration time series (somewhat inappropriately called emission scenarios) are based on assumptions about the global carbon and biogeochemical cycles that are likely invalid as the climate changes. Further, the correct simulation of these additional processes, and more importantly, the feedback between the carbon cycle and climate system, requires improved simulation of the physical climate system to remove remaining systematic error, or “biases”, particularly those pertaining to simulating precipitation events.

The success of the SciDAC 1 team in software engineering for performance portability, the development of a new coupler, rewriting and optimizing the land model for vector computers and providing complete ocean and ice components, show a productive engagement and collaboration. The addition of atmospheric chemistry to the CAM3 under SciDAC was also a major contribution expanding the capabilities of the model. A prototype carbon-climate-biogeochemistry model was assembled as a demonstration of the readiness to undertake coupled Earth system simulation at this dramatically new level of complexity. In this first step towards a comprehensive Earth system model, CO<sub>2</sub> fluxes were exchanged between components and the oceanic flux of dimethylsulfide (DMS) was used in the atmospheric model to create sulfate aerosols. These aerosols interacted and affected the physical climate system, the oceanic carbon cycle, and terrestrial ecosystems. The team of researchers assembled in this proposal is ready to address the scientific and computational challenges posed by the need for a coupled carbon-climate Earth system simulation capability.

## ***1.2 Technical Approach***

### *1.2.1 Earth System Model*

Two important human inputs---fossil fuel emissions and land use/land cover change---are known to contribute significantly to atmospheric CO<sub>2</sub>. Meanwhile, the world's oceans act as a carbon sink and serve as the largest reservoir of CO<sub>2</sub> in the climate system. The goal of our work is to quantify the effects of fossil fuel emissions and land cover change on the global carbon cycle and to quantify the feedbacks among the biogeochemical processes and climate. We will pursue this goal by development and research in terrestrial and oceanic biogeochemistry.

#### *1.2.1.1 Terrestrial Biogeochemistry and Dynamic Vegetation*

##### *Development of a community terrestrial biosphere model*

Our first and primary objective is to develop a community terrestrial biosphere model in collaboration with the CCSM community and other DOE-funded efforts. This model will combine representations of the major biophysical, biogeochemical, and ecological processes that determine the physical and chemical evolution of the land surface and soils. In contrast to traditional physical land-surface models, the biosphere model will include a comprehensive carbon cycle coupled to a dynamic implementation of vegetation. This activity is intended to address major goals of the U.S. Climate Change Science Program (CCSP), the assessment needs of the U.S. Department of Energy (DOE) Climate Change Research Division (CCRD), and, in particular, the research needs of the DOE Terrestrial Carbon Program (TCP) and the larger climate/carbon cycle community. This model could serve as the foundation for a National Terrestrial Carbon Model (NTCM)--an objective of the DOE TCP--for studying parameterization, appropriate initial conditions, carbon data assimilation, and fast and slow carbon pools.

The community terrestrial biosphere model will be developed based upon a thorough intercomparison of existing biogeochemistry models now underway by SciDAC investigators in partnership with the CCSM Biogeochemistry Working Group. The intercomparison is based upon a series of experiments with systematic increases in the coupling among terrestrial and oceanic biogeochemical processes and the rest of the climate system. These experiments will be used to identify the components from existing models with greatest fidelity to theory and observations of the carbon cycle. The community terrestrial biosphere model will be assembled from those components, and it is expected to serve as the biosphere model within CCSM4. The new biogeochemistry module will then be validated against a variety of datasets, released as a part of CCSM4, and used in the next suite of IPCC simulations.

In addition to the terrestrial biogeochemistry module, the biogeophysics of the land model will undergo a significant change. The Community Land Model Version 3 (CLM3) presently solves near-surface state equations for prognostic temperature and humidity using an iterative scheme. For the next version of the

model, CLM4, we will implement an analytical method of solving the same set of equations using a matrix solver. This method employs an explicit coefficient/implicit temperature scheme of Kalnay and Kanamitsu. Commonly referred to as Prognostic Canopy Air Space (PCAS) following Vidale and Stöckli, this analytical method will reduce large sections of code and simplify the implementation of water isotope tracer capabilities in the model.

The new PCAS algorithm will make future developments within the biogeophysics of the model easier to incorporate and test. For example, a multi-layered canopy scheme will be implemented to permit the representation of overlapping vegetation (as is done in IBIS and other biosphere models). This development and other specific process work will be integrated into the CLM4, depending upon the priorities of the CCSM Land Model Working Group.

#### *Novel methods for observational evaluation of terrestrial biosphere models*

Model performance has traditionally been assessed by comparing statistics of individual variables or the relationships among two or three variables to that observed. The team will collaborate with a **SAP (Carbon Data Assimilation and Parameter Estimation Using Local Ensemble Transform Kalman Filter (LETKF). PI: Eugenia Kalnay (UMD))**, that will build a carbon-climate reanalysis model constructed of selected CCSM modules and Ensemble Kalman Filters. The main goal of this SAP is to develop an efficient and flexible system to assess Earth system models *in toto*, and to quantify, in a self-consistent way, uncertainties in the biogeochemical simulations in terms of the observations as well as uncertainties in the physics/mathematics of the model. This proposal uses a coupled carbon-climate model in the DOE-NCAR CCSM framework to prototype the approach. In this SAP, we propose to take advantage of three scientific advancements to create, for the first time, a carbon data assimilation system that includes carbon cycle parameter estimations, and estimations of uncertainty. In recent years a realistic global atmosphere-ocean-land model in the DOE-NCAR CCSM framework has been coupled to interactive terrestrial and oceanic carbon cycles to project the co-evolution of CO<sub>2</sub> and climate [Fung et al 2005]. At the same time, the University of Maryland has developed an advanced Ensemble Kalman Filtering (EnKF) system that is model independent, accurate and computationally very efficient and parallel, and that provides an estimate of the uncertainty of the analysis. The third development is the maturity of carbon-relevant observations beyond the ~100 CO<sub>2</sub> mixing ratios in the marine boundary layer at remote locations around the globe. The observations include DOE's in situ measurements of terrestrial carbon dynamics [AmeriFlux and FACE programs, Running et al. 1999], aircraft data from COBRA [Gerbig et al. 2003], in situ and aircraft data from the forthcoming North American Carbon Program (NACP), and the forthcoming observations of total column daytime CO<sub>2</sub> throughout the globe from orbiting satellites. This makes it possible, for the first time, to perform data assimilation of the carbon cycle in conjunction with conventional meteorological data assimilation to synthesize all carbon and meteorological observations into a single framework. An outcome of this SAP will be an estimation of the distribution of CO<sub>2</sub> in space and time with much more accuracy than possible before and to provide reliable, self-consistent data-based and process-based information about CO<sub>2</sub> distributions and CO<sub>2</sub> sources and sinks for testing models and informing policy makers.

#### *Interaction of atmospheric chemistry and aerosols with terrestrial biogeochemistry*

Atmospheric chemistry and aerosols can interact with the biosphere, producing potentially important feedbacks on the mean and variance of the climate system. These feedbacks can only be studied within a coupled Earth system model, and CCSM4 will be ideally suited for this application. After completing our effort to create a community terrestrial biosphere model, we will focus on modeling these interactions, including:

- Biogenic emissions (mainly isoprene and monoterpenes) from the land, which affect ozone and the oxidizing power of the atmosphere. Recent observations have indicated that the ozone-biogenic emissions feedback could even be positive [Velikova et al., 2005].
- Leaf damage by ozone, reducing plant growth.

- Deposition of reactive nitrogen on land, which can fertilize growth. The multi-model study we led showed that deposition of reactive nitrogen over land may increase 2.5 times by 2100 [Lamarque *et al.*, 2005b], and recent simulations with the Community Land Model (CLM) indicate a dramatic impact on the amount of sequestered carbon.
- Changes in the ratio of direct to diffuse radiation due to aerosol scattering, since diffuse radiation illuminates a greater leaf area and thereby promotes growth.

### 1.2.1.2 Ocean Biogeochemistry

The ocean component of an Earth system model must include an ocean ecosystem model that can not only simulate the uptake and processing of carbon dioxide and other greenhouse gases, but also the exchange of trace gases like dimethyl sulfide (DMS) that can directly or indirectly participate in aerosol feedbacks [Chu, 2004]. During the past several years of support under SciDAC, we worked to incorporate the Doney-Moore-Lindsay (DML) ecosystem model into POP and subsequently added a flexible geocycling module for trace volatiles.

We will build directly from these past accomplishments in several ways. Early work will include refinement of the existing coupled sulfur cycle. DMS concentrations are currently over-predicted in the Southern Ocean, but tests indicate that segregation of small phytoplankton into a cyanobacterial component will improve the situation. Reproduction of polar maxima will require the implementation of a phaeocystis parameterization. While optimizing and improving existing code, we will also work to couple carbon monoxide and at least some non-methane hydrocarbons across the sea air interface and into CAM atmospheric chemistry. The possibility for construction of a separate geochemical module, devoted to the treatment of specialist prokaryotic producers and consumers will be explored. Several of the trace species at hand happen to be strongly processed photochemically in the mixed layer. A concerted effort will be made to begin the appropriate simulation of open ocean photochemistry. We will also collaborate with CCSM Biogeochemistry Working Group to incorporate iron chemistry in the ocean component. We will work on coupling the module for iron chemistry with the atmosphere, because much of the surface ocean iron is supplied by dust deposited by the atmosphere. Deposition of iron and other nutrients to the oceans through dust deposition is important in the large regions of the ocean deficient in these nutrients [Erickson *et al.* 2003].

Software infrastructure will be required to more effectively extend ocean biogeochemical models for specific application. Our primary objective is to generalize the ocean biogeochemistry infrastructure. Current software approaches require coding each specific species and process individually. However, many of these processes are represented by very similar forms and only differ due to inputs of various coefficients and data. We plan to design and test an automated system which combines features of genomic models and data bases to reduce complex global biogeochemistry and the attendant information, energy and mass balance considerations to a highly tabular form. Once a choice of species or elemental cycles is made, such a framework will automatically setup the relevant parameters by retrieving the information from such a table without requiring individual components or routines for each species or process.

### 1.2.1.3 The Chemical Climate Balance

Both atmospheric chemistry and aerosols affect climate directly and indirectly, and strongly affect each other. They are also controlled to a large degree by various anthropogenic emissions (SO<sub>2</sub>, NO<sub>x</sub>, CO, etc.). Since emissions are likely to change significantly over the next century, as reflected in the various SRES scenarios [Nakicenovic *et al.* 2000] it is vital to properly treat chemistry and aerosols for climate change simulations with an Earth system model. It is conjectured that by inclusion of more realistic treatment of the chemical atmosphere and the interaction of aerosols with clouds, the uncertainty of model predictions can be reduced. Utilizing research from the DOE Atmospheric Radiation Measurement (ARM) program, the global modeling effort will be further enriched with results from the DOE measurement programs.

The direct effects of atmospheric chemistry and aerosols include greenhouse absorption by CH<sub>4</sub>, N<sub>2</sub>O, CFCs, and ozone, plus the reflection and absorption of sunlight by aerosols. The indirect effects of atmospheric chemistry and aerosols include their impact on cloud properties (reflectivity, lifetime, precipitation, etc.), and the biosphere (ozone damage to plants, iron fertilization of the ocean by dust, nitrogen fertilization of the land, changes to photosynthetic atmospheric radiation (PAR), etc.) with consequential implications for CO<sub>2</sub>. These direct and indirect effects involve more W/m<sup>2</sup> than anthropogenic CO<sub>2</sub> emissions, with both positive and negative forcing [IPCC, 2001 – Summary for Policy Makers, Figure 3]. Inclusion of atmospheric chemistry and aerosols in CCSM, including their connections to radiation, clouds, and the biosphere, will provide self-consistent inclusion of their direct and indirect effects under variable emission scenarios, and allow the earth system feedbacks mediated by atmospheric chemistry & aerosols to operate on the mean and variability of the climate state. To bring these capabilities into the CCSM we propose the tasks described in the following sections, and will continue to work closely with the Chemistry and Biogeochemistry Working Groups.

*Development of a faster chemistry package for reactive transport of radiatively active species in the troposphere and lower stratosphere.*

The oxidizing power of the atmosphere is crucial to the abundance and/or lifetime of the reactive greenhouse gases, as well as the abundance and properties of many aerosols (especially sulfate, ammonium, nitrate, the oxidation state of iron in mineral dust, and the conversion of aerosols from hydrophobic to hydrophilic). We added a flexible state-of-the-art atmospheric chemistry transport capability for the troposphere to CCSM under SciDAC 1 (based on the MOZART model) that is radiatively active. Because the computational cost of the full chemistry scheme is likely to be prohibitive for long climate simulations (a factor of 6, ie ~500% increase over basic CAM3), we also developed a fast chemical mechanism, based on the IMPACT model [Rotman, *et al*, 2004], that is designed to provide the required capabilities for climate change simulations with a significantly reduced computational cost (60-70% less). Initial tests of this fast mechanism within CAM are very promising, with ozone and sulfate agreeing with observations about as well as the full chemical mechanism. In addition to predicting ozone and sulfate interactively, both our chemistry schemes offer the possibility of interactively calculating the lifetimes of reactive greenhouse gases (CH<sub>4</sub>, N<sub>2</sub>O, & CFCs), which is central to their global warming potential (GWP), and will be needed if, as expected, the emission scenarios used for the fifth IPCC assessment (AR5) specify emissions rather than concentrations.

Under SciDAC 2, we will continue to validate, optimize, and refine our fast mechanism in the troposphere, as well as extend the mechanism into the stratosphere. We will also modify the chemistry scheme to provide the necessary interactions with aerosols and the biosphere.

*Extension of CCSM aerosol parameterizations, including interactions with atmospheric chemistry and clouds.*

Aerosols play key roles in the climate system through their influence on the energy balance (directly by scattering and absorbing radiation in the atmosphere and on snow, and indirectly by influencing the optical and microphysical properties of clouds) and through fertilization and acidification of the land and ocean surface (by wet and dry deposition of nitrate, ammonium, sulfate, organic carbon, and soil dust). The current treatment of aerosols in the CCSM predicts the mass concentrations of all of the important aerosol species (sulfate, nitrate, ammonium, hydrophilic and hydrophobic organic carbon (OC) and black carbon (BC), soil dust, and sea salt), but suffers from a number of serious limitations. Offline aerosol modeling by several groups [Easter *et al.*, 2004; Liu *et al.*, 2005] has produced a suite of improved, documented and validated aerosol modules that can be readily applied to the CCSM. We propose to adapt these modules to CCSM to improve the treatment of a variety of aerosol properties and processes.

The aerosol size distribution will initially be represented by seven different internally mixed log-normal modes. For CCSM4, only the total number concentration and the mass concentrations of each component will be predicted for each mode (a modal scheme); A more accurate but more expensive sectional scheme (*aka* a bin scheme) that has already been developed in a standalone global chemistry/aerosol model under collaboration with DOE-ARM will be implemented in CCSM to help validate the modal scheme, and for use in CCSM5. The



processes we will incorporate include are particle nucleation; coagulation; condensational growth; hydrophilic growth (water uptake, including hysteresis effects); and oxidation of volatile organic compounds (VOC) in collaboration with DOE ASP. Aerosol optical properties will be expressed in terms of relative humidity and internal mixtures of components for each mode to improve the estimated direct effect [Ghan et al., 2001a, Zaveri et al., 2006]. The first and second indirect effect will be treated using physically-based parameterizations of droplet nucleation and auto-conversion [Ghan et al., 1997, 2001b; Liu et al., 2005], and nucleation scavenging of each component of each mode will be related to droplet nucleation [Abdul-Razzak and Ghan, 2000]. The quadrature method of moments (QMOM), developed in recent years in collaborations between BNL scientists and SUNY-SB mathematicians, provides a statistically based alternative to modal and sectional methods for aerosol simulation. The **SAP (Statistical Approaches to Aerosol Dynamics for Climate Simulation, PI: McGraw (BNL))** will investigate this approach to modeling aerosols. Key moments of the aerosol population, including number, mass, and mixed moments entering the covariance matrix of a principal components analysis, are tracked in place of the distribution itself. The new approach is highly efficient, yet provides the comprehensive representation of natural and anthropogenic aerosols, and of their mixing states and direct and indirect effects, that the CCSM will require. If it pans out as we expect, QMOM will be an attractive option for handling aerosols for CCSM5. In addition to furthering its partnership with SUNY-SB, the proposed SAP will leverage findings from current BNL science programs related to aerosols (DOE/ASP), aerosol-cloud interaction (DOE/ARM), and climate simulation (NASA-GISS) to the maximum extent possible to meet CCPP objectives in collaboration with the inter-laboratory science team.

*Evaluation of new capabilities and their effect on mean climate and climate variability.*

The evaluation of the added features related to chemistry and aerosols (including impact on clouds) will consist of two separate and complementary exercises: the first will be a comparison to recent and present-day observations of concentrations and aerosol properties, the second will be a study of the response of the new model to the added features, under present-day, pre-industrial and future conditions.

In the first phase, the simulated (using emissions relevant for the period of observations, mostly post-1980) chemical and aerosol fields will be compared to available observations: these include surface, aircraft and satellite observations (MOPITT, TES, MLS, GOME, SCHIAMACHY, OMI). Measurements of aerosol concentration, size distribution and composition are available from surface (IMPROVE, EMEP and isolated sites) and aircraft observations (NASA-GTE and DOE-ARM campaigns). To maximize the relevance of the comparison with observations, we will use a recently produced version of CAM that is driven by analyzed meteorology from NCEP or ECMWF.

In the second phase, we will perform a set of sensitivity experiments to evaluate the model response to the added features. For that purpose, we will study the behavior of the model chemistry and aerosols between the pre-industrial period and present-day (see Lamarque et al., 2005a and references therein). This is an important test for the evaluation of the model response to changes in anthropogenic influence. It is likely that the emissions scenarios used for the fifth IPCC assessment (AR5) will differ significantly from the projections in the Special Report on Emissions Scenarios (SRES) [Nakicenovic *et al.*, 2000]. These scenarios will feature recent advances in socio-economic projections and will emphasize mitigation strategies for emissions of radiatively active species. The team will evaluate the new representations of chemistry and the carbon cycle using one or more of these scenarios. These evaluation runs will be started from the end of the 20<sup>th</sup> century integrations. We will isolate the effects of new representations from changes in the model physics by running the same simulations using CCSM3 forced by our projections for the important species.

The team will quantify the effects of the new features on the mean state and climate variability of the simulated physical and chemical climate. This evaluation will focus first on short-lived radiatively active species, in particular natural tropospheric aerosols and ozone. The evaluation will occur in three phases for each major class of species. First, the model will be integrated with specified SSTs and no radiative feedbacks to quantify the variability in the forcing agents caused by unforced variability of the climate system. Second, the model will

be integrated including the radiative forcing from the time-varying distributions of the species from the first experiment. This second test will quantify the changes in regional and global variability introduced by the radiatively active species. In the third test, the model will be integrated with interactive species in order to isolate and quantify the feedbacks between the forcing agents and the rest of the climate system. An analogous evaluation process will be applied to the (long-lived) carbon dioxide produced by the oceanic and terrestrial biogeochemical packages.

The principal goal of the research is to simulate the past, present, and future climate including the interactions with gas chemistry, aerosols, and carbon cycle. In order to understand these simulations, the team will quantify the response of the model to idealized changes in the concentrations or emissions of important forcing agents. The team will quantify the sensitivity of the climate to the new short-lived radiatively active gaseous and particulate species. The team will also quantify the climate feedbacks and transient climate response of the new carbon cycle to changes in anthropogenic emissions.

### *1.2.2 Model Integration and Evaluation*

One of the strengths of a community model effort like the CCSM is the ability to incorporate new methods and components developed by a variety of investigators at institutions geographically distant. Current and future development efforts include substantial new capabilities in the physics and chemistry and in the dynamical formulation planned for CCSM4. We propose to develop new software functionality to facilitate the prototyping, development, integration, and rigorous evaluation of new physics and dynamics. One element of the software effort will be focused on systematic development and testing of new physics, chemistry, and biogeochemistry in a user-friendly framework. A second element will be focused on enabling the generalizations and enhancements to the dynamics needed for speed, accuracy, and model configurations targeting higher spatial resolution. A third element will include integration of entire new components, especially an ice sheet component. In essence, the software will accelerate integration both at the level of a single column and across an entire component model.

#### *1.2.2.1 Frameworks for Integration and Unit Testing of New Parameterizations*

Our goal is to make developers more self-sufficient so that entrepreneurial research efforts can proceed without the direct assistance of the limited human resources developing CCSM. Ideally, a developer will be able to perform substantial amounts of integration and evaluation on their own before involving one of the CCSM working groups. A system of unit and integration test codes will make this possible. A unit test is a component of a simulation system for testing individual subroutines or procedures. An integration test combines several software modules, such as all of the CAM column physics, and tests them as a group. A unit or integration test requires the creation of test harness software, which feeds input into the individual subroutines, and outputs computed values for comparison.

The atmosphere model CAM currently has an integration test code called the Single Column Atmosphere Model (SCAM), which is widely used for CAM development and the central avenue for inclusion of results from the DOE Atmospheric Radiation Measurement (ARM) program. We will work to extend the SCAM framework to all CCSM components. This will involve creating a sequential CCSM in addition to the existing concurrent configuration with a single code base for all the major components. Development of the sequential version will produce the software superstructure required to build a SCAM that encompasses all CCSM components. We will work to include new physics, chemistry, and biogeochemistry (collectively, the “column physics”) introduced elsewhere in this proposal into the SCAM framework. We will develop interface standards that will generate flexible environments for running the SCAM with a wide variety of interactive or “data” components and boundary conditions.

The unit and integration tests will be small pieces of software, compared to the full CCSM, that will provide an easier point-of-entry for new developers. Since the unit and integration tests will employ exactly the same

subroutine calls and arguments as are used in the full model, a developer who has made their new scheme execute with unit and integration tests will be ready for system testing with the full model and the help of the working groups. All unit and integration tests will follow the *initialize/run/finalize* programming convention of component technologies. The defined test case data will also help developers evaluate their new schemes. We will also develop standard methods and protocols for automatic comparisons against benchmark data sets, e.g., radiative fluxes calculated with line-by-line spectral radiative transfer codes.

This functionality will accelerate the development of an Earth system model by providing rigorous, extensible, and user-friendly methods to insure the scientific and numerical fidelity of parameterizations for column physics on new and existing computational platforms.

The CCSM Coupler component, cpl6, and the Model Coupling Toolkit (MCT) provide an efficient framework for integration of complete model components. Currently, cpl6 is used by the full CCSM while MCT is used by the standalone CAM. As we merge these two systems (see below), we will unify the use of MCT, cpl6 and other supporting utility layer components (from the Earth System Modeling Framework (ESMF), for example). The result will be a single integration software framework at the full model level. This unification will also enable us to more easily extend the coupled model integration framework.

#### *1.2.2.2 Frameworks for Integration of New Dynamics and Components*

We propose to address the goal of integration and evaluation as an integral part of the development of the CCSM through attention to componentization and well-defined interfaces for new components and dynamical cores. Two new classes of components will be developed and integrated in this task.

The first components we will integrate are new dynamical cores for the atmosphere in a three-phase process. A dynamical core is the numerical implementation of the methods that solve the flow equations and conservation laws of mass, momentum, energy and species. New atmospheric dynamics written in flux form are required to conserve the long-lived chemical species required for the chemistry and biogeochemistry. In addition, incorporation of comprehensive tropospheric and stratospheric chemistry will require order-of-magnitude enhancements in the computational performance of the atmosphere code. For these reasons, we will develop methods to incorporate three new dynamical formulations that meet these requirements and provide near-, medium-, and long-term enhancements to CCSM. We will start with generalizations of the present Finite Volume dynamical core to improve its scaling to large processor counts. We will continue by integrating and testing discontinuous Galerkin formulations of the atmospheric dynamics in collaboration with other DOE and NSF-funded investigations. The effort will culminate in the incorporation of a new non-hydrostatic dynamical core that is capable of supporting adaptive mesh refinement. This is the subject of a SAP led by Phil Colella.

Second, we will focus on the oceans and cryosphere by incorporating a new model of terrestrial ice sheets and new versions of the ocean and sea-ice components. The treatment of land ice is a high priority in order to address questions of sea level rise and feedback between ice melt and the thermohaline circulation.

The team will accomplish these two objectives by:

- Generalizing and abstracting the interfaces between component-level dynamics and column physics;
- Creating the software infrastructure to support more general grids, including component model data structures and tools for creation, input, and interpolation of data sets;
- Generalizing the coupling methodologies to permit rapid, localized interpolation of fluxes and state information among components operating on very different grids; and
- Optimizing these coupling methodologies for sequential and/or concurrent versions of CCSM ported to a representative set of vector and scalar systems.

### 1.2.2.3 Atmosphere model integration

For the AR5 IPCC simulations, CCSM4 will require scalability to the 5000-processor level and the accurate prediction of fifty to one hundred chemical and aerosol species. Due to the fast time scales of the atmosphere, at the AR5 target resolutions of 0.5 to 1 degree, the atmospheric model will be the dominant component of these simulations and thus its performance is a key concern. Because of these considerations, highly-scalable flux-form dynamics will play an increasingly important role in CCSM. The team will address the requirements for improved atmospheric dynamics in three phases.

#### *Phase 1: Integration of the Finite Volume (FV) dynamical core:*

The FV dycore has been provisionally ported to the CCSM system, but its computational and scientific performance is an ongoing, long-term development. We propose to optimize the performance on available computing platforms. Points of emphasis would be the efficiency for large numbers of tracers and for high horizontal resolution. We will also develop a performance model for the FV dycore to facilitate the optimization process. We will generalize the dycore to alternative horizontal discretizations including the cubed-sphere grid. The cubed sphere approach has the advantage of eliminating the polar singularity while offering increased concurrency and scalability. Preliminary estimates suggest that timely execution of the suite of simulations for the AR5 will certainly require as much scalability as possible in the atmospheric model.

#### *Phase 2: Integration of a discontinuous Galerkin and other dynamical cores:*

For SciDAC 2 we propose to integrate NCAR's cubed sphere modeling environment (HOMME) into CAM. HOMME provides all the software necessary to handle cubed sphere grids and associated domain decomposition and solvers, as well as proven performance on tens of thousands of processors. The use of HOMME will also make it possible for individual investigators to develop and evaluate the performance of other unstructured grid methods within CAM with substantially less effort than is required now. We will focus on integrating other SciDAC efforts on Discontinuous Galerkin methods, which extend the finite volume method to higher order and more general flux solvers. This work will also allow CAM to take advantage of other advances in unstructured grids, such as the SciDAC supported work on icosahedral methods. It is a necessary step towards ensuring a DOE climate capability that will scale to petascale computing platforms.

#### *Phase 3: Integration of an adaptive mesh dynamical core:*

For applications beyond the AR5, the team will begin work to shift the atmospheric model in CCSM to a single dynamical core offering both hydrostatic and non-hydrostatic modes of operation. Towards this end, we will collaborate with a SAP proposal headed by **Dr. Phillip Colella (LBNL)** entitled **Local Refinement Methods for Atmospheric Modeling**. The method we propose to develop will be based on well-proven adaptive mesh techniques. This will allow simulations achieving regional resolution for selected areas. This is currently only accomplished through a nested grid approach and we believe the more advanced block-structured AMR approach is the correct way to introduce regional resolution. Fundamentally new mathematical techniques developed by the PI [Gatti-Bono2005] for treating the fast gravity and acoustic waves in stratified flows will allow for ultra high resolution in a computationally efficient manner. These methods will address the multi-scale problem in climate modeling with more sophisticated techniques than have previously been available to the climate research community.

### 1.2.2.4 Cryosphere and ocean model integration

The CCSM lacks an interactive ice sheet model and therefore cannot simulate ice sheet melting and its effects on sea level rise under climate change scenarios. Recent modeling and observations suggest that the Greenland and Antarctic ice sheets could respond to greenhouse warming on time scales of decades to a few centuries, potentially raising global sea level by several meters and altering the thermohaline circulation. Treating these processes will require the coupling of an interactive ice sheet model with the CCSM. The ability to predict the effects of melting ice sheets on sea level and climate will be an added benefit. As part of SciDAC2, we will integrate a state-of-the-art ice sheet model (*Glimmer*) developed at the University of Bristol into the CCSM.

Once the model integration is complete, we will validate the ice sheet model in control climate simulations at various resolutions. The model will then be used for multi-century greenhouse warming simulations that will be included in AR5. *Glimmer* also will be used for paleoclimate studies of ice sheet advance and retreat—for example, the collapse of the Laurentide ice sheet following the Last Glacial Maximum. The current version of *Glimmer* uses the “shallow-ice approximation,” which is not valid for transition zones such as ice streams and grounding lines. We will improve the model by incorporating a three-dimensional dynamical solver that is valid throughout the ice sheet. We will also implement *Glimmer* on an adaptive, unstructured grid with smaller cells near the ice sheet margin where finer resolution is needed. On-line downscaling will provide the fine-resolution atmospheric conditions needed for this work based upon a subgrid orography scheme [Ghan et al., 2002] applied to CCSM during SciDAC1.

Integration of new methods in the ocean model will be particularly important over the next five years. In recent work, several groups both within SciDAC [Randall, 2002] and outside of SciDAC have been testing new horizontal grids for use in ocean modeling. Such grids have advantages in their ability to create locally refined or nested grids for regional downscaling or to resolve relatively localized processes like Western boundary currents. We plan to take advantage of the expertise in the SciDAC community in unstructured grids and grid standards development SciDAC CETs ITAPS, TOPS and APDEC to implement new data structures for support of new horizontal grids and begin to test and evaluate these grids in a climate or ocean context. New infrastructure for alternative grids, and their associated discretized operators, will enable ocean models to more easily integrate developments from outside the traditional ocean modeling community. It has also been shown recently [Dennis, private communication] that the linear data structures necessary for these grids improve the computational performance on standard dipole and tripole grids through better load balancing and land point elimination (see performance section 1.2.3). Thus, a beneficial short-term improvement results while we continue to evaluate grid alternatives.

Besides improved grid infrastructure, the addition of ocean ecosystems and biogeochemistry require better advection or transport schemes that are monotone and conservative as well as inexpensive for large tracer counts. Several candidate schemes exist in the DOE and larger academic community and are currently being examined, including incremental remapping [Dukowicz and Baumgardner, 2000], weighted differencing schemes with limiters and other compact discretization schemes. A new tracer transport infrastructure will be needed for these schemes and will be developed under this proposal.

#### 1.2.2.5 Frameworks for Model Evaluation

Once a new method is integrated into the model, the new model must be evaluated against observational data and against other models. Currently, model evaluations require expert knowledge and detailed examination by the model developers. We will pursue innovative ideas for new approaches to quantitatively evaluate how a model performs when compared to observational and reanalysis data.

Evaluation frameworks must encapsulate expert knowledge of the climate system. This requires defining standard metrics for quantitative comparison and the development of scripts and analysis software to compute standard metrics. Much of this is already encapsulated in tools developed by the Program for Climate Model Diagnosis and Intercomparison (PCMDI) and we will work with them to extend these standard metrics, particularly for components other than the atmosphere where common metrics are not as well defined. In addition, new tools to capture features of the climate system must be developed, including statistical, spectral and comparative visualization tools to quantitatively evaluate spatial patterns and time evolution, particularly in cases where features are present, but are shifted in time and/or space.

To enable participation by more researchers in the universities and national laboratories in model testing and development, diagnostics and evaluation tools must be easier to use and understand. We will work collaboratively with the proposed CET “Scaling the Earth System Grid to Petascale Data” and the related **SAP**

**(Facilitating Climate Modeling Research by Joining Earth Science Analysis/Visualization Tools and Frameworks (PI: Dean Williams [ LLNL]).** The Earth System Grid has become an indispensable tool for managing and remotely accessing climate data. The new proposals will be extending ESG functionality to perform more analyses of distributed data and integrate ESG functionality with existing desktop analysis tools like CDAT, NCL and Ferret. We will work with them to define standard quantitative metrics and implement standard diagnostics for model evaluation. Making these tools more widely available throughout the community through the ESG will enable external developers to access standard data sets to perform their own analyses and model evaluation.

### *1.2.3 Computational Performance*

The computational performance of the CCSM is a key factor in its fidelity. As the CCSM evolves into a comprehensive Earth system model, it will require increased resolution and the ability to model additional chemistry and ecological processes, all the while retaining an integration rate of at least five simulated years per day. This will ultimately demand petascale levels of performance, and thus we propose aggressive scalability and performance goals to ensure that the CCSM can effectively utilize the upcoming DOE petascale computational platforms. We will build on our previous work extending the scalability of the CCSM3 with advanced data decompositions and load balancing, and we will exploit the new avenues of parallelism made possible by the addition of tracers and new chemical mechanisms in the atmospheric model and the enhanced scalability of the proposed new dynamical formulations in both the atmosphere and ocean models.

A petascale computer system will necessarily employ tens of thousands of processors. Two major issues face the CCSM code structure as we move from systems with 1000 to 10,000 and 50,000 processors: the first is parallel scalability and the second is load balancing. In multi-physics codes such as the CCSM, the way to address these issues is not trivial. To obtain scalability to 1000 processors with CCSM3, process parallelism and data parallelism through domain decomposition were both employed. In order to maintain high per processor performance, we adopted a data transpose approach allowing each aspect of the numerical algorithm to operate with an efficient, natural data layout. This had the advantage of localizing communication in the code and allowing highly optimized communicators to be employed. It was also possible to introduce load balancing by migrating processes between processors in the transpose step. This approach will extend in the near term to five thousand processors. But a different tact is required to achieve processor counts of fifty thousand. Both targets will be addressed.

#### *1.2.3.1 Atmosphere model*

The new features of supercomputer architectures offer opportunities and challenges for optimizing performance of the dynamical cores. Our work under the first SciDAC project parallelized the FV dycore in CAM with two-dimensional domain decompositions in both latitude-vertical and longitude-latitude. Remap phases connect the two decompositions. Additional concurrency may be achieved through OpenMP. The ability to multithread effectively varies considerably across platforms, with the IBM and SGI architectures offering a true hybrid programming capability on clusters of shared memory multiprocessors, and non-SGI Linux machines being very limited in their OpenMP implementations. Additionally, vector architectures such as the Cray X1E and Earth Simulator incur reduced throughput at fine domain decompositions due to shorter vector lengths resulting from smaller sub-domain size.

Present concurrency in the FV dycore is limited by the number of sub-domains, which is limited by the coarseness of the vertical grid. In contrast, dynamical cores utilizing a cubed sphere computational grid do not require a polar filter and are amenable to a strictly horizontal decomposition. This enables finer domain decomposition and eliminates the need for inter-decomposition data transposes. It also eliminates the load-imbalance introduced by the fast Fourier transforms (FFTs) used in the FV dynamical core as a polar filter. Therefore we will implement support for unstructured spherical grids in the CAM. The cubed sphere grid is the leading candidate for new versions of the FV dycore but other methods will also find this support important for scalability.

The chemical calculations for tropospheric and stratospheric models will permit 3-D data decomposition and this has not yet been investigated in the CCSM. We will start by investigating optimizations with the 2-D decomposition and load balancing of the physics, taking care to exploit vectorization of the chemistry calculations. Afterward we will investigate further parallelism that will improve performance on non-vector architectures with more significant processor counts. With chemistry calculations, there is also the need to run with large numbers of tracers. This region of parameter space has yet to be explored. Algorithms currently implemented will not scale well to this regime. On the other hand, the large number of constituents offers a further dimension for parallelism. This dimension will be investigated and exploited for optimization and scalability.

The calculation of the physical parameterizations will not permit efficient 3-D data decomposition. However, the physics code can be written in such a way that local and shared memory parallelism can be exploited. We have already restructured the code to take advantage of cache and vector constructs by the introduction of chunked/blocked data structures. One remaining degree of freedom to increase performance and give better scalability is to exploit thread level parallelism. With the new dual and quad core chips slated to be used in future versions of the Cray architecture, attention to exposing thread parallelism should start immediately. Towards the end of the proposal period there may be multi-threading architectures available at the chip level and, though speculative at this point, some parts of the physics calculation may be able to take advantage of this type of system. We will explore the use of hybrid processing power in the single source, performance portable programming methodologies of the CCSM as these systems become available.

From the model integration effort (described in section 1.2.2), we expect a different grid system for the dynamical cores of CAM. After the separation of physics and dynamics accomplished during the SciDAC 1 project, the optimizations and load balance of the physics are independent of the optimizations introduced for atmospheric dynamics. However, the number of processors used for each phase is not entirely independent. We will generalize the parallelism of the CAM and perform the necessary development and code integration to assure that a version of the FV dycore with the relevant technology is available to the climate community.

Performance engineering will be crucial in achieving the scientific and computational goals of this proposal. We will introduce further performance instrumentation, analysis, and tracking of CAM as it evolves, so as to identify problems early in the development process; porting and optimizing the new code on the target platforms; cleaning up interfaces and generalizing current performance tuning options (such as load balancing) for incorporating new dynamical cores or new computational grids, all of this targeting the near term utilization of 5000 processors for CCSM. These activities, while vital, will not achieve the required scalability to run on 50,000 processors. For work in new parallel algorithms and the exploitation of next generation architectures, we are depending on contributions from a Science Application Partnership project. The **SAP (Performance Engineering for the Next Generation Community Climate System Model, PI: Patrick Worley [ORNL])** will target large-scale scalability and portability to the IBM BG/L and future large configurations of the Cray XT-series. Specific activities will be implementation and analysis of more extreme decompositions, of both the domain (2D for physical parameterizations, 3D for chemistry) and species (across tracers in the dynamical core and across species in the chemistry) and porting the full CCSM to the IBM BG/L system at Argonne, to identify other roadblocks to exploiting next generation architectures such as unacceptable scaling of memory requirements. The SAP will also examine scalability when running at range of grid resolutions, to anticipate issues that may arise if the grid resolutions were to increase dramatically. Finally, we will also collaborate with the Performance Engineering Research Center for Enabling Technology (PERC) on applying performance prediction techniques in order to anticipate the impact of changes in the model and in the target architectures.

### *1.2.3.2 Ocean Model*

Ocean model performance is determined by the performance of the explicit solution of the full 3-D baroclinic equation and the solution of the very fast 2-d first barotropic wave mode. The baroclinic calculation is dominated by floating point operations and single-processor memory bandwidth. The barotropic equation is currently solved implicitly using a preconditioned conjugate gradient solver that often limits scalability due to the large iteration count, global reduction operations and low floating point operation count per solver iteration. As part of our previous SciDAC project, the performance of the baroclinic part of the code was improved, particularly at high resolution, by introducing a sub-blocking data decomposition scheme that eliminated some land points, permitted some load balancing and enabled cache blocking with hybrid parallelism. To improve performance further, we will need to move to a linear data structure and a more unstructured approach that will enable the elimination of all land points and much improved load balancing. Such an effort will utilize ideas and software developed under other SciDAC efforts. The performance of the barotropic solver will require work on more advanced pre-conditioners and solvers that will occur as part of a proposed SciDAC CET, A center for PRedictive SIMulation of Multiphysics Systems (PRISIMS – PI: Dana Knoll).

The methods for solving and decomposing implicit systems will also be addressed. One approach is to generalize the decomposition of these solvers to allow them to run efficiently on a smaller set of processors than the entire set associated with the component. To offset the potential load imbalance introduced by more general decompositions, the solvers adopted must be highly optimized.

As with the atmospheric model work, careful instrumentation and analysis will drive the further optimization of the ocean model, to determine both how to set the many tuning options on the different target platforms, and to identify remaining bottlenecks in scalability. Initial ports of POP to BG/L have been promising, but a number of issues still remain with regard to production runs. The SAP (Worley) will address these issues. In collaboration with PERC, the SAP will apply performance prediction technologies to anticipate future scalability problems.

### *1.2.3.3 Sea Ice and Land Ice*

The performance of the sea ice model has not been as extensively studied as the other CCSM components. We will instrument and characterize the performance of the sea ice model to identify bottlenecks and test the impacts of model improvements. Sea ice and land ice models are largely two-dimensional and pose a challenge when scaling to large processor counts; the work load is small compared to the larger 3D components and there are fewer dimensions over which to exploit parallelism. However, sea and land ice processes occur in a relatively limited domain on the Earth's surface, offering possibilities for performance improvement through more flexible data decomposition and distribution schemes. Land ice, in the form of ice sheets, poses an additional challenge for coupling. Changes in ice sheets are likely to occur on much longer timescales, requiring less frequent coupling. Such changes over long integrations result in significant changes in surface topography and land masks, possibly requiring dynamic online computation of interpolation and merging weights. Adding this capability will eliminate the need to stop and restart climate change simulations with different boundary condition and regriding files. We will prototype and optimize new coupling methodologies for these situations.

### *1.2.3.4 Coupled Model*

In the concurrently coupled mode of CCSM, performance is limited by the serialization of the land, atmosphere and sea ice models created by their data dependencies. Consequently, there is little time during a simulated day when all five components are executing concurrently. This load imbalance of the concurrent system on new platforms with high processor counts continues to be a challenge. We will explore the use of sequential and hybrid (ocean concurrent with sequential atmosphere-land-sea ice) coupling modes that remove these obstacles and should provide decreased total idle time on large numbers of processors. We will continue to explore the



use of portable tools such as jumpshot/MPE and TAU for load balancing the system. The SAP (Worley) will also collaborate with PERC to assess whether a performance model of the CCSM can be constructed suitable for optimizing CCSM load balance.

Performance of the fully coupled model is also limited by the data transfer time, as the number of chemical constituents exchanged between the components increases. We will optimize coupler performance for this case. In the case of the ice/coupler communication, we will develop new capabilities within cpl6 and MCT to remove ice-free regions from the transferred data. MCT is currently based on MPI-1 and uses two-sided message passing. We will add a one-sided message passing ability to MCT based on MPI-2 capabilities and explore how it can improve performance of the concurrent system.

As resolution increases, the I/O performed by the coupler, both reading interpolation weights and writing *history* and *restart*, will become an obstacle on platforms with low memory such as the IBM BG/L. We will add parallel NetCDF capability to cpl6 to remove any potential I/O bottlenecks. This latter task will be performed in collaboration with the SAP, which has primary responsibility for porting CCSM to BG/L.

### **1.3 Consortium Arrangements**

#### **1.3.1 Why This Team?**

To effectively perform the proposed work, we are building on an already successful collaboration between the DOE national laboratories and National Center for Atmospheric Research (NCAR). This proposal will complement and leverage efforts at NCAR funded by the National Science Foundation and will be compatible with the scientific goals of the CCSM as well as directly addressing the goals of the DOE OBER Climate Change Prediction Program (CCPP). The success of the SciDAC 1 teams in software engineering, the development of a new coupler, re-factoring and optimizing the land model, development of the interactive chemistry capability and providing complete ocean and ice components, demonstrate a productive engagement and collaboration. This work contributed to the release of the CCSM3 in June 2004.

#### **1.3.2 Project Management**

We currently follow a working management plan available on the web at [www.scidac.org/CCSM](http://www.scidac.org/CCSM). The co-PI's coordinate effort through site contacts at each of the national laboratories. In addition, the project has liaisons to the relevant CCSM Working Groups that meet several times each year. The PI is responsible for overall coordination with the CCSM project management at NCAR.

The project is managed within the scope of the Climate Change Prediction Program (CCPP) so coordination with the DOE program manager (Dr. Anjuli Bamzai) and the CCPP Chief Scientist (Dr. Dave Bader) is essential. Funding decisions are solely the responsibility of the program office, though the PI will raise issues affecting the deliverables of the project. The SciDAC program office, and in particular, the SAP program manager, will also be kept informed with regular (yearly) progress reports and (quarterly) highlights of the collaborative accomplishments.

#### **1.3.3 Software Management and Software Engineering**

As a software development project, this part of the management is particularly important. Mariana Vertenstein at NCAR manages access to the development team repository. Each component model is quality assured by a gatekeeper or change review board. Permission to commit changes to the development trunk is, however, a critical item for the rapid advancement of the model by researchers on this proposal. This permission was granted and exercised in SciDAC 1. The distribution of code under development outside this consortium is strictly prohibited, though researchers engaged with the CCSM Working groups have the ability to manage

branches and perform simulations using the development code. Released, validated code is publicly available and freely distributed.

### 1.3.4 Simulation Schedule and Coordination of Model Development

This proposal follows a schedule that is driven by a firm release date for the CCSM4 model in June of 2009. Several significant simulations are planned along the development path in support of the Climate Change Working Group and the Biogeochemistry Working Group. The tasks of the proposal are coordinated to feed and support this schedule and it is the goal of our work to deliver the best climate modeling system capable of effectively utilizing the targeted supercomputing platforms. The relevant simulations with their required added capabilities are given in the table.

<b>Year</b>	<b>Simulation</b>	<b>Added capability</b>
2006	Ice Sheet Development	Ice sheet
2006	High resolution historical FV1x1	High resolution atmosphere
2007	Ice sheet de-stabilization and sea level rise	Ice sheet coupling
2007	WG3 carbon scenarios	Biogeochemical carbon models
2008	Mitigation CCSM3&carbon	BGC control run
2008	Transient simulation of pre-industrial through 2100 using prescribed emission	Fast atmospheric chemistry scheme
2008	High res future simulations	Coupled FV 1x1
2008	Special DOE scenarios and energy use	Coupled climate carbon models
2009	The impact of interactive aerosol forcing (including the indirect effect) on climate	Interactive modal representation of aerosols; indirect effects
2009	AR5 preliminary runs	CCSM4 preliminary model
2009	Ultra high resolution historical runs	FV0.5x0.5 coupled. Scalability to 5K processors.
2009	Special DOE Scenarios for energy strategies	CCSM4 with special forcing
2010	IPCC AR5 Simulations	IPCC version of CCSM4
2011	Sensitivity of climate model to interactions between biogeochemistry and atmospheric chemistry & aerosol	Interactions between biogeochemistry and atmospheric chemistry & aerosols.

### 1.3.5 Institutional Roles and Budget Discussion

It is helpful to give a broad description of which DOE Laboratory leads particular efforts, though collaboration on tasks among the laboratories and NCAR is an enforced practice under this proposal. The atmospheric chemistry is the primary responsibility of LLNL while aerosols are the responsibility of PNNL. The ocean, sea ice and land ice components are the responsibility of LANL. The land model and land biogeochemistry developments are lead by ORNL and LBNL while LANL leads the ocean biogeochemistry work of this proposal. Couplers and utility toolkits are lead by ANL. Computational performance is primarily the responsibility of ORNL with atmospheric algorithm development and scalability involving SNL, ORNL and LLNL. The scalability of the ocean, sea ice and land ice are lead from LANL.

Budgets at each laboratory are commensurate with tasks to be performed and adequate support of our core teams. We are mindful of the need for institutional highlights and accomplishments and will manage the milestones/highlights of the project so that institutional contributions are acknowledged. Sharing credit is always a challenge but one that can be successfully navigated.

### *1.3.6 Other SciDAC Interactions*

Through interactions with computer science and mathematics teams in SciDAC 1, we have built two very important collaborations with the Earth System Grid (ESG) team and with the Performance Evaluation Research Center (PERC). We will continue this close relationship under this proposal using the ESG to distribute and catalog model output and the performance tools that PERC has developed to guide our optimization and load balancing efforts.

The interactions with other SciDAC Centers for Enabling Technology (CET) proposals and SciDAC Institutes are acknowledged and detailed in the Appendix.

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### 3 Budgets and Budget Explanations

#### 3.1 Overall Budget Summary

The budgets are calculated by each laboratory on a “base” year cost as given in the first column of the table. Since the proposal period begins in the middle of FY06 (July 1,2006), the FY06 cost is for 3 months of the base budget. Out year (FY07 and beyond) reflect the same base budget but adjusted as per Laboratory conventions for overhead and rates. The SAP budgets are for three years with institutional breakdown as shown. The detailed SAP budgets (along with project narrative) are included in the Appendix. Each SAP also submitted a matching, full proposal in response to the LAB 06-04 call.

<b>OBER Request</b>	<b>4310</b>	<b>505</b>	<b>4340</b>	<b>4491</b>	<b>4640</b>	<b>4808</b>	<b>4303</b>	<b>23087</b>
<b>Institution</b>	<b>Base</b>	<b>FY06</b>	<b>FY07</b>	<b>FY08</b>	<b>FY09</b>	<b>FY10</b>	<b>FY11</b>	<b>Total</b>
ORNL	750	187	772	795	819	844	653	4071
ANL	320		320	330	340	350	360	1700
LANL	990	238	996	1044	1094	1147	902	5421
LBNL	302		302	312	322	332	334	1601
LLNL	560		563	578	595	610	628	2974
NCAR	750		750	784	812	849	834	4027
PNNL	330		330	330	330	330	330	1650
SNL	307	80	307	318	328	346	262	1643

<b>OASCR SAP Request</b>	<b>2373</b>	<b>27</b>	<b>2372</b>	<b>2414</b>	<b>2427</b>			<b>7240</b>
<b>Institution</b>	<b>Base</b>	<b>FY06</b>	<b>FY07</b>	<b>FY08</b>	<b>FY09</b>	<b>FY10</b>	<b>FY11</b>	<b>Total</b>
ORNL (Worley)	105	27	108	108	81			324
ANL (Worley)	224		224	224	224			672
LLNL (Worley)	168		168	168	168			504
<b>Total (Worley)</b>	497	27	500	500	473			1500
LLNL (Williams)	350		350	360	371			1081
BNL (McGraw)	190		190	199	207			597
SUNY –SB (McGraw)	125		125	127	130			382
<b>Total (McGraw)</b>	315		315	326	337			979
LBNL(Kalnay)	211		211	219	226			657
U.C.-Berkeley (Kalnay)	250		250	250	250			750
U. Maryland (Kalnay)	250		250	250	250			750
<b>Total (Kalney)</b>	711		711	719	726			2156
LBNL (Colella)	500		496	509	520			1526

**U. S. Department of Energy  
Budget Page**  
(See reverse for Instructions)  
(Amounts in Thousands)

ORGANIZATION <b>OAK RIDGE NATIONAL LABORATORY</b>				Budget Page No: <u>FY2006</u>		
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>John Drake</b>				Requested Duration: <u>3</u> (Months)		
A. SENIOR PERSONNEL: PI/PI, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Amounts in Whole Dollars	
			CAL	ACAD	SUMR	
					Funds Requested by Applicant	
					Funds Granted by DOE	
1.	John Drake		2.2			26,695
2.	Pat Worley		1.5			15,604
3.	David Erickson		1.5			15,604
4.	Forrest Hoffman		1.5			13,033
5.						
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7.	( 4 ) TOTAL SENIOR PERSONNEL (1-6)		6.7			70,937
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)						
1.	( ) POST DOCTORAL ASSOCIATES					
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3.	( ) GRADUATE STUDENTS					
4.	( ) UNDERGRADUATE STUDENTS					
5.	( ) SECRETARIAL - CLERICAL					
6.	( ) OTHER (CRAFTS)					
TOTAL SALARIES AND WAGES (A+B)						70,937
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)						
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)						24,828
						95,765
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)						
TOTAL PERMANENT EQUIPMENT						
E. TRAVEL						
			1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)			
			2. FOREIGN			
TOTAL TRAVEL						4,750
F. TRAINEE/PARTICIPANT COSTS						
1. STIPENDS (Itemize levels, types + totals on budget justification page)						
2. TUITION & FEES						
3. TRAINEE TRAVEL						
4. OTHER (fully explain on justification page)						
TOTAL PARTICIPANTS ( )			TOTAL COST			
G. OTHER DIRECT COSTS						
1. MATERIALS AND SUPPLIES						1,500
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION						
3. CONSULTANT SERVICES						
4. COMPUTER (ADPE) SERVICES						
5. SUBCONTRACTS						
6. OTHER Division Organization Burden and Labor Burden						30,405
TOTAL OTHER DIRECT COSTS						31,905
TOTAL DIRECT COSTS (A THROUGH G)						132,420
I. INDIRECT COSTS (SPECIFY RATE AND BASE)						
G&A 35.0%, Legacy Tax 4.8% Management Fee 2.90%						
TOTAL INDIRECT COSTS						54,985
TOTAL DIRECT AND INDIRECT COSTS (H+I)						187,406
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES						
TOTAL COST OF PROJECT (J+K)						187,406



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(Amounts in Thousands)

ORGANIZATION <b>OAK RIDGE NATIONAL LABORATORY</b>			Budget Page No: <u>    FY2007    </u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>John Drake</b>			Requested Duration: <u>    12    </u> (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Amounts in Whole Dollars
	CAL	ACAD	SUMR	Funds Requested by Applicant      Funds Granted by DOE
1. <b>John Drake</b>	8.5			107,320
2. <b>Pat Worley</b>	6.0			65,172
3. <b>David Erickson</b>	6.0			65,172
4. <b>Forrest Hoffman</b>	6.0			54,697
5.				
6. (    ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)				
7. ( <b>4</b> ) TOTAL SENIOR PERSONNEL (1-6)	26.5			292,362
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)				
1. (    ) POST DOCTORAL ASSOCIATES				
2. (    ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3. (    ) GRADUATE STUDENTS				
4. (    ) UNDERGRADUATE STUDENTS				
5. (    ) SECRETARIAL - CLERICAL				
6. (    ) OTHER (CRAFTS)				
TOTAL SALARIES AND WAGES (A+B)				292,362
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				103,788
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				396,150
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)				
TOTAL PERMANENT EQUIPMENT				
E. TRAVEL				
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				
2. FOREIGN				
TOTAL TRAVEL				20,000
F. TRAINEE/PARTICIPANT COSTS				
1. STIPENDS (Itemize levels, types + totals on budget justification page)				
2. TUITION & FEES				
3. TRAINEE TRAVEL				
4. OTHER (fully explain on justification page)				
TOTAL PARTICIPANTS (    )			TOTAL COST	
G. OTHER DIRECT COSTS				
1. MATERIALS AND SUPPLIES				6,000
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				
3. CONSULTANT SERVICES				
4. COMPUTER (ADPE) SERVICES				
5. SUBCONTRACTS				
6. OTHER Division Organization Burden and Labor Burden				126,101
TOTAL OTHER DIRECT COSTS				132,101
H. TOTAL DIRECT COSTS (A THROUGH G)				548,251
I. INDIRECT COSTS (SPECIFY RATE AND BASE)				
G&A 34.0%, Legacy Tax 4.8% Management Fee 2.90%				
TOTAL INDIRECT COSTS				223,904
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				772,155
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES				
L. TOTAL COST OF PROJECT (J+K)				772,155

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(Amounts in Thousands)

ORGANIZATION <b>OAK RIDGE NATIONAL LABORATORY</b>				Budget Page No: <u>    FY2008    </u>			
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>John Drake</b>				Requested Duration: <u>    12    </u> (Months)			
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Amounts in Whole Dollars		
			CAL	ACAD	SUMR		
			Funds Requested				
			Funds Granted				
			by Applicant				
			by DOE				
1.	John Drake		8.2			108,054	
2.	Pat Worley		6.0			68,225	
3.	David Erickson		6.0			68,225	
4.	Forrest Hoffman		6.0			57,255	
5.							
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)						
7.	( 4 ) TOTAL SENIOR PERSONNEL (1-6)		26.2			301,759	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)							
1.	( ) POST DOCTORAL ASSOCIATES						
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)						
3.	( ) GRADUATE STUDENTS						
4.	( ) UNDERGRADUATE STUDENTS						
5.	( ) SECRETARIAL - CLERICAL						
6.	( ) OTHER (CRAFTS)						
TOTAL SALARIES AND WAGES (A+B)						301,759	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)						108,633	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)						410,392	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)							
TOTAL PERMANENT EQUIPMENT							
E. TRAVEL			1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				
			2. FOREIGN				
TOTAL TRAVEL						20,000	
F. TRAINEE/PARTICIPANT COSTS							
1. STIPENDS (Itemize levels, types + totals on budget justification page)							
2. TUITION & FEES							
3. TRAINEE TRAVEL							
4. OTHER (fully explain on justification page)							
TOTAL PARTICIPANTS ( ) TOTAL COST							
G. OTHER DIRECT COSTS							
1. MATERIALS AND SUPPLIES						6,000	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION							
3. CONSULTANT SERVICES							
4. COMPUTER (ADPE) SERVICES							
5. SUBCONTRACTS							
6. OTHER Division Organization Burden and Labor Burden						130,626	
TOTAL OTHER DIRECT COSTS						136,626	
H. TOTAL DIRECT COSTS (A THROUGH G)						567,019	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) G&A 35.0%, Legacy Tax 2.9% Management Fee 2.50%							
TOTAL INDIRECT COSTS						228,018	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)						795,037	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES							
L. TOTAL COST OF PROJECT (J+K)						795,037	

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(Amounts in Thousands)

ORGANIZATION <b>OAK RIDGE NATIONAL LABORATORY</b>				Budget Page No: <u>    FY2009    </u>		
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>John Drake</b>				Requested Duration: <u>    12    </u> (Months)		
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Amounts in Whole Dollars	
			CAL	ACAD	SUMR	
			Funds Requested			
			Funds Granted			
			by Applicant			
			by DOE			
1.	John Drake		8.1			111,447
2.	Pat Worley		6.0			70,783
3.	David Erickson		6.0			70,783
4.	Forrest Hoffman		6.0			59,402
5.						
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7.	( 4 ) TOTAL SENIOR PERSONNEL (1-6)		26.1			312,415
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)						
1.	( ) POST DOCTORAL ASSOCIATES					
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3.	( ) GRADUATE STUDENTS					
4.	( ) UNDERGRADUATE STUDENTS					
5.	( ) SECRETARIAL - CLERICAL					
6.	( ) OTHER (CRAFTS)					
TOTAL SALARIES AND WAGES (A+B)						312,415
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)						112,469
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)						424,884
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)						
TOTAL PERMANENT EQUIPMENT						
E. TRAVEL			1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)			
			2. FOREIGN			
TOTAL TRAVEL						20,000
F. TRAINEE/PARTICIPANT COSTS						
1. STIPENDS (Itemize levels, types + totals on budget justification page)						
2. TUITION & FEES						
3. TRAINEE TRAVEL						
4. OTHER (fully explain on justification page)						
TOTAL PARTICIPANTS ( ) TOTAL COST						
G. OTHER DIRECT COSTS						
1. MATERIALS AND SUPPLIES						6,000
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION						
3. CONSULTANT SERVICES						
4. COMPUTER (ADPE) SERVICES						
5. SUBCONTRACTS						
6. OTHER Division Organization Burden and Labor Burden						130,600
TOTAL OTHER DIRECT COSTS						136,600
H. TOTAL DIRECT COSTS (A THROUGH G)						581,484
I. INDIRECT COSTS (SPECIFY RATE AND BASE) G&A 35.0%, Legacy Tax 2.9% Management Fee 2.50%						
TOTAL INDIRECT COSTS						237,700
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)						819,184
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES						
L. TOTAL COST OF PROJECT (J+K)						819,184

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(Amounts in Thousands)

ORGANIZATION <b>OAK RIDGE NATIONAL LABORATORY</b>				Budget Page No: <u>FY2010</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>John Drake</b>				Requested Duration: <u>12</u> (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Amounts in Whole Dollars
			CAL	ACAD	SUMR
					Funds Requested by Applicant
					Funds Granted by DOE
1.	John Drake		8.1		114,942
2.	Pat Worley		6.0		73,438
3.	David Erickson		6.0		73,438
4.	Forrest Hoffman		6.0		61,630
5.					
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)				
7.	( 3 ) TOTAL SENIOR PERSONNEL (1-6)				323,446
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1.	( ) POST DOCTORAL ASSOCIATES				
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER (CRAFTS)				
TOTAL SALARIES AND WAGES (A+B)					323,446
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					116,441
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					439,887
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL					
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL					20,000
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					6,000
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER Division Organization Burden and Labor Burden					130,579
TOTAL OTHER DIRECT COSTS					136,579
H. TOTAL DIRECT COSTS (A THROUGH G)					596,466
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
G&A 35.0%, Legacy Tax 2.9% Management Fee 2.50%					
TOTAL INDIRECT COSTS					247,866
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					844,332
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					844,332

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(Amounts in Thousands)

ORGANIZATION <b>OAK RIDGE NATIONAL LABORATORY</b>				Budget Page No: <u>    FY2011    </u>		
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>John Drake</b>				Requested Duration: <u>    9    </u> (Months)		
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Amounts in Whole Dollars	
			CAL	ACAD	SUMR	
					Funds Requested by Applicant	
					Funds Granted by DOE	
1.	John Drake		8.1		89,439	
2.	Pat Worley		6.0		57,144	
3.	David Erickson		6.0		57,144	
4.	Forrest Hoffman		6.0		47,956	
5.						
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7.	( 4 ) TOTAL SENIOR PERSONNEL (1-6)					251,682
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)						
1.	( ) POST DOCTORAL ASSOCIATES					
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3.	( ) GRADUATE STUDENTS					
4.	( ) UNDERGRADUATE STUDENTS					
5.	( ) SECRETARIAL - CLERICAL					
6.	( ) OTHER (CRAFTS)					
TOTAL SALARIES AND WAGES (A+B)					251,682	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					90,605	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					342,287	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)						
TOTAL PERMANENT EQUIPMENT						
E. TRAVEL						
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)						
2. FOREIGN						
TOTAL TRAVEL					14,250	
F. TRAINEE/PARTICIPANT COSTS						
1. STIPENDS (Itemize levels, types + totals on budget justification page)						
2. TUITION & FEES						
3. TRAINEE TRAVEL						
4. OTHER (fully explain on justification page)						
TOTAL PARTICIPANTS ( ) TOTAL COST						
G. OTHER DIRECT COSTS						
1. MATERIALS AND SUPPLIES					4,500	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION						
3. CONSULTANT SERVICES						
4. COMPUTER (ADPE) SERVICES						
5. SUBCONTRACTS						
6. OTHER Division Organization Burden and Labor Burden					98,107	
TOTAL OTHER DIRECT COSTS					102,607	
H. TOTAL DIRECT COSTS (A THROUGH G)					459,145	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)						
G&A 35.0%, Legacy Tax 2.9% Management Fee 2.50%						
TOTAL INDIRECT COSTS					194,223	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					653,368	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES						
L. TOTAL COST OF PROJECT (J+K)					653,368	

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ORGANIZATION <b>OAK RIDGE NATIONAL LABORATORY</b>				Budget Page No: <u>YRS 1 - 5</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>John Drake</b>				Requested Duration: <u>60</u> (Months)	
A. SENIOR PERSONNEL: PI/PI, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Amounts in Whole Dollars
			CAL	ACAD	SUMR
					Funds Requested by Applicant
					Funds Granted by DOE
1.	John Drake		35.1		557,897
2.	Pat Worley		25.5		350,366
3.	David Erickson		25.5		350,366
4.	Forrest Hoffman		25.5		293,972
5.					
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)				
7.	( 4 ) TOTAL SENIOR PERSONNEL (1-6)		111.6		1,552,601
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1.	( ) POST DOCTORAL ASSOCIATES				
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER (CRAFTS)				
TOTAL SALARIES AND WAGES (A+B)					1,552,601
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					556,765
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					2,109,366
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL					
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL					99,000
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					30,000
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER Division Organization Burden and Labor Burden					646,419
TOTAL OTHER DIRECT COSTS					676,419
H. TOTAL DIRECT COSTS (A THROUGH G)					2,884,785
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
G&A 35.0%, Legacy Tax 2.9% Management Fee 2.50%					
TOTAL INDIRECT COSTS					1,186,696
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					4,071,481
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					4,071,481

## ORNL Budget Explanation

Cost estimates presented in the "budget pages" of this proposal have been reclassified in order to be comparable to proposals submitted by other research institutions. At the Oak Ridge National Laboratory (ORNL), costs are collected and reported in accordance with approved Department of Energy (DOE) accounting guidelines. Although costs have been reclassified in this proposal, integrity has been maintained in total and between direct versus indirect costs.

### A. (1-7) Senior Personnel

The ORNL's cost accounting system utilizes wage pools based upon salary ranges. For purposes of this budget, the wage pool cost estimate is divided by the fringe benefits rate. The labor component is being reported in Item A and the fringe component is being reported in Item C.

The list of senior personnel participating in this project is as follows: John B. Drake, Patrick Worley, David Erickson, Forrest Hoffman, Mac Post

### B.1 Post-Doctoral Associates

Post-BS subcontractors, who work on the ORNL site, are assessed a \$1,075 per month organization burden charge for FY2006, \$1120 for FY2007 and \$1130 for FY2008 and out years. This charge recovers the division's costs associated with working on-site (primarily space and utilities). This is being reported in Item G.6.

### C. Fringe Benefits

Fringe Benefits for ORNL employees are estimated to be 35% of labor costs for FY 2006, 35.5% for FY2007 and 36% for FY2008 and out years.

### D. Permanent Equipment

### E. (1-2) Travel

Travel funds are requested to attend the CCPP Science Team meeting, the CCSM Workshop, one CCSM Working Group meeting, the AGU (or similar professional society meeting) and a project meeting each year. Estimated cost per domestic travel is \$1,250 and includes plane fare, housing, meals, registration, and other allowable costs under government per diem rules.

### G.6 Other - Organization Burden Administration

Use of cost collection centers in ORNL R&D divisions is the approved method for collection and distribution of organization burden costs. These accounts are established to collect costs associated with an R&D division. The types of costs which can be charged to organization burden cost collection centers are unfunded paid hours; division administration; and general materials/service costs, including, but not limited to telecommunications, space, utilities, word processing, and copying which are not directly attributable or chargeable to R&D projects. Division Administration costs include: (i) managerial, technical, and administrative oversight; and (ii) support personnel such as facilities and operations, environmental, safety, and health, finance and budget, quality, and health physics provided for the general benefit of a division.

For ORNL staff, the labor and fringe components have been estimated and reported in items A - C. For Post-BS subcontractors, the subcontract costs have been reported in Item B.1. For ORNL staff and Post-BS subcontractors, the organization burden component has been estimated and is being reported in Item G.6. Inclusion of these costs is necessary to provide a full accounting of estimated cost for the project period. All cost will be collected and reported in ORNL's cost accounting system.

#### I. Indirect Costs

Full General & Administrative (G&A), Legacy Charge, and Management Fee are assessed on ORNL labor costs (Items A, C, and G.6), Materials and Supplies, and Equipment less than \$35,000 unit value. Full G&A is estimated to be 35.0% for FY2006, 34.0% for FY2007 and 36.50% for FY2008, with an estimated 3% increase each year after that for additional fiscal years. Legacy Charge is estimated to be 4.8% for each year. Management Fee is estimated to be 2.9% for FY2006, 3.2% for FY2007 and 3.5% for FY2008 and out years.

Non-DOE-contractor subcontract costs are assessed Subcontract G&A and Management Fee. Subcontract G&A is estimated to be 1.1% each year. Management Fee is estimated to be 2.9% for FY2006, 3.2% for FY2007 and 3.5% for FY2008 and out years.

Travel costs are assessed Travel G&A and Management Fee. Travel G&A is estimated to be 7.0% each year. Management Fee is estimated to be 2.9% for FY2006, 3.2% for FY2007 and 3.5% for FY2008 and out years.



**Cover Page**

**Title of Proposed Project:**

A Scalable and Extensible Earth System Model  
for Climate Change Science  
FWP # 57645

**Office of Science Program Announcement Title/#:**

Lab 06-04  
Scientific Discovery through Advanced Computing

**Name of Laboratory:**

Argonne National Laboratory

**Principal Investigator(s):**

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(T) 630-252-2983 (Fax) 630-252-6104  
[jacob@mcs.anl.gov](mailto:jacob@mcs.anl.gov)

**Official signing for Laboratory:**

Rick L. Stevens, Associate Laboratory Director-PBCS  
Argonne National Laboratory  
Mathematics and Computer Science Division  
9700 So. Cass Avenue - Bld.221  
Argonne, IL 60439  
(T) 630-252-3378, ( Fax) 630-252-6333  
stevens@mcs.anl.gov

**Requested funding for Argonne National Laboratory  
for Proposed Project:**

Year 1	\$	320,000
Year 2	\$	330,000
Year 3	\$	340,000
Year 4	\$	350,000
Year 5	\$	360,000
Total:	\$	<u>1,700,000</u>

**Duration of Entire Project Period:**

07/01/2006 to 06/30/2011

**Use of human subjects in proposed project:**

No

**Use of vertebrate animals in proposed project:**

No

**Signature of PI, Date of Signature:**

PI's electronic signature on file

March 6, 2006

**Signature of Official, Date of Signature:**



March 6, 2006

**U.S. Department of Energy**  
**Budget Page**  
(See reverse for Instructions)

ORGANIZATION <b>The University of Chicago, Operator of Argonne National Laboratory</b>				Budget Page No: <u>pg 1 of 6</u> Yr 1 of 5	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Robert L. Jacob</b>				Requested Duration: <u>12</u> (Months) FWP # 57645	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested
			CAL	ACAD	SUMR
					by Applicant
					by DOE
1. Robert L. Jacob, PI			12.00		
2.					
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. ( 1 ) TOTAL SENIOR PERSONNEL (1-6)			12.00		
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)					\$212,159
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$212,159
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL					
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					\$4,200
2. FOREIGN					\$2,600
TOTAL TRAVEL					\$6,800
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					\$15,613
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					\$1,000
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS					\$16,613
H. TOTAL DIRECT COSTS (A THROUGH G)					\$235,571
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
Section H. Direct cost X Aggregate rate of: 35.840%					
TOTAL INDIRECT COSTS					\$84,429
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$320,000
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					\$320,000

**U.S. Department of Energy**  
**Budget Page**  
(See reverse for Instructions)

ORGANIZATION <b>The University of Chicago, Operator of Argonne National Laboratory</b>				Budget Page No: <u>2 of 6</u> Yr. 2 of 5			
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Robert L. Jacob</b>				Requested Duration: <u>12</u> (Months) FWP # 57645			
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded				
			Person-mos.			Funds Requested	Funds Granted
			CAL	ACAD	SUMR	by Applicant	by DOE
1. Robert L. Jacob, PI			12.00			\$224,076	
2.							
3.							
4.							
5.							
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)							
7. ( 1 ) TOTAL SENIOR PERSONNEL (1-6)			12.00			\$224,076	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)							
1. ( ) POST DOCTORAL ASSOCIATES							
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)							
3. ( ) GRADUATE STUDENTS							
4. ( ) UNDERGRADUATE STUDENTS							
5. ( ) SECRETARIAL - CLERICAL							
6. ( ) OTHER							
TOTAL SALARIES AND WAGES (A+B)						\$224,076	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)							
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)						\$224,076	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)							
TOTAL PERMANENT EQUIPMENT							
E. TRAVEL			1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)			\$4,389	
			2. FOREIGN			\$2,717	
TOTAL TRAVEL						\$7,106	
F. TRAINEE/PARTICIPANT COSTS							
1. STIPENDS (Itemize levels, types + totals on budget justification page)							
2. TUITION & FEES							
3. TRAINEE TRAVEL							
4. OTHER (fully explain on justification page)							
TOTAL PARTICIPANTS ( ) TOTAL COST							
G. OTHER DIRECT COSTS							
1. MATERIALS AND SUPPLIES						\$10,751	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION						\$1,000	
3. CONSULTANT SERVICES							
4. COMPUTER (ADPE) SERVICES							
5. SUBCONTRACTS							
6. OTHER							
TOTAL OTHER DIRECT COSTS						\$11,751	
H. TOTAL DIRECT COSTS (A THROUGH G)						\$242,933	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)							
Section H. Direct cost X Aggregate rate of: 35.840%							
TOTAL INDIRECT COSTS						\$87,067	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)						\$330,000	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES							
L. TOTAL COST OF PROJECT (J+K)						\$330,000	

**U.S. Department of Energy**  
**Budget Page**  
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ORGANIZATION <b>The University of Chicago, Operator of Argonne National Laboratory</b>				Budget Page No: <u>3 of 6</u> Yr 3 of 5	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Robert L. Jacob</b>				Requested Duration: <u>12</u> (Months) FWP # 57645	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested
			by Applicant	Funds Granted by DOE	
1. Robert L. Jacob, PI			12.00		\$232,278
2.					
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. ( 1 ) TOTAL SENIOR PERSONNEL (1-6)			12.00		\$232,278
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)					\$232,278
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$232,278
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL					
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					\$4,587
2. FOREIGN					\$2,839
TOTAL TRAVEL					\$7,426
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					\$9,591
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					\$1,000
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS					\$10,591
H. TOTAL DIRECT COSTS (A THROUGH G)					\$250,294
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
Section H. Direct cost X Aggregate rate of: 35.840%					
TOTAL INDIRECT COSTS					\$89,706
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$340,000
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					\$340,000

**U.S. Department of Energy**  
**Budget Page**  
(See reverse for Instructions)

ORGANIZATION <b>The University of Chicago, Operator of Argonne National Laboratory</b>				Budget Page No: <u>4 of 6</u> Yr 4 of 5			
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Robert L. Jacob</b>				Requested Duration: <u>12</u> (Months) FWP # 57645			
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested		
			by Applicant	Funds Granted by DOE			
			CAL	ACAD	SUMR		
1.	Robert L. Jacob, PI		12.00			\$240,781	
2.							
3.							
4.							
5.							
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)						
7.	( 1 ) TOTAL SENIOR PERSONNEL (1-6)		12.00			\$240,781	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)							
1.	( ) POST DOCTORAL ASSOCIATES						
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)						
3.	( ) GRADUATE STUDENTS						
4.	( ) UNDERGRADUATE STUDENTS						
5.	( ) SECRETARIAL - CLERICAL						
6.	( ) OTHER						
TOTAL SALARIES AND WAGES (A+B)						\$240,781	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)							
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)						\$240,781	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)							
TOTAL PERMANENT EQUIPMENT							
E. TRAVEL							
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)						\$4,793	
2. FOREIGN						\$2,967	
TOTAL TRAVEL						\$7,760	
F. TRAINEE/PARTICIPANT COSTS							
1. STIPENDS (Itemize levels, types + totals on budget justification page)							
2. TUITION & FEES							
3. TRAINEE TRAVEL							
4. OTHER (fully explain on justification page)							
TOTAL PARTICIPANTS ( ) TOTAL COST							
G. OTHER DIRECT COSTS							
1. MATERIALS AND SUPPLIES						\$8,115	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION						\$1,000	
3. CONSULTANT SERVICES							
4. COMPUTER (ADPE) SERVICES							
5. SUBCONTRACTS							
6. OTHER							
TOTAL OTHER DIRECT COSTS						\$9,115	
H. TOTAL DIRECT COSTS (A THROUGH G)						\$257,656	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)							
Section H. Direct cost X Aggregate rate of: 35.840%							
TOTAL INDIRECT COSTS						\$92,344	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)						\$350,000	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES							
L. TOTAL COST OF PROJECT (J+K)						\$350,000	

**U.S. Department of Energy**  
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ORGANIZATION <b>The University of Chicago, Operator of Argonne National Laboratory</b>				Budget Page No: <u>5 of 6</u> Yr 5 of 5		
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Robert L. Jacob</b>				Requested Duration: <u>12</u> (Months) FWP # 57645		
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested	
			CAL	ACAD	SUMR	
					by Applicant	
					by DOE	
1.	Robert L. Jacob, PI		12.00			\$249,597
2.						
3.						
4.						
5.						
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7.	( 1 ) TOTAL SENIOR PERSONNEL (1-6)		12.00			\$249,597
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)						
1.	( ) POST DOCTORAL ASSOCIATES					
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3.	( ) GRADUATE STUDENTS					
4.	( ) UNDERGRADUATE STUDENTS					
5.	( ) SECRETARIAL - CLERICAL					
6.	( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)						\$249,597
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)						
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)						\$249,597
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)						
TOTAL PERMANENT EQUIPMENT						
E. TRAVEL						
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)						\$5,009
2. FOREIGN						\$3,101
TOTAL TRAVEL						\$8,109
F. TRAINEE/PARTICIPANT COSTS						
1. STIPENDS (Itemize levels, types + totals on budget justification page)						
2. TUITION & FEES						
3. TRAINEE TRAVEL						
4. OTHER (fully explain on justification page)						
TOTAL PARTICIPANTS ( ) TOTAL COST						
G. OTHER DIRECT COSTS						
1. MATERIALS AND SUPPLIES						\$6,312
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION						\$1,000
3. CONSULTANT SERVICES						
4. COMPUTER (ADPE) SERVICES						
5. SUBCONTRACTS						
6. OTHER						
TOTAL OTHER DIRECT COSTS						\$7,312
H. TOTAL DIRECT COSTS (A THROUGH G)						\$265,018
I. INDIRECT COSTS (SPECIFY RATE AND BASE)						
Section H. Direct cost X Aggregate rate of: 35.840%						
TOTAL INDIRECT COSTS						\$94,982
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)						\$360,000
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES						
L. TOTAL COST OF PROJECT (J+K)						\$360,000

## U.S. Department of Energy

## Budget Page

(See reverse for Instructions)

ORGANIZATION The University of Chicago, Operator of Argonne National Laboratory				Budget Page No: <u>6 of 6</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Robert L. Jacob				5-Yr. ANL Total Project Requested Duration: <u>60</u> (Months) FWP # 57645	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested
			CAL	ACAD	SUMR
					by Applicant
					by DOE
1. Robert L. Jacob, PI			60.00		
2.					
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. ( 1 ) TOTAL SENIOR PERSONNEL (1-6)			60.00		\$1,158,890
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)					\$1,158,890
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$1,158,890
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL			1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)		\$22,977
			2. FOREIGN		\$14,224
TOTAL TRAVEL					\$37,201
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					\$50,382
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					\$5,000
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS					\$55,382
H. TOTAL DIRECT COSTS (A THROUGH G)					\$1,251,472
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS					\$448,528
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$1,700,000
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					\$1,700,000

**Lab 06-04: Scientific Discovery through Advanced Computing**  
**A Scalable and Extensible Earth System Model**  
**for Climate Change Science**

**Robert L. Jacob, PI**  
**FWP # 57645**  
**Budget Explanation**

**A-C Salaries and Fringe Benefits**

Argonne National Laboratory is a government-owned facility operated by the University of Chicago. As a contractor for the Department of Energy, Argonne National Laboratory must comply with DOE general policies and procedures on budgeting and accounting. The Laboratory's costing procedures are based on the assumption that all costs incurred will be recovered. The costing procedures use standard rates, which are used throughout the Laboratory on a consistent basis and uniformly applied to all work supported by the Department of Energy and other federal agencies.

Standard rates are established at the beginning of the fiscal year for each research division, and are monitored and revised as necessary. All labor costs are distributed using standard rates which are developed by the laboratory's budget office for each major payroll classification within the lab. The division-wide rates are based on pay bands ( salary ranges ) and fringe benefits (35.2% for a regular staff and clerical, and 11% for post/pre doctoral appointees), plus a factor for divisional overhead and for paid absences. Graduate and undergraduate students costs include housing allowance and fringe benefits( 7.65%). Effort is escalated each year by a rate provided by the Argonne Budget Department.

The principal investigator for this proposal is: Robert L. Jacob  
The PI's effort charged per year to this proposal is : 12.00 man-months

**E Travel**

Domestic: \$1.4 K per trip/escalate 4.5% per yr.  
Foreign: \$2.6 K per trip/escalate 4.5% per yr.

**G Other Direct Costs**

1. Materials and Supplies:  
Hardware/software maintenance, software, low-end computers (<\$5k), computer and misc.supplies.
2. Publication Costs:  
Books/literature, subscriptions, publishing costs related to research.

**I Indirect Costs**

Standard rates are also developed for Laboratory General and Administrative (G&A) expense. The procedures for distributing Laboratory G&A and program expense is applied on the basis of the total cost of the work performed. The following indirect rates are provisional and have been estimated for each fiscal year budget period:

PBCS Program Expenses @ 3.7%  
Laboratory G&A:  
Common Support @ 27.3%  
Service Centers @ 21.3%  
Equipment/Subcontracts@ 8.1%  
G&A Burden @ 2.9%

Argonne' s indirect rates are continuously reviewed and audited by  
Cognizant Federal Agency:

Martin Straka 630-252-7724 Department of Energy-Chicago Operations Office



### 3.3 Los Alamos National Laboratory Detail Budgets & Budget Explanation

#### A Scalable and Extensible Earth System Model for Climate Change Science Scientific Discovery through Advanced Computing, LAB-06-04 Los Alamos National Laboratory

Principal Investigator	Official Signing for the Laboratory
Philip W Jones	James M. Hyman
Position	Position
Project Leader	Group Leader
Mailing Address	Mailing Address
T-3, MS B216 PO Box 1663 Los Alamos, NM 87545	T-7, MS B284 PO Box 1663 Los Alamos, NM 87545
Telephone	Telephone
505-667-6387	505-667-6294
Fax Number	Fax Number
505-665-5926	505-665-5757
Email	Email
<a href="mailto:pwjones@lanl.gov">pwjones@lanl.gov</a>	<a href="mailto:jh@lanl.gov">jh@lanl.gov</a>

Requested funding for each year: \$990k

Total funding: \$4,950k

Use of human subjects in proposed project?			Yes		No	x
IRB Approval date:		Assurance of Compliance Number:				

Use of vertebrate animals in proposed project?			Yes		No	x
IACUC Approval date:		Animal Welfare Assurance number:				



\_\_\_\_\_  
Signature of Principal Investigator

24 February 2006

\_\_\_\_\_  
Date

\_\_\_\_\_  
Signature of Official

\_\_\_\_\_  
Date

**U.S. Department of Energy**  
**Budget Page**  
(See reverse for Instructions)

ANIZATION <b>Los Alamos National Laboratory</b>				<b>Budget Page No:</b> <u>2</u>	
ICIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Philip Jones SCFY061019</b>				Requested Duration: <u>3</u> (Months) Year 1 FY06	
SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)				DOE Funded	
				Person-mos.	
				Funds Requested	
				Funds Granted	
				by Applicant	
				by DOE	
Philip Jones				1.50	\$15,027
Maltrud				2.50	\$23,142
Lipscomb				2.50	\$23,142
Elliott				2.50	\$23,142
) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
( ) TOTAL SENIOR PERSONNEL (1-6)					
OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
) POST DOCTORAL ASSOCIATES					
) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
) GRADUATE STUDENTS					
) UNDERGRADUATE STUDENTS					
) SECRETARIAL - CLERICAL					
) OTHER					
TOTAL SALARIES AND WAGES (A+B)					\$84,452
FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					\$21,777
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$106,229
PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
TRAVEL				1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)	
				2. FOREIGN	
TOTAL TRAVEL					
TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					\$10,623
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS					\$10,623
TOTAL DIRECT COSTS (A THROUGH G)					\$116,852
INDIRECT COSTS (SPECIFY RATE AND BASE)					
Infrastructure Tax 20% X 160,576 \$32,115					
Program Overhead 1.75% X 229,030 = 4,008 Division Tax 32.0% x 113,558 \$36,339					
TOTAL INDIRECT COSTS G&A Overhead 36% X 186,020 = 66,967					\$121,311
TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$238,163
AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
TOTAL COST OF PROJECT (J+K)					\$238,163

**U.S. Department of Energy**  
**Budget Page**  
(See reverse for Instructions)

ORGANIZATION <b>Los Alamos National Laboratory</b>				Budget Page No: <u>3</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Philip Jones SCFY061019</b>				Requested Duration: <u>12</u> (Months) Year 2 FY07	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested
			CAL	ACAD	SUMR
					by Applicant
					by DOE
1.	Philip Jones		6.00		\$63,033
2.	Maltrud		10.00		\$96,760
3.	Lipscomb		10.00		\$96,760
4.	Elliott		10.00		\$96,760
5.					
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)				
7.	( ) TOTAL SENIOR PERSONNEL (1-6)				
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1.	( ) POST DOCTORAL ASSOCIATES				
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER				
TOTAL SALARIES AND WAGES (A+B)					\$353,313
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					\$91,106
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$444,419
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL					
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL					
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( )					TOTAL COST
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					\$44,442
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS					\$44,442
H. TOTAL DIRECT COSTS (A THROUGH G)					\$488,861
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
		Infrastructure Tax	20% X 160,576	\$32,115	
		Program Overhead 1.75% X 229,030 = 4,008	Division Tax 32.0% x 113,558	\$36,339	
TOTAL INDIRECT COSTS G&A Overhead 36% X 186,020 = 66,967					\$507,516
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$996,377
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					\$996,377

**U.S. Department of Energy  
Budget Page**  
(See reverse for Instructions)

ORGANIZATION <b>Los Alamos National Laboratory</b>				Budget Page No: <u>4</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Philip Jones SCFY061019</b>				Requested Duration: <u>12</u> (Months) Year 3 FY08	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested
			CAL	ACAD	SUMR
					by Applicant
					by DOE
1.	Philip Jones		6.00		\$66,059
2.	Maltrud		10.00		\$101,403
3.	Lipscomb		10.00		\$101,403
4.	Elliott		10.00		\$101,403
5.					
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)				
7.	( ) TOTAL SENIOR PERSONNEL (1-6)				
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1.	( ) POST DOCTORAL ASSOCIATES				
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER				
TOTAL SALARIES AND WAGES (A+B)					\$370,269
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					\$95,478
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$465,747
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL			1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)		
			2. FOREIGN		
TOTAL TRAVEL					
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( )			TOTAL COST		
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					\$46,575
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS					\$46,575
H. TOTAL DIRECT COSTS (A THROUGH G)					\$512,322
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
Infrastructure Tax 20% X 160,576					\$32,115
Program Overhead 1.75% X 229,030 = 4,008					
Division Tax 32.0% x 113,558					\$36,339
TOTAL INDIRECT COSTS G&A Overhead 36% X 186,020 = 66,967					\$531,873
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$1,044,195
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					\$1,044,195

**U.S. Department of Energy  
Budget Page**  
(See reverse for Instructions)

ORGANIZATION <b>Los Alamos National Laboratory</b>				Budget Page No: <u>5</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Philip Jones SCFY061019</b>				Requested Duration: <u>12</u> (Months) Year 4 FY09	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested
			CAL	ACAD	SUMR
					by Applicant
					by DOE
1.	Philip Jones		6.00		\$69,229
2.	Maltrud		10.00		\$106,276
3.	Lipscomb		10.00		\$106,276
4.	Elliott		10.00		\$106,276
5.					
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)				
7.	( ) TOTAL SENIOR PERSONNEL (1-6)				
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1.	( ) POST DOCTORAL ASSOCIATES				
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER				
TOTAL SALARIES AND WAGES (A+B)					\$388,058
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					\$100,065
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$488,123
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL			1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)		
			2. FOREIGN		
TOTAL TRAVEL					
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( )			TOTAL COST		
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					\$48,812
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS					\$48,812
H. TOTAL DIRECT COSTS (A THROUGH G)					\$536,935
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
Infrastructure Tax 20% X 160,576					\$32,115
Program Overhead 1.75% X 229,030 = 4,008					
Division Tax 32.0% x 113,558					\$36,339
TOTAL INDIRECT COSTS G&A Overhead 36% X 186,020 = 66,967					\$557,426
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$1,094,361
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					\$1,094,361

**U.S. Department of Energy  
Budget Page**  
(See reverse for Instructions)

ORGANIZATION <b>Los Alamos National Laboratory</b>				Budget Page No: <u>6</u>		
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Philip Jones SCFY061019</b>				Requested Duration: <u>12</u> (Months) Year 5 FY10		
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested	
			CAL	ACAD	SUMR	
					by Applicant	
					by DOE	
1.	Philip Jones		6.00			\$72,552
2.	Maltrud		12.00			\$111,379
3.	Lipscomb		12.00			\$111,379
4.	Elliott		12.00			\$111,379
5.						
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7.	( ) TOTAL SENIOR PERSONNEL (1-6)					
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)						
1.	( ) POST DOCTORAL ASSOCIATES					
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3.	( ) GRADUATE STUDENTS					
4.	( ) UNDERGRADUATE STUDENTS					
5.	( ) SECRETARIAL - CLERICAL					
6.	( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)						\$406,689
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)						\$104,870
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)						\$511,559
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)						
TOTAL PERMANENT EQUIPMENT						
E. TRAVEL			1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)			
			2. FOREIGN			
TOTAL TRAVEL						
F. TRAINEE/PARTICIPANT COSTS						
1. STIPENDS (Itemize levels, types + totals on budget justification page)						
2. TUITION & FEES						
3. TRAINEE TRAVEL						
4. OTHER (fully explain on justification page)						
TOTAL PARTICIPANTS ( )			TOTAL COST			
G. OTHER DIRECT COSTS						
1. MATERIALS AND SUPPLIES						\$51,156
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION						
3. CONSULTANT SERVICES						
4. COMPUTER (ADPE) SERVICES						
5. SUBCONTRACTS						
6. OTHER						
TOTAL OTHER DIRECT COSTS						\$51,156
H. TOTAL DIRECT COSTS (A THROUGH G)						\$562,715
I. INDIRECT COSTS (SPECIFY RATE AND BASE)			Infrastrurcture Tax	20% X 160,576	\$32,115	
Program Overhead 1.75% X 229,030 = 4,008			Division Tax	32.0% x 113,558	\$36,339	
TOTAL INDIRECT COSTS			G&A Overhead 36% X 186,020 = 66,967			\$584,188
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)						\$1,146,903
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES						
L. TOTAL COST OF PROJECT (J+K)						\$1,146,903

**U.S. Department of Energy  
Budget Page**  
(See reverse for Instructions)

ORGANIZATION <b>Los Alamos National Laboratory</b>				Budget Page No: <u>6</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Philip Jones SCFY061019</b>				Requested Duration: <u>12</u> (Months) Year 6 FY11	
A. SENIOR PERSONNEL: PI/PI, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested by Applicant
			CAL	ACAD	SUMR
1. <b>Philip Jones</b>			4.50		
2. <b>Maltrud</b>			7.50		
3. <b>Lipscomb</b>			7.50		
4. <b>Elliott</b>			7.50		
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. ( ) TOTAL SENIOR PERSONNEL (1-6)					
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)					\$319,739
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					\$82,448
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$402,187
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL			1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)		
			2. FOREIGN		
TOTAL TRAVEL					
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					\$40,219
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS					\$40,219
H. TOTAL DIRECT COSTS (A THROUGH G)					\$442,406
I. INDIRECT COSTS (SPECIFY RATE AND BASE)			Infrastrurcture Tax	20% X 160,576	\$32,115
Program Overhead 1.75% X 229,030 = 4,008			Division Tax	32.0% x 113,558	\$36,339
TOTAL INDIRECT COSTS			G&A Overhead 36% X 186,020 = 66,967		\$459,286
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$901,692
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					\$901,692

Budget Explanations  
Los Alamos National Laboratory

Year 1  
FY06

B. OTHER PERSONNEL

Philip Jones	\$15,027
Matthew Maltrud	\$23,142
William H. Lipscomb	\$23,142
Scott M. Elliott	\$23,142

Total Salaries and wages \$84,453

C. FRINGE BENEFITS \$21,777

Rate applied to salaries included in the above total 20.5% \$21,777

Total salaries, wages and fringe benefits \$106,230

G. OTHER

Travel	\$4,249
Materials & Supplies	\$6,373

Total Other expenses \$10,622

H. TOTAL DIRECT COSTS \$116,852

I. TOTAL INDIRECT COSTS

	Rate	Base	Cost
Division overhead	32%	\$106,230	\$34,206
Infrastructure rate	21%	\$106,229	\$22,308
Program rate	1.76%	\$173,352	\$3,051
G&A rate	35%	\$176,417	\$61,746

Total Indirect Costs \$121,311

J. TOTAL DIRECT AND INDIRECT COSTS \$238,163



Budget Explanations  
Los Alamos National Laboratory

Year 2  
FY07

B. OTHER PERSONNEL

Philip Jones		\$63,033
Matthew Maltrud		\$96,760
William H. Lipscomb		\$96,760
Scott M. Elliott		\$96,760

Total Salaries and wages		<u>\$353,313</u>
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C. FRINGE BENEFITS \$91,106

Rate applied to salaries included in the above total	20.5		\$91,106
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Total salaries, wages and fringe benefits		<u>\$444,419</u>
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G. OTHER

Travel		\$17,777
Materials & Supplies		\$26,665

Total Other expenses		<u>\$44,442</u>
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H. TOTAL DIRECT COSTS \$488,861

I. TOTAL INDIRECT COSTS

	Rate	Base	Cost
Division overhead	32%	\$444,419	\$143,103
Infrastructure rate	21%	\$444,419	\$93,328
Program rate	1.76%	\$725,284	\$12,765
G&A rate	35%	\$738,057	\$258,320

Total Indirect Costs		<u>\$507,516</u>
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J. TOTAL DIRECT AND INDIRECT COSTS \$996,377

Budget Explanations  
Los Alamos National Laboratory

Year 3  
FY08

B. OTHER PERSONNEL

Philip Jones	\$66,059
Matthew Maltrud	\$101,403
William H. Lipscomb	\$101,403
Scott M. Elliott	\$101,403

Total Salaries and wages	<u>\$370,269</u>
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C. FRINGE BENEFITS \$95,478

Rate applied to salaries included in the above total	20.5	\$95,478
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Total salaries, wages and fringe benefits	<u>\$465,747</u>
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G. OTHER

Travel	\$18,630
Materials & Supplies	\$27,945

Total Other expenses	<u>\$46,575</u>
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H. TOTAL DIRECT COSTS \$512,322

I. TOTAL INDIRECT COSTS

Division overhead  
Infrastructure rate  
Program rate  
G&A rate

Rate	Base	Cost
32%	\$465,748	\$149,971
21%	\$465,748	\$97,807
1.76%	\$760,114	\$13,378
35%	\$773,477	\$270,717

Total Indirect Costs	<u>\$531,873</u>
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J. TOTAL DIRECT AND INDIRECT COSTS \$1,044,195

Budget Explanations  
Los Alamos National Laboratory

Year 4  
FY09

B. OTHER PERSONNEL

Philip Jones	\$69,229
Matthew Maltrud	\$106,276
William H. Lipscomb	\$106,276
Scott M. Elliott	\$106,276

Total Salaries and wages	<u>\$388,058</u>
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C. FRINGE BENEFITS \$100,065

Rate applied to salaries included in the above total	20.5	\$100,065
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Total salaries, wages and fringe benefits	<u>\$488,123</u>
---	------------------

G. OTHER

Travel	\$19,525
Materials & Supplies	\$29,287

Total Other expenses	<u>\$48,812</u>
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H. TOTAL DIRECT COSTS \$536,935

I. TOTAL INDIRECT COSTS

Division overhead  
Infrastructure rate  
Program rate  
G&A rate

Rate	Base	Cost
32%	\$488,125	\$157,176
21%	\$488,124	\$102,506
1.76%	\$796,597	\$14,020
35%	\$810,638	\$283,723

Total Indirect Costs	<u>\$557,426</u>
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J. TOTAL DIRECT AND INDIRECT COSTS \$1,094,361

Budget Explanations  
Los Alamos National Laboratory

Year 5  
FY10

B. OTHER PERSONNEL

Philip Jones	\$72,552
Matthew Maltrud	\$111,379
William H. Lipscomb	\$111,379
Scott M. Elliott	\$111,379

Total Salaries and wages	<u>\$406,689</u>
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C. FRINGE BENEFITS \$104,870

Rate applied to salaries included in the above total	20.5	\$104,870
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Total salaries, wages and fringe benefits	<u>\$511,559</u>
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G. OTHER

Travel	\$20,462
Materials & Supplies	\$30,694

Total Other expenses	<u>\$51,156</u>
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H. TOTAL DIRECT COSTS \$562,715

I. TOTAL INDIRECT COSTS

	Rate	Base	Cost
Division overhead	32%	\$511,559	\$164,722
Infrastructure rate	21%	\$511,557	\$107,427
Program rate	1.76%	\$834,886	\$14,694
G&A rate	35%	\$849,557	\$297,345

Total Indirect Costs	<u>\$584,188</u>
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J. TOTAL DIRECT AND INDIRECT COSTS \$1,146,903

Budget Explanations  
Los Alamos National Laboratory

Year 6  
FY11

B. OTHER PERSONNEL

Philip Jones	\$57,091
Matthew Maltrud	\$87,549
William H. Lipscomb	\$87,549
Scott M. Elliott	\$87,549

Total Salaries and wages	<u>\$319,739</u>
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C. FRINGE BENEFITS \$82,448

Rate applied to salaries included in the above total	20.5	\$82,448
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Total salaries, wages and fringe benefits	<u>\$402,187</u>
---	------------------

G. OTHER

Travel	\$16,088
Materials & Supplies	\$24,131

Total Other expenses	<u>\$40,219</u>
----------------------	-----------------

H. TOTAL DIRECT COSTS \$442,406

I. TOTAL INDIRECT COSTS

Division overhead  
Infrastructure rate  
Program rate  
G&A rate

Rate	Base	Cost
32%	\$402,186	\$129,504
21%	\$402,186	\$84,459
1.76%	\$656,364	\$11,552
35%	\$667,919	\$233,772

Total Indirect Costs	<u>\$459,286</u>
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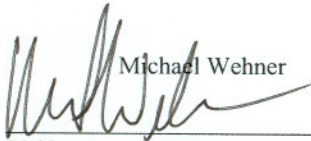
J. TOTAL DIRECT AND INDIRECT COSTS \$901,692

## A Scalable and Extensible Earth System Model for Climate Change Science

For the period July 1, 2006 – June 30, 2011

### Principal Investigator

Michael Wehner, Staff Computer Scientist  
Computational Research Division  
Lawrence Berkeley National Laboratory  
(510) 495-2527 (Voice)  
(510) 486-5812 (Fax)  
MFWehner@lbl.gov

  
Michael Wehner  
\_\_\_\_\_  
PI Signature and Date

### Official Signing for LBNL

Horst D. Simon, Director  
NERSC Center and Computational Research Division  
Lawrence Berkeley National Laboratory  
(510) 486-7377 (Voice)  
(510) 486-4300 (Fax)  
HDSimon@lbl.gov

Horst Simon  
 2/27/06  
\_\_\_\_\_  
Official Signature and Date

### Lead Principal Investigator

John Drake, Oak Ridge National Laboratory

### LBNL Co PI's:

Yun He  
Yu-Heng Tseng  
Michael Wehner

Requested Funding:      Year 1: \$302,272  
                                    Year 2: \$311,872  
                                    Year 3: \$322,300  
                                    Year 4: \$332,170  
                                    Year 5: \$332,753

Total Funding Requested: \$1,601,359

Use of Human Subjects: No  
Use of Vertebrate Animals: No

**U.S. Department of Energy**  
**Budget Page**  
(See reverse for Instructions)

ORGANIZATION <b>Lawrence Berkeley National Laboratory</b>				Budget Page No: <u>1</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Michael Wehner</b>				Requested Duration: <u>12</u> (Months) Year 1	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)				DOE Funded	
				Person-mos.	
				CAL	ACAD
				SUMR	
				Funds Requested	
				Funds Granted	
				by Applicant	
				by DOE	
1.	Michael Wehner, Computer Staff Scientist			0.10	
2.	Yu-Heng Tseng, Computer Systems Engineer II			0.35	
3.	Yun He, Computer Systems Engineer III			0.75	
4.					
5.					
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE) TSM 110-119				
7.	( 3 ) TOTAL SENIOR PERSONNEL (1-6)			1.20	
B. ( ) OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1.	( ) POST DOCTORAL ASSOCIATES				
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER				
TOTAL SALARIES AND WAGES (A+B)					\$108,541
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$108,541
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					\$3,000
E. TRAVEL					\$5,000
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL					\$5,000
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					\$1,662
5. SUBCONTRACTS					
6. OTHER					\$2,266
TOTAL OTHER DIRECT COSTS					\$3,928
H. TOTAL DIRECT COSTS (A THROUGH G)					\$120,469
I. INDIRECT COSTS					
Org Burden 17.6% -Base 157,600 Tvl Rate 14% - Base 5,000					
Proc. Burden 8.4% Base 3,000 LDRD Rate 9.1% - Base 193,694					
Gen Rate 46.3% -Base 188,184 Payroll Rate (Var.) - Base 108,541					
TOTAL INDIRECT COSTS					\$181,803
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$302,272
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					\$302,272

**U.S. Department of Energy**  
**Budget Page**  
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ORGANIZATION <b>Lawrence Berkeley National Laboratory</b>				Budget Page No: <u>2</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Michael Wehner</b>				Requested Duration: <u>12</u> (Months) Year 2	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested
			CAL	ACAD	SUMR
					by Applicant
					by DOE
1.	Michael Wehner, Computer Staff Scientist		0.10		\$12,425
2.	Yu-Heng Tseng, Computer Systems Engineer II		0.35		\$29,815
3.	Yun He, Computer Systems Engineer III		0.75		\$69,558
4.					
5.					
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE) TSM 110-119				
7.	( 3 ) TOTAL SENIOR PERSONNEL (1-6)		1.20		\$111,797
B.	( ) OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)				
1.	( ) POST DOCTORAL ASSOCIATES				
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER				
TOTAL SALARIES AND WAGES (A+B)					\$111,797
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$111,797
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					\$3,000
E. TRAVEL					\$5,000
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL					\$5,000
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					\$1,677
5. SUBCONTRACTS					
6. OTHER					\$2,372
TOTAL OTHER DIRECT COSTS					\$4,049
H. TOTAL DIRECT COSTS (A THROUGH G)					\$123,846
I. INDIRECT COSTS (SPECIFY BASE AND RATE)					
Gen Rate 5.6% - Base 162,749 Tvl Rate 14% - Base 5,000					
Proc. Burden 8.4% Base 3,000 LDRD Rate 9.1% - Base 199,871					
Gen Rate 46.3% - Base 194,357 Payroll Rate (Var.) - Base 111,797					
TOTAL INDIRECT COSTS					\$188,026
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$311,872
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					\$311,872



**U.S. Department of Energy**  
**Budget Page**  
(See reverse for Instructions)

ORGANIZATION <b>Lawrence Berkeley National Laboratory</b>				Budget Page No: <u>3</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Michael Wehner</b>				Requested Duration: <u>12</u> (Months) Year 3	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested
			CAL	ACAD	SUMR
					by Applicant
					by DOE
1.	Michael Wehner, Computer Staff Scientist		0.10		\$12,797
2.	Yu-Heng Tseng, Computer Systems Engineer II		0.35		\$30,709
3.	Yun He, Computer Systems Engineer III		0.75		\$71,645
4.					
5.					
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE) TSM 110-119				
7.	( 3 ) TOTAL SENIOR PERSONNEL (1-6)		1.20		\$115,151
B.	( ) OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)				
1.	( ) POST DOCTORAL ASSOCIATES				
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER				
TOTAL SALARIES AND WAGES (A+B)					\$115,151
C.	FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$115,151
D.	PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)				
TOTAL PERMANENT EQUIPMENT					\$3,000
E.	TRAVEL		1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)		\$5,000
			2. FOREIGN		
TOTAL TRAVEL					\$5,000
F.	TRAINEE/PARTICIPANT COSTS				
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G.	OTHER DIRECT COSTS				
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					\$1,680
5. SUBCONTRACTS					
6. OTHER					\$2,376
TOTAL OTHER DIRECT COSTS					\$4,055
H.	TOTAL DIRECT COSTS (A THROUGH G)				\$127,207
I.	INDIRECT COSTS (SPECIFY CATEGORY AND RATE)-Base		168,450	Tvl Rate 14% - Base	5,000
Proc. Burden 8.4% Base			3,000	LDRD Rate 9.1% - Base	206,582
TOTAL INDIRECT COSTS			201,067	Payroll Rate (Var.) - Base	115,151
J.	TOTAL DIRECT AND INDIRECT COSTS (H+I)				\$322,300
K.	AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES				
L.	TOTAL COST OF PROJECT (J+K)				\$322,300

**U.S. Department of Energy**  
**Budget Page**  
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ORGANIZATION <b>Lawrence Berkeley National Laboratory</b>				Budget Page No: <u>4</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Michael Wehner</b>				Requested Duration: <u>12</u> (Months) Year 4	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested
			CAL	ACAD	SUMR
					by Applicant
					by DOE
1.	Michael Wehner, Computer Staff Scientist		0.10		\$13,181
2.	Yu-Heng Tseng, Computer Systems Engineer II		0.35		\$31,630
3.	Yun He, Computer Systems Engineer III		0.75		\$73,794
4.					
5.					
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE) TSM 110-119				
7.	( 3 ) TOTAL SENIOR PERSONNEL (1-6)		1.20		\$118,606
B. ( ) OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1.	( ) POST DOCTORAL ASSOCIATES				
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER				
TOTAL SALARIES AND WAGES (A+B)					\$118,606
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$118,606
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					\$3,000
E. TRAVEL					\$5,000
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL					\$5,000
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					\$1,680
5. SUBCONTRACTS					
6. OTHER					\$1,343
TOTAL OTHER DIRECT COSTS					\$3,022
H. TOTAL DIRECT COSTS (A THROUGH G)					\$129,628
I. INDIRECT COSTS (SPECIFY ON GLE AND BAE)-Base			174,729	Tvl Rate 14% - Base	5,000
Proc. Burden 8.4% Base			3,000	LDRD Rate 9.1% - Base	212,933
TOTAL INDIRECT COSTS Gen Rate 46.3% -Base			207,418	Payroll Rate (Var). - Base	118,606
					\$202,542
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$332,170
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					\$332,170

**U.S. Department of Energy  
Budget Page**  
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ORGANIZATION <b>Lawrence Berkeley National Laboratory</b>				Budget Page No: <u>5</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Michael Wehner</b>				Requested Duration: <u>12</u> (Months) Year 5	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested
			CAL	ACAD	SUMR
					by Applicant
					by DOE
1.	Michael Wehner, Computer Staff Scientist		0.10		\$13,181
2.	Yu-Heng Tseng, Computer Systems Engineer II		0.35		\$31,630
3.	Yun He, Computer Systems Engineer III		0.75		\$73,794
4.					
5.					
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE) TSM 110-119				
7.	( 3 ) TOTAL SENIOR PERSONNEL (1-6)		1.20		\$118,606
B.	( ) OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)				
1.	( ) POST DOCTORAL ASSOCIATES				
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER				
TOTAL SALARIES AND WAGES (A+B)					\$118,606
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$118,606
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					\$3,000
E. TRAVEL			1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)		\$5,000
			2. FOREIGN		
TOTAL TRAVEL					\$5,000
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					\$1,680
5. SUBCONTRACTS					
6. OTHER					\$1,343
TOTAL OTHER DIRECT COSTS					\$3,022
H. TOTAL DIRECT COSTS (A THROUGH G)					\$129,628
I. INDIRECT COSTS (SPECIFY ON THE ATTACHED PAGE)					
Gen Rate 5.6% - Base 175,048 Tvl Rate 14% - Base 5,000					
Proc. Burden 8.4% Base 3,000 LDRD Rate 9.1% - Base 213,308					
Gen Rate 46.3% - Base 207,793 Payroll Rate (Var.) - Base 118,606					
TOTAL INDIRECT COSTS					\$203,125
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$332,753
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					\$332,753

**Budget Page**

(See reverse for Instructions)

ORGANIZATION <b>Lawrence Berkeley National Laboratory</b>				Budget Page No: <u>6</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Michael Wehner</b>				Requested Duration: <u>60</u> (Months) Summary - All Years	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)				DOE Funded	
				Person-mos.	
				Funds Requested	
				Funds Granted	
				by Applicant	
				by DOE	
1.	Michael Wehner, Computer Staff Scientist	0.50		\$63,647	
2.	Yu-Heng Tseng, Computer Systems Engineer II	1.75		\$152,731	
3.	Yun He, Computer Systems Engineer III	3.75		\$356,323	
4.					
5.					
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE) TSM 110-119				
7.	( 3 ) TOTAL SENIOR PERSONNEL (1-6)	6.00		\$572,701	
B. ( ) OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1.	( ) POST DOCTORAL ASSOCIATES				
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER				
TOTAL SALARIES AND WAGES (A+B)				\$572,701	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				\$572,701	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT				\$15,000	
E. TRAVEL					
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				\$25,000	
2. FOREIGN					
TOTAL TRAVEL				\$25,000	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES				\$8,379	
5. SUBCONTRACTS					
6. OTHER				\$9,692	
TOTAL OTHER DIRECT COSTS				\$18,070	
H. TOTAL DIRECT COSTS (A THROUGH G)				\$630,771	
I. INDIRECT COSTS					
Org Burden 17.6% -Base 838,578 Tvl Rate 14% - Base 25,000					
Proc. Burden 8.4% Base 15,000 LDRD Rate 9.1% - Base 1,026,388					
Gen Rate 46.3% -Base 998,819 Payroll Rate (Var.) - Base 572,701					
TOTAL INDIRECT COSTS				\$970,588	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				\$1,601,359	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				\$1,601,359	


### 3.5 Lawrence Livermore National Laboratory Detail Budget & Budget Explanation

#### A Scalable and Extensible Earth System Model for Climate Change Science

Proposal Submitted to Application: **Climate Modeling and Simulation**  
Program Announcement LAB06-04

By  
Lawrence Livermore National Laboratory  
Livermore, CA

#### Principal Investigator:

 24 Feb 2006  
Dr. Philip Cameron-Smith      Date  
Physicist/Atmospheric Scientist  
Energy and Environmental Directorate  
Lawrence Livermore National Laboratory  
Tel: 925-423-6634  
Fax: 925-422-6388  
Email: [cameronsmith1@llnl.gov](mailto:cameronsmith1@llnl.gov)


#### Amount Requested:

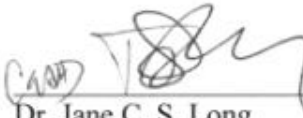
#### Budget:

1 <sup>st</sup> year: \$563,083	2 <sup>nd</sup> year: \$578,564	3 <sup>rd</sup> year: 594,600
4 <sup>th</sup> year: \$610,677	5 <sup>th</sup> year: \$627,230	Total: \$2,974,154

Use of human subjects or vertebrate animals is proposed project: No

Use of vertebrate animals in proposed project: No

 2/24/06  
Dr. Douglas Rotman      Date  
Program Leader  
Earth Systems Science & Engineering  
Energy & Environmental Directorate  
Lawrence Livermore National Laboratory  
Tel: 925-422-7746  
Fax: 925-423-0153  
Email: [rotman1@llnl.gov](mailto:rotman1@llnl.gov)

 2/24/06  
Dr. Jane C. S. Long      Date  
Associate Director  
Energy and Environmental Directorate  
Lawrence Livermore National Laboratory  
Tel: 925-422-0315  
Fax: 925-422-0096  
Email: [long36@llnl.gov](mailto:long36@llnl.gov)

**U.S. Department of Energy**  
**Budget Page**  
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ORGANIZATION <b>Lawrence Livermore National Lab</b>				Budget Page No: <u>1 of 6</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Philip Cameron-Smith</b>				Requested Duration: <u>12</u> (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested
			CAL	ACAD	SUMR
					by Applicant
					by DOE
1. Cameron-Smith, PI, Physicist			7.80		\$67,174
2. Mirin, Computational Physicist			5.40		\$64,412
3. Chuang, Physicist			1.20		\$11,366
4. Atherton, Physicist			1.20		\$12,614
5. Connell, Physicist			1.20		\$11,366
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. ( ) TOTAL SENIOR PERSONNEL (1-6)			16.80		\$166,932
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)					\$166,932
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					\$71,451
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$238,383
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL			1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)		\$11,500
			2. FOREIGN		
TOTAL TRAVEL					\$11,500
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					\$6,000
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					\$4,000
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER - OFC					\$27,356
TOTAL OTHER DIRECT COSTS					\$37,356
H. TOTAL DIRECT COSTS (A THROUGH G)					\$287,239
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS					\$275,844
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$563,083
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					\$563,083

**U.S. Department of Energy**  
**Budget Page**  
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ORGANIZATION <b>Lawrence Livermore National Lab</b>				Budget Page No: <u>2 of 6</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Philip Cameron-Smith</b>				Requested Duration: <u>12</u> (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested
			CAL	ACAD	SUMR
					by Applicant
					by DOE
1. Cameron-Smith, PI, Physicist			7.80		\$69,189
2. Mirin, Computational Physicist			5.40		\$66,344
3. Chuang, Physicist			1.20		\$11,706
4. Atherton, Physicist			1.20		\$12,993
5. Connell, Physicist			1.20		\$11,706
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. ( ) TOTAL SENIOR PERSONNEL (1-6)			16.80		\$171,938
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)					\$171,938
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					\$74,412
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$246,350
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL			1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)		\$11,500
			2. FOREIGN		
TOTAL TRAVEL					\$11,500
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					\$6,000
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					\$4,000
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER - OFC					\$27,356
TOTAL OTHER DIRECT COSTS					\$37,356
H. TOTAL DIRECT COSTS (A THROUGH G)					\$295,206
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS					\$283,358
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$578,564
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					\$578,564

**U.S. Department of Energy**  
**Budget Page**  
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ORGANIZATION <b>Lawrence Livermore National Lab</b>				Budget Page No: <u>3 of 6</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Philip Cameron-Smith</b>				Requested Duration: <u>12</u> (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)				DOE Funded Person-mos.	
				Funds Requested	
				Funds Granted	
				by Applicant	
				by DOE	
1.	Cameron-Smith, PI, Physicist	7.80	0.00	0.00	\$71,264
2.	Mirin, Computational Physicist	5.40	0.00	0.00	\$68,335
3.	Chuang, Physicist	1.20	0.00	0.00	\$12,058
4.	Atherton, Physicist	1.20	0.00	0.00	\$13,382
5.	Connell, Physicist	1.20	0.00	0.00	\$12,058
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)				
7.	( ) TOTAL SENIOR PERSONNEL (1-6)	16.80	0.00	0.00	\$177,097
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1.	( ) POST DOCTORAL ASSOCIATES				
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER				
TOTAL SALARIES AND WAGES (A+B)				\$177,097	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				\$76,860	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				\$253,957	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT				\$0	
E. TRAVEL				\$11,500	
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL				\$11,500	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)				\$0	
2. TUITION & FEES				\$0	
3. TRAINEE TRAVEL				\$0	
4. OTHER (fully explain on justification page)				\$0	
TOTAL PARTICIPANTS                   0 )                   TOTAL COST				\$0	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				\$6,000	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				\$4,000	
3. CONSULTANT SERVICES				\$0	
4. COMPUTER (ADPE) SERVICES				\$0	
5. SUBCONTRACTS				\$0	
6. OTHER - OFC				\$27,356	
TOTAL OTHER DIRECT COSTS				\$37,356	
H. TOTAL DIRECT COSTS (A THROUGH G)				\$302,813	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS				\$291,787	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				\$594,600	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES				\$0	
L. TOTAL COST OF PROJECT (J+K)				\$594,600	



**U.S. Department of Energy**  
**Budget Page**  
(See reverse for Instructions)

ORGANIZATION				<b>Budget Page No:</b> <u>4 of 6</u>				
Lawrence Livermore National Lab								
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR				Requested Duration: <u>12</u> (Months)				
Philip Cameron-Smith								
A. SENIOR PERSONNEL: PI/PI, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)				DOE Funded			Funds Requested	Funds Granted
				Person-mos.			by Applicant	by DOE
	CAL	ACAD	SUMR					
1.	Cameron-Smith, PI, Physicist	7.80	0.00	0.00	\$73,403			
2.	Mirin, Computational Physicist	5.40	0.00	0.00	\$70,385			
3.	Chuang, Physicist	1.20	0.00	0.00	\$12,420			
4.	Atherton, Physicist	1.20	0.00	0.00	\$13,784			
5.	Connell, Physicist	1.20	0.00	0.00	\$12,420			
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)							
7.	( ) TOTAL SENIOR PERSONNEL (1-6)	16.80	0.00	0.00	\$182,412			
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)								
1.	( ) POST DOCTORAL ASSOCIATES							
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)							
3.	( ) GRADUATE STUDENTS							
4.	( ) UNDERGRADUATE STUDENTS							
5.	( ) SECRETARIAL - CLERICAL							
6.	( ) OTHER							
TOTAL SALARIES AND WAGES (A+B)					\$182,412			
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					\$79,166			
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$261,578			
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)								
TOTAL PERMANENT EQUIPMENT					\$0			
E. TRAVEL					\$11,500			
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)								
2. FOREIGN								
TOTAL TRAVEL					\$11,500			
F. TRAINEE/PARTICIPANT COSTS								
1. STIPENDS (Itemize levels, types + totals on budget justification page)					\$0			
2. TUITION & FEES					\$0			
3. TRAINEE TRAVEL					\$0			
4. OTHER (fully explain on justification page)					\$0			
TOTAL PARTICIPANTS <u>0</u> ) TOTAL COST					\$0			
G. OTHER DIRECT COSTS								
1. MATERIALS AND SUPPLIES					\$6,000			
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					\$4,000			
3. CONSULTANT SERVICES					\$0			
4. COMPUTER (ADPE) SERVICES					\$0			
5. SUBCONTRACTS					\$0			
6. OTHER - OFC					\$27,356			
TOTAL OTHER DIRECT COSTS					\$37,356			
H. TOTAL DIRECT COSTS (A THROUGH G)					\$310,434			
I. INDIRECT COSTS (SPECIFY RATE AND BASE)								
TOTAL INDIRECT COSTS					\$300,243			
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$610,677			
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					\$0			
L. TOTAL COST OF PROJECT (J+K)					\$610,677			

**U.S. Department of Energy**  
**Budget Page**  
(See reverse for Instructions)

ORGANIZATION <b>Lawrence Livermore National Lab</b>				Budget Page No: <u>5 of 6</u>		
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Philip Cameron-Smith</b>				Requested Duration: <u>12</u> (Months)		
A. SENIOR PERSONNEL: PI/PI, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested	
			CAL	ACAD	SUMR	
					by Applicant	
					by DOE	
1.	Cameron-Smith, PI, Physicist		7.80	0.00	0.00	\$75,604
2.	Mirin, Computational Physicist		5.40	0.00	0.00	\$72,496
3.	Chuang, Physicist		1.20	0.00	0.00	\$12,792
4.	Atherton, Physicist		1.20	0.00	0.00	\$14,197
5.	Connell, Physicist		1.20	0.00	0.00	\$12,792
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7.	( ) TOTAL SENIOR PERSONNEL (1-6)		16.80	0.00	0.00	\$187,881
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)						
1.	( ) POST DOCTORAL ASSOCIATES					
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3.	( ) GRADUATE STUDENTS					
4.	( ) UNDERGRADUATE STUDENTS					
5.	( ) SECRETARIAL - CLERICAL					
6.	( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)						\$187,881
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)						\$81,542
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)						\$269,423
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)						
TOTAL PERMANENT EQUIPMENT						\$0
E. TRAVEL						\$11,500
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)						
2. FOREIGN						
TOTAL TRAVEL						\$11,500
F. TRAINEE/PARTICIPANT COSTS						
1. STIPENDS (Itemize levels, types + totals on budget justification page)						\$0
2. TUITION & FEES						\$0
3. TRAINEE TRAVEL						\$0
4. OTHER (fully explain on justification page)						\$0
TOTAL PARTICIPANTS 0 ) TOTAL COST						\$0
G. OTHER DIRECT COSTS						
1. MATERIALS AND SUPPLIES						\$6,000
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION						\$4,000
3. CONSULTANT SERVICES						\$0
4. COMPUTER (ADPE) SERVICES						\$0
5. SUBCONTRACTS						\$0
6. OTHER - OFC						\$27,356
TOTAL OTHER DIRECT COSTS						\$37,356
H. TOTAL DIRECT COSTS (A THROUGH G)						\$318,279
I. INDIRECT COSTS (SPECIFY RATE AND BASE)						
TOTAL INDIRECT COSTS						\$308,951
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)						\$627,230
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES						\$0
L. TOTAL COST OF PROJECT (J+K)						\$627,230

**U.S. Department of Energy**  
**Budget Page**  
(See reverse for Instructions)

ORGANIZATION <b>Lawrence Livermore National Lab</b>				Budget Page No: <u>6 of 6</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Philip Cameron-Smith</b>				Requested Duration: <u>60</u> (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested
			CAL	ACAD	SUMR
					by Applicant
					by DOE
1.	Cameron-Smith, PI, Physicist		39.00		\$356,634
2.	Mirin, Computational Physicist		27.00		\$341,972
3.	Chuang, Physicist		6.00		\$60,342
4.	Atherton, Physicist		6.00		\$66,970
5.	Connell, Physicist		6.00		\$60,342
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)				
7.	( ) TOTAL SENIOR PERSONNEL (1-6)		84.00		\$886,260
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1.	( ) POST DOCTORAL ASSOCIATES				
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER				
TOTAL SALARIES AND WAGES (A+B)					\$886,260
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$1,269,691
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL					
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					57500.00
2. FOREIGN					
TOTAL TRAVEL					\$57,500
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					\$30,000
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					\$20,000
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER - space, telephone, computer, electricity recharges					\$136,780
TOTAL OTHER DIRECT COSTS					\$186,780
H. TOTAL DIRECT COSTS (A THROUGH G)					\$1,513,971
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS					\$1,460,183
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$2,974,154
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					\$2,974,154

## Budget Justification

### Lawrence Livermore National Laboratory

#### A. Senior Personnel

**Philip Cameron-Smith:** Site contact for the project at Lawrence Livermore National Laboratory. Lead the implementation of atmospheric chemistry, and its iterations with biogeochemistry, in the Community Climate System Model (CCSM).

**Art Mirin:** Improved performance and scalability and software engineering aspects of the Community Atmosphere Model (CAM) and the Community Climate System Model (CCSM).

**Cathy Chuang:** Collaborate on implementation of aerosols capabilities in CAM. Connection to DOE-

**Cyndi Atherton:** Collaborate on implementation of aerosol capabilities, especially secondary organic aerosols. Connection to DOE-ASP program.

**Peter Connell:** Development and analysis of atmospheric chemistry mechanisms.

#### C. Fringe Benefits

The Laboratory's Payroll Burden Rate is 42.5% and is applied to the non-leave standard salary of all Laboratory employees, including overtime. PostDocs are charged a 35% Payroll Burden, and students are charged 9.5%.

#### D. Equipment

None planned.

#### E. Travel

##### Domestic Travel:

Four trips per FTE per year, estimated at \$11.5k per year

#### F. Trainee/Participant Costs

N/A.

#### G. Other Costs

- 1.) Software/Hardware maintenance for hard disk server
- 2.) Poster printing; Academic journal publication charges, estimated at \$4k per year
- 4) Computer services-N/A
- 6.) Office space is estimated at \$27,356 per year

#### H. Total Direct Costs

Total direct costs are estimated at \$1,513,971

#### I. Indirect Costs

Total Indirect Costs are estimated at \$1,460,183 LLNL rate amounts and their definitions are explained in Attachment A. Note that rates are applied in a specified order and not all taxes apply to each direct cost.



# Face Page

**TITLE OF PROPOSED RESEARCH:**

A Scalable and Extensible Earth System Model for Climate Change Science

1. CATALOG OF FEDERAL DOMESTIC ASSISTANCE #  
81.049

2. CONGRESSIONAL DISTRICT:  
Applicant Organization's District: District #2  
Project Site's District: \_\_\_\_\_

3A. I.R.S. ENTITY IDENTIFICATION OR SSN:  
840421668

3B. DUNS Number:  
0783395870000

4. AREA OF RESEARCH OR ANNOUNCEMENT TITLE#:  
DEFG02-06ER06-04

5. HAS THIS RESEARCH PROPOSAL BEEN SUBMITTED  
TO ANY OTHER FEDERAL AGENCY?  
 YES  NO

PLEASE LIST \_\_\_\_\_

6. DOE/OER PROGRAM STAFF CONTACT (if known):  
\_\_\_\_\_

7. TYPE OF APPLICATION:  
 New  Renewal  
 Continuation  Revision  
 Supplement

8. ORGANIZATION TYPE:  
 Local Govt.  State Govt.  
 Non-Profit  Hospital  
 Indian Tribal Govt.  Individual  
 Other  Inst. of Higher Educ.  
 For-Profit  Disadvan. Business  
 Small Business  8(a)  
 Women-Owned

9. CURRENT DOE AWARD # (IF APPLICABLE):  
\_\_\_\_\_

10. WILL THIS RESEARCH INVOLVE:  
10A. Human Subjects  No  If yes  
Exemption No. \_\_\_\_\_ or  
IRB Approval Date \_\_\_\_\_  
Assurance of Compliance No: \_\_\_\_\_  
10B. Vertebrate Animals  No  If yes  
IACUC Approval Date \_\_\_\_\_ or  
Animal Welfare Assurance No: \_\_\_\_\_

11. AMOUNT REQUESTED FROM DOE FOR ENTIRE  
PROJECT PERIOD \$ 4,085,183.00

12. DURATION OF ENTIRE PROJECT PERIOD:  
07/01/06 to 06/30/11  
MM/DD/YY MM/DD/YY

13. REQUESTED AWARD START DATE  
07/01/06  
MM/DD/YY

14. IS APPLICANT DELINQUENT ON ANY FEDERAL DEBT?  
 Yes (attach an explanation)  No

15. PRINCIPAL INVESTIGATOR/PROGRAM DIRECTOR  
NAME Dr. William Collins  
TITLE Scientist III  
ADDRESS 1850 Table Mesa Drive  
Boulder, CO 80305  
PHONE NUMBER 303-497-1381

William Collins  
SIGNATURE OF PRINCIPAL INVESTIGATOR/ PROGRAM DIRECTOR  
(please type in full name if electronically submitted)  
Date 03/06/06

PI/PD ASSURANCE: I agree to accept responsibility for the scientific conduct of the project and to provide the required progress reports if an award is made as a result of this submission. Willful provision of false information is a criminal offense. (U.S. Code, Title 18, Section 1001).

16. ORGANIZATION'S NAME UCAR  
ADDRESS P. O. Box 3000  
Boulder, CO 80305

CERTIFYING REPRESENTATIVE'S  
NAME Ms. Gina Taberski  
TITLE Manager, Sponsored Agreements  
PHONE NUMBER 303-497-2132

SIGNATURE OF ORGANIZATION'S CERTIFYING REPRESENTATIVE  
(please type in full name if electronically submitted)  
Date \_\_\_\_\_

CERTIFICATION and ACCEPTANCE: I certify that the statements herein are true and complete to the best of my knowledge, and accept the obligation to comply with DOE terms and conditions if an award is made as the result of this submission. A willfully false certification is a criminal offense. (U.S. Code, Title 18, Section 1001).

**NOTICE FOR HANDLING PROPOSALS**

This submission is to be used only for DOE evaluation purposes and this notice shall be affixed to any reproduction or abstract thereof. All Government and non-Government personnel handling this submission shall exercise extreme care to ensure that the information contained herein is not duplicated, used, or disclosed in whole or in part for any purpose other than evaluation without written permission except that if an award is made based on this submission, the terms of the award shall control disclosure and use. This notice does not limit the Government's right to use information contained in the submission if it is obtainable from another source without restriction. This is a Government notice, and shall not itself be construed to impose any liability upon the Government or Government personnel for any disclosure or use of data contained in this submission.

**PRIVACY ACT STATEMENT**

If applicable, you are requested, in accordance with 5 U.S.C., Sec. 562A, to voluntarily provide your Social Security Number (SSN). However, you will not be denied any right, benefit, or privilege provided by law because of a refusal to disclose your SSN. We request your SSN to aid in accurate identification, referral and review of applications for research/training support for efficient management of Office of Science grant/contract programs.

**A Scalable and Extensible Earth System Model  
for Climate Change Science**

W. Collins, Principal Investigator  
YEAR 1: 1 July 2006-30 June 2007

**MODIFIED TOTAL DIRECT COSTS (MTDC):**

	CGD	FTE	NSF Cosponsorship	FTE	Total
SALARIES (85%)*					
Sci. III PI (.20 total)	\$9,702	0.10	\$9,702	0.10	\$19,404
Sr. Scientist (.16 total)	\$7,555	0.06	\$12,592	0.10	20,148
Sr. Scientist (.05 total)	\$0	0.00	6,919	0.05	6,919
Scientist II	\$78,481	1.00	-	0.00	78,481
Software Engineer IV	\$91,543	1.00	-	0.00	91,543
Software Engineer II	\$76,807	1.00	-	0.00	76,807
STAFF SUBTOTAL	<u>\$264,088</u>		\$ 29,213		\$ 293,302
 BENEFITS (48.8%)*	 <u>128,875</u>		 <u>14,256</u>		 <u>143,131</u>
SUBTOTAL	\$392,963		\$43,469		\$ 436,433
 MATERIALS/SUPPLIES	 5,000		 0		 5,000
(page charges based on avg. \$110-\$115/page)					
 PURCHASED SERVICES:	 500		 0		 500
(commun. costs incl. LD phone, fax, copy center)					-
Subcontract (Craig--first \$25k/year)	25000				25,000
 TRAVEL (3 domestic trips)	 <u>6,000</u>		 <u>0</u>		 <u>6,000</u>
(estimated travel based on previous DOE costs)					
<b>SUBTOTAL, MTDC</b>	\$429,463		\$43,469		\$472,933
 INDIRECT COSTS (50.6%)*	 217,308		 21,995		 239,304
COMPUTER SERVICE CENTER*	30,573		1,932		32,505
SCD COMPUTING (500 GAUs @ \$5)	<u>0</u>		<u>2,500</u>		<u>2,500</u>
SUBTOTAL	\$677,344		\$69,896		\$747,242
 UCAR Management Fee (3%)*	 <u>20,320</u>		 <u>0</u>		 <u>20,320</u>
SUBTOTAL	\$697,665		\$69,896		\$767,562
 <b>EXCLUSIONS FROM MTDC:</b>					
<b>Subcontract, balance (Craig)</b>	41560		<u>0</u>		41,560
EQUIPMENT (Sun workstation)	<u>10,000</u>		<u>0</u>		<u>10,000</u>
<b>TOTAL FUNDING TO UCAR</b>	\$749,224		\$69,896		\$819,122

\*See attached footnote page.

**A Scalable and Extensible Earth System Model  
for Climate Change Science**

W. Collins, Principal Investigator  
YEAR 2: 1 July 2007-30 June 2008

**MODIFIED TOTAL DIRECT COSTS (MTDC):**

	CGD	FTE	NSF Cosponsorship	FTE	Total
SALARIES (85%)*					
Sci. III PI (.20 total)	\$10,187	0.10	\$10,187	0.10	\$20,374
Sr. Scientist (.16 total)	8,400	0.06	13,222	0.10	21,622
Sr. Scientist (.05 total)	-	0.00	7,265	0.05	7,265
Scientist II	82,405	1.00	-	0.00	82,405
Software Engineer IV	96,120	1.00	-	0.00	96,120
Software Engineer II	80,647	1.00	-	0.00	80,647
STAFF SUBTOTAL	\$277,759		\$ 30,674		\$ 308,434
 BENEFITS (48.8%)*	 <u>135,546</u>		 <u>14,969</u>		 <u>150,515</u>
SUBTOTAL	\$413,305		\$45,643		\$ 458,949
 MATERIALS/SUPPLIES	 5,300		 0		 5,300
(page charges based on avg. \$110-\$115/page)					
 PURCHASED SERVICES:	 500		 0		 500
(commun. costs incl. LD phone, fax, copy center)					-
Subcontract (Craig) first \$25K/year	25000				25,000
 TRAVEL (3 domestic trips)					
(estimated travel based on previous DOE costs)	<u>6,300</u>		<u>0</u>		<u>6,300</u>
<b>SUBTOTAL, MTDC</b>	\$450,405		\$45,643		\$496,049
 INDIRECT COSTS (50.6%)*	 227,905		 23,095		 251,001
COMPUTER SERVICE CENTER*	30,507		1,931		32,438
SCD COMPUTING (500 GAUs @ \$5)	<u>0</u>		<u>2,500</u>		<u>2,500</u>
SUBTOTAL	\$708,817		\$73,169		\$781,988
 UCAR Management Fee (3%)*	 <u>21,264</u>		 <u>0</u>		 <u>21,264</u>
SUBTOTAL	\$730,081		\$73,169		\$803,252
 <b>EXCLUSIONS FROM MTDC:</b>					
<b>Subcontract, balance of Craig</b>	44,888				44,888
EQUIPMENT (Sun workstation)	<u>10,000</u>		<u>0</u>		<u>10,000</u>
<b>TOTAL FUNDING TO UCAR</b>	\$784,969		\$73,169		\$858,140

\*See attached footnote page.

**A Scalable and Extensible Earth System Model  
for Climate Change Science**

W. Collins, Principal Investigator

YEAR 3: 1 July 2008-30 June 2009

**MODIFIED TOTAL DIRECT COSTS (MTDC):**

	CGD	FTE	NSF Cosponsorship	FTE	Total
SALARIES (85%)*					
Sci. III PI (.20 total)	\$10,697	0.10	\$10,697	0.10	\$21,393
Sr. Scientist (.16 total)	8,820	0.06	13,883	0.10	22,703
Sr. Scientist (.05 total)	-	0.00	7,628	0.05	7,628
Scientist II	86,526	1.00	-	0.00	86,526
Software Engineer IV	100,926	1.00	-	0.00	100,926
Software Engineer II	84,679	1.00	-	0.00	84,679
STAFF SUBTOTAL	\$291,648		\$ 32,208		\$ 323,856
 BENEFITS (48.8%)*	 <u>142,324</u>		 <u>15,718</u>		 <u>158,042</u>
SUBTOTAL	\$433,972		\$47,926		\$ 481,898
 MATERIALS/SUPPLIES	 5,600		 0		 5,600
(page charges based on avg. \$110-\$115/page)					
 PURCHASED SERVICES:	 500		 0		 500
(commun. costs incl. LD phone, fax, copy center)					-
Subcontract (Craig) first \$25k/year	25,000				25,000
 TRAVEL (3 domestic trips)					
(estimated travel based on previous DOE costs)	<u>6,600</u>		<u>0</u>		<u>6,600</u>
<b>SUBTOTAL, MTDC</b>	\$471,672		\$47,926		\$519,598
 INDIRECT COSTS (50.6%)*	 238,666		 24,251		 262,916
COMPUTER SERVICE CENTER*	30,505		1,929		32,434
SCD COMPUTING (500 GAUs @ \$5)	<u>0</u>		<u>2,500</u>		<u>2,500</u>
SUBTOTAL	\$740,843		\$76,606		\$817,448
 UCAR Management Fee (3%)*	 <u>22,225</u>		 <u>0</u>		 <u>22,225</u>
SUBTOTAL	\$763,068		\$76,606		\$839,673
 <b>EXCLUSIONS FROM MTDC:</b>					
<b>Subcontract, balance of Craig</b>	48,382				48,382
EQUIPMENT	<u>0</u>		<u>0</u>		<u>-</u>
<b>TOTAL FUNDING TO UCAR</b>	\$811,450		\$76,606		\$888,056

\*See attached footnote page.



**A Scalable and Extensible Earth System Model  
for Climate Change Science**

W. Collins, Principal Investigator  
YEAR 4: 1 July 2009-30 June 2010

**MODIFIED TOTAL DIRECT COSTS (MTDC):**

	CGD	FTE	NSF Cosponsorship	FTE	Total
SALARIES (85%)*					
Sci. III PI (.20 total)	\$11,231	0.10	\$11,231	0.10	\$22,463
Sr. Scientist (.16 total)	9,261	0.06	14,577	0.10	23,838
Sr. Scientist (.05 total)	-	0.00	8,010	0.05	8,010
Scientist II	90,852	1.00	-	0.00	90,852
Software Engineer IV	105,973	1.00	-	0.00	105,973
Software Engineer II	88,913	1.00	-	0.00	88,913
STAFF SUBTOTAL	<u>\$306,230</u>		<u>\$ 33,818</u>		<u>\$ 340,048</u>
BENEFITS (48.8%)*	<u>149,440</u>		<u>16,503</u>		<u>165,944</u>
SUBTOTAL	\$455,670		\$50,322		\$ 505,992
MATERIALS/SUPPLIES	5,900		0		5,900
(page charges based on avg. \$110-\$115/page)					
PURCHASED SERVICES:	500		0		500
(commun. costs incl. LD phone, fax, copy center)					-
Subcontract (Craig) first \$25k	25,000				25,000
TRAVEL (3 domestic trips)					
(estimated travel based on previous DOE costs)	<u>6,900</u>		<u>0</u>		<u>6,900</u>
<b>SUBTOTAL, MTDC</b>	<b>\$493,970</b>		<b>\$50,322</b>		<b>\$544,292</b>
INDIRECT COSTS (50.6%)*	249,949		25,463		275,412
COMPUTER SERVICE CENTER*	30,505		1,931		32,436
SCD COMPUTING (500 GAUs @ \$5)	<u>0</u>		<u>2,500</u>		<u>2,500</u>
SUBTOTAL	\$774,424		\$80,215		\$854,639
UCAR Management Fee (3%)*	<u>23,233</u>		<u>0</u>		<u>23,233</u>
SUBTOTAL	\$797,657		\$80,215		\$877,872
<b>EXCLUSIONS FROM MTDC:</b>					
<b>Subcontract, balance of Craig</b>	52,051				52,051
EQUIPMENT	<u>0</u>		<u>0</u>		<u>-</u>
<b>TOTAL FUNDING TO UCAR</b>	<b>\$849,708</b>		<b>\$80,215</b>		<b>\$929,923</b>

\*See attached footnote page.

**A Scalable and Extensible Earth System Model  
for Climate Change Science**

W. Collins, Principal Investigator  
YEAR 5: 1 July 2010-30 June 2011

**MODIFIED TOTAL DIRECT COSTS (MTDC):**

	CGD	FTE	NSF Cosponsorship	FTE	Total
SALARIES (85%)*					
Sci. III PI (.20 total)	\$11,793	0.10	\$11,793	0.10	\$23,586
Sr. Scientist (.16 total)	9,724	0.06	15,306	0.10	25,030
Sr. Scientist (.05 total)	-	0.00	8,410	0.05	8,410
Scientist II	95,395	1.00	-	0.00	95,395
Software Engineer IV	111,271	1.00	-	0.00	111,271
Software Engineer II	<u>93,359</u>	1.00	-	0.00	<u>93,359</u>
STAFF SUBTOTAL	\$321,542		\$ 35,509		\$ 357,051
 BENEFITS (48.8%)*	 <u>156,912</u>		 <u>17,328</u>		 <u>174,240</u>
SUBTOTAL	\$478,454		\$52,837		\$ 531,291
 MATERIALS/SUPPLIES	 6,200		 0		 6,200
(page charges based on avg. \$110-\$115/page)					
 PURCHASED SERVICES:	 500		 0		 500
(commun. costs incl. LD phone, fax, copy center)					-
Subcontract (Craig) first \$25k	25,000				25,000
 TRAVEL (3 domestic trips)					
(estimated travel based on previous DOE costs)	<u>7,200</u>		<u>0</u>		<u>7,200</u>
<b>SUBTOTAL, MTDC</b>	\$517,354		\$52,837		\$570,191
 INDIRECT COSTS (50.6%)*	 261,781		 26,736		 288,517
COMPUTER SERVICE CENTER*	30,504		1,931		32,435
SCD COMPUTING (500 GAUs @ \$5)	<u>0</u>		<u>2,500</u>		<u>2,500</u>
SUBTOTAL	\$809,639		\$84,004		\$893,643
 UCAR Management Fee (3%)*	 <u>24,289</u>		 <u>0</u>		 <u>24,289</u>
SUBTOTAL	\$833,929		\$84,004		\$917,932
 <b>EXCLUSIONS FROM MTDC:</b>					
<b>Subcontract, balance of Craig</b>	55,904				55,904
EQUIPMENT	<u>0</u>		<u>0</u>		<u>-</u>
<b>TOTAL FUNDING TO UCAR</b>	\$889,832		\$84,004		\$973,836

\*See attached footnote page.

U.S. Department of Energy  
OFFICE OF SCIENCE (SC)

**PROPOSAL**

**1. TITLE OF PROPOSED PROJECT:** A Scalable and Extensible Earth System Model for Climate Change Science

**1a. SC PROGRAM ANNOUNCEMENT TITLE:** Scientific Discovery through Advanced Computing

**2. NUMBER OF SOLICITATION:** LAB 06-04

**3. NAME OF LABORATORY:** Pacific Northwest National Laboratory

**4. NAME OF PRINCIPAL INVESTIGATOR (PI):** Steven J. Ghan

**5. POSITION/TITLE OF PI:** Staff Scientist

**6. MAILING ADDRESS OF PI:** Battelle, Pacific Northwest National Laboratory, P.O. Box 999, MSIN K9-24, Richland, WA 99352-0999

**7. TELEPHONE NUMBER OF PI:** 509/372-6169

**8. FAX NUMBER:** 509/372-6168

**9. ELECTRONIC MAIL ADDRESS OF PI:** steve.ghan@pnl.gov

**10. NAME OF OFFICIAL SIGNING FOR LABORATORY:** Charlette A. Geffen

**11. TITLE OF OFFICIAL:** Director, Atmospheric Science & Global Change Division

**12. TELEPHONE NUMBER OF OFFICIAL:** 509/375-3646

**13. FAX NUMBER:** 509/372-6153

**14. ELECTRONIC MAIL ADDRESS OF OFFICIAL:** ca.geffen@pnl.gov

**15. REQUESTED FUNDING FOR EACH YEAR; TOTAL REQUEST:**

YEAR 1: \$330,000 YEAR 2: \$330,000 YEAR 3: \$330,000 YEAR 4: \$330,000 YEAR 5: \$330,000 TOTAL: \$1,650,000

NOTE: See budget section for detailed information. Per lead institution, funding requested by project year. FWP and budget details by fiscal year.

**16. COLLABORATORS REQUESTED FUNDING FOR EACH YEAR; TOTAL REQUEST:**

Total Collaborator Budget Requests: YEAR 1: YEAR 2: YEAR 3: YEAR 4: YEAR 5: TOTAL:

NOTE: See appendix for collaborator(s) detailed budget information.

**17. (a) USE OF HUMAN SUBJECTS IN PROPOSED PROJECT:**

If activities involving human subjects are not planned at any time during the proposed project period, check "NO"; otherwise check "YES", provide the IRB Approval date and Assurance of Compliance Number and include all necessary information with the application.

( ) YES IRB APPROVAL DATE: (X) NO ASSURANCE OF COMPLIANCE NUMBER:

**(b) USE OF VERTEBRATE ANIMALS IN PROPOSED PROJECT:**

If activities involving vertebrate animals are not planned at any time during this project, check "No"; otherwise check "YES" and provide the IACUC Approval date and Animal Welfare Assurance number and include all necessary information with the application.

( ) YES IACUC APPROVAL DATE: (X) NO ANIMAL WELFARE ASSURANCE NUMBER:

**18. SIGNATURE OF PI:**

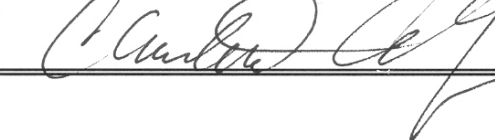
**DATE:**



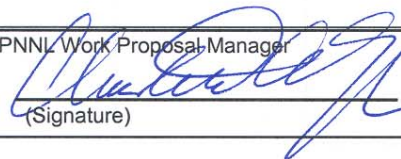
3-2-06

**19. SIGNATURE OF OFFICIAL:**

**DATE:**



3-2-06

U.S. DEPARTMENT OF ENERGY Pacific Northwest Site Office		
FIELD WORK PROPOSAL		
1. Work Proposal Number 42333	2. Revision No.	3. Date Prepared 03-06-06
4. Work Proposal Title A Scalable and Extensible Earth System Model for Climate Change Science		
5. Budget and Reporting Code KP-12-01-01-0	6. Work Proposal Term Begin: 07-01-06                      End: OPEN	
7. Headquarters/Operations Office Program Manager (Name: Last, First, Middle Initial; Phone: Area code 7 digit #) Bamzai, Anjuli (301) 903-0294	8. Headquarters Organization  SC	
9. DOE Field Element Work Proposal Reviewer (Name: Last, First, Middle Initial; Phone: area code-7 digit #) Williams, Kimberly (509) 372-4829	10. DOE Field Element  Pacific Northwest Site Office	
11. PNNL Work Proposal Manager and Principal Investigator (Name: Last, First, Middle Initial; Phone: area code-7 digit #) Geffen, Charlette A. (509) 375-3646 (PM) Ghan, Steven J. (509) 372-6169 (PI)	12. Contractor Name  Battelle Memorial Institute Pacific Northwest National Laboratory	
13. Work Proposal Description (Approach, Anticipated Benefit, in 200 Words or Less)		
<p>Our challenge for SciDAC is to create a first generation Earth system model based on the Community Climate System Model (CCSM) that treats the coupling between the physical, chemical, and biogeochemical processes in the climate system. The model will include comprehensive treatments of the processes governing well-mixed greenhouse gases, natural and anthropogenic aerosols, the aerosol indirect effect and tropospheric ozone for climate change studies. We will improve the representation of carbon and chemical processes, particularly for treatment of greenhouse gas emissions and aerosol feedbacks in collaboration with the DOE Atmospheric Science Program and DOE Terrestrial Carbon Programs.</p> <p>We will also improve the software and testing infrastructure of the CCSM to enable the rapid integration and evaluation of new numerical methods and model improvements. To focus these efforts, specific integration tasks are proposed for methods that improve scalability to thousands of processors, permit more flexibility in horizontal and vertical grids and advance dynamical formulations. To evaluate and validate new methods, we will create a testing and evaluation infrastructure through updated unit and system tests and new data analysis capabilities. Integration and evaluation work will rely on collaboration with other SciDAC CETs and SAPs.</p> <p>During the integration of new methods and new chemical and biogeochemical processes, we will ensure that the model continues to perform well on DOE computational platforms to maximize the length of simulations and number of ensembles that can be used for assessment products. This will facilitate the aggressive schedule of climate change simulations required for upcoming assessment products.</p>		
14. PNNL Work Proposal Manager  (Signature)                      3/02/06 (Date)		15. DOE Operations Office Review Official  _____ (Signature)                      _____ (Date)

WORK PROPOSAL REQUIREMENTS FOR OPERATING/EQUIPMENT OBLIGATIONS AND COSTS								
Contractor Name Battelle Memorial Institute Pacific Northwest National Laboratory			Work Proposal No. 42333		Rev. No.		Date Prepared 03-06-06	
	FY 2006	FY 2007	FY 2008	FY 2009	FY 2010	FY 2011	FY 2012	FY 2013
16. Staffing* (in Staff Years)								
A. Scientific	0.3	1.1	1.1	1.1	1.1	0.8		
B. Other Direct	0.0	0.0	0.0	0.0	0.0	0.0		
C. Total Direct	0.3	1.1	1.1	1.1	1.1	0.8		
17. Operating Expense* (in Thousands)								
A. Total Obligations	76	333	335	330	330	247		
B. Total Costs	76	333	335	330	330	247		
18. Equipment (in Thousands)								
A. Obligations								
B. Costs								
19. Tasks or Milestones					Proposed Dollars			
					FY 2006	FY 2007	FY 2008	
*Staffing and funding proposed are for PNNL only and does not include partners.								

ORGANIZATION Battelle, Pacific Northwest National Laboratory			Budget Page No: 1		
PRINCIPAL INVESTIGATOR (PI)/PROJECT DIRECTOR (PD) Steven J. Ghan			Requested Duration: <u>60</u> (Months)		
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates List each separately with title, A.8 show number in bracket(s)			DOE Funded Person - mos		
	CAL	ACAD	SUMR	Funds Requested by Applicant	Funds Granted by DOE
1. Ghan, Steven J - 64 - SCIENTIST/ENGINEER E	11.5			\$ 163,279	
2. Easter, Richard C - 63 - SCIENTIST/ENGINEER D	10.5			\$ 116,441	
3. Zaveri, Rahul A - 62 - SCIENTIST/ENGINEER C	10.3			\$ 94,723	
4. Liu, Xiaohong - 63 - SCIENTIST/ENGINEER D	33.2			\$ 368,073	
5. -	0.0			\$ -	
6. -	0.0			\$ -	
7. -	0.0			\$ -	
8. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)	0.0			\$ -	
9. ( ) TOTAL SENIOR PERSONNEL (1-8)	65.5			\$ 742,516	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES *	0.0			\$ -	
2. ( ) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)				\$ -	
3. ( ) GRADUATE STUDENTS *				\$ -	
4. ( ) UNDERGRADUATE STUDENTS *				\$ -	
5. (1) SECRETARIAL - CLERICAL				\$ 2,880	
6. (1) OTHER - Project Specialist				\$ 2,240	
TOTAL SALARIES AND WAGES (A+B)				\$ 747,635	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)			Included in Above		
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				\$ 747,635	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM)					
TOTAL PERMANENT EQUIPMENT				\$ -	
E. TRAVEL					
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				\$ 34,306	
2. FOREIGN				\$ -	
TOTAL TRAVEL				\$ 34,306	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)				\$ -	
2. TUITION & FEES				\$ -	
3. TRAINEE TRAVEL				\$ -	
4. OTHER (fully explain on justification page)				\$ -	
TOTAL PARTICIPANTS ( ) TOTAL COST				\$ -	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				\$ 38,127	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				\$ 11,207	
3. CONSULTANT SERVICES				\$ -	
4. COMPUTER (ADP) SERVICES				\$ 20,770	
5. SUBCONTRACTS				\$ -	
6. OTHER				\$ -	
TOTAL OTHER DIRECT COSTS				\$ 70,103	
H. TOTAL DIRECT COSTS (ATHROUGH G)				\$ 852,044	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)			See attachment "Indirect Cost" for explanation.		
TOTAL INDIRECT COSTS				\$ 797,982	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				\$ 1,650,026	
K. AMOUNT OF ANY REQUIRED COST-SHARING FROM NON-FEDERAL SOURCES				\$ -	
L. TOTAL COST OF PROJECT (J+K)				\$ 1,650,026	

**U.S. Department of Energy**  
**Budget Page**  
Year 1  
July 1, 2006 - June 30, 2007

ORGANIZATION Battelle, Pacific Northwest National Laboratory			Budget Page No: <u>2</u>		
PRINCIPAL INVESTIGATOR (PI)/PROJECT DIRECTOR (PD) Steven J. Ghan			Requested Duration: <u>12</u> (Months)		
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates List each separately with title. A.8 show number in bracket(s)			DOE Funded Person - mos	Funds Requested	Funds Granted
	CAL	ACAD	SUMR	by Applicant	by DOE
1. Ghan, Steven J - 64 - SCIENTIST/ENGINEER E	2.3			\$ 30,931	
2. Easter, Richard C - 63 - SCIENTIST/ENGINEER D	2.1			\$ 21,883	
3. Zaveri, Rahul A - 62 - SCIENTIST/ENGINEER C	2.1			\$ 18,154	
4. Liu, Xiaohong - 63 - SCIENTIST/ENGINEER D	6.6			\$ 70,025	
5. -	0.0			\$ -	
6. -	0.0			\$ -	
7. -	0.0			\$ -	
8. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)	0.0			\$ -	
9. ( ) TOTAL SENIOR PERSONNEL (1-8)	13.1			\$ 140,992	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES *	0.0			\$ -	
2. ( ) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)				\$ -	
3. ( ) GRADUATE STUDENTS *				\$ -	
4. ( ) UNDERGRADUATE STUDENTS *				\$ -	
5. (1) SECRETARIAL - CLERICAL				\$ 594	
6. (1) OTHER - Project Specialist				\$ 445	
TOTAL SALARIES AND WAGES (A+B)				\$ 142,031	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)			Included in Above		
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				\$ 142,031	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM)					
TOTAL PERMANENT EQUIPMENT				\$ -	
E. TRAVEL					
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				\$ 6,527	
2. FOREIGN				\$ -	
TOTAL TRAVEL				\$ 6,527	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)				\$ -	
2. TUITION & FEES				\$ -	
3. TRAINEE TRAVEL				\$ -	
4. OTHER (fully explain on justification page)				\$ -	
TOTAL PARTICIPANTS ( ) TOTAL COST				\$ -	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				\$ 26,925	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				\$ 2,132	
3. CONSULTANT SERVICES				\$ -	
4. COMPUTER (ADP) SERVICES				\$ 4,154	
5. SUBCONTRACTS				\$ -	
6. OTHER				\$ -	
TOTAL OTHER DIRECT COSTS				\$ 33,211	
H. TOTAL DIRECT COSTS (ATHROUGH G)				\$ 181,768	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) See attachment "Indirect Cost" for explanation.					
TOTAL INDIRECT COSTS				\$ 148,235	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				\$ 330,003	
K. AMOUNT OF ANY REQUIRED COST-SHARING FROM NON-FEDERAL SOURCES				\$ -	
L. TOTAL COST OF PROJECT (J+K)				\$ 330,003	

**U.S. Department of Energy**  
**Budget Page**  
Year 2  
July 1, 2007 - June 30, 2008

ORGANIZATION Battelle, Pacific Northwest National Laboratory			Budget Page No: <u>3</u>		
PRINCIPAL INVESTIGATOR (PI)/PROJECT DIRECTOR (PD) Steven J. Ghan			Requested Duration: <u>12</u> (Months)		
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates List each separately with title. A.8 show number in bracket(s)			DOE Funded Person - mos	Funds Requested	Funds Granted
	CAL	ACAD	SUMR	by Applicant	by DOE
1. Ghan, Steven J - 64 - SCIENTIST/ENGINEER E	2.4			\$ 32,468	
2. Easter, Richard C - 63 - SCIENTIST/ENGINEER D	2.2			\$ 23,925	
3. Zaveri, Rahul A - 62 - SCIENTIST/ENGINEER C	2.1			\$ 18,608	
4. Liu, Xiaohong - 63 - SCIENTIST/ENGINEER D	6.6			\$ 71,775	
5. -	0.0			\$ -	
6. -	0.0			\$ -	
7. -	0.0			\$ -	
8. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)	0.0			\$ -	
9. ( ) TOTAL SENIOR PERSONNEL (1-8)	13.3			\$ 146,776	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES *	0.0			\$ -	
2. ( ) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)				\$ -	
3. ( ) GRADUATE STUDENTS *				\$ -	
4. ( ) UNDERGRADUATE STUDENTS *				\$ -	
5. (1) SECRETARIAL - CLERICAL				\$ 516	
6. (1) OTHER - Project Specialist				\$ 456	
TOTAL SALARIES AND WAGES (A+B)				\$ 147,748	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)			Included in Above		
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				\$ 147,748	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM)					
TOTAL PERMANENT EQUIPMENT				\$ -	
E. TRAVEL					
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				\$ 6,690	
2. FOREIGN				\$ -	
TOTAL TRAVEL				\$ 6,690	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)				\$ -	
2. TUITION & FEES				\$ -	
3. TRAINEE TRAVEL				\$ -	
4. OTHER (fully explain on justification page)				\$ -	
TOTAL PARTICIPANTS ( ) TOTAL COST				\$ -	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				\$ 11,202	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				\$ 2,185	
3. CONSULTANT SERVICES				\$ -	
4. COMPUTER (ADP) SERVICES				\$ 4,154	
5. SUBCONTRACTS				\$ -	
6. OTHER				\$ -	
TOTAL OTHER DIRECT COSTS				\$ 17,541	
H. TOTAL DIRECT COSTS (ATHROUGH G)				\$ 171,978	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) See attachment "Indirect Cost" for explanation.					
TOTAL INDIRECT COSTS				\$ 158,025	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				\$ 330,003	
K. AMOUNT OF ANY REQUIRED COST-SHARING FROM NON-FEDERAL SOURCES				\$ -	
L. TOTAL COST OF PROJECT (J+K)				\$ 330,003	



**U.S. Department of Energy**  
**Budget Page**  
Year 3  
July 1, 2008 - June 30, 2009

ORGANIZATION Battelle, Pacific Northwest National Laboratory			Budget Page No: <u>4</u>		
PRINCIPAL INVESTIGATOR (PI)/PROJECT DIRECTOR (PD) Steven J. Ghan			Requested Duration: <u>12</u> (Months)		
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates List each separately with title. A.8 show number in bracket(s)			DOE Funded Person - mos	Funds Requested	Funds Granted
	CAL	ACAD	SUMR	by Applicant	by DOE
1. Ghan, Steven J - 64 - SCIENTIST/ENGINEER E	2.4			\$ 33,964	
2. Easter, Richard C - 63 - SCIENTIST/ENGINEER D	2.2			\$ 24,523	
3. Zaveri, Rahul A - 62 - SCIENTIST/ENGINEER C	2.1			\$ 19,708	
4. Liu, Xiaohong - 63 - SCIENTIST/ENGINEER D	6.6			\$ 73,570	
5. -	0.0			\$ -	
6. -	0.0			\$ -	
7. -	0.0			\$ -	
8. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)	0.0			\$ -	
9. ( ) TOTAL SENIOR PERSONNEL (1-8)	13.4			\$ 151,765	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES *	0.0			\$ -	
2. ( ) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)				\$ -	
3. ( ) GRADUATE STUDENTS *				\$ -	
4. ( ) UNDERGRADUATE STUDENTS *				\$ -	
5. (1) SECRETARIAL - CLERICAL				\$ 563	
6. (1) OTHER - Project Specialist				\$ 467	
TOTAL SALARIES AND WAGES (A+B)				\$ 152,796	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)			Included in Above		
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				\$ 152,796	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM)					
TOTAL PERMANENT EQUIPMENT				\$ -	
E. TRAVEL					
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				\$ 6,857	
2. FOREIGN				\$ -	
TOTAL TRAVEL				\$ 6,857	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)				\$ -	
2. TUITION & FEES				\$ -	
3. TRAINEE TRAVEL				\$ -	
4. OTHER (fully explain on justification page)				\$ -	
TOTAL PARTICIPANTS ( ) TOTAL COST				\$ -	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				\$ -	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				\$ 2,240	
3. CONSULTANT SERVICES				\$ -	
4. COMPUTER (ADP) SERVICES				\$ 4,154	
5. SUBCONTRACTS				\$ -	
6. OTHER				\$ -	
TOTAL OTHER DIRECT COSTS				\$ 6,394	
H. TOTAL DIRECT COSTS (ATHROUGH G)				\$ 166,047	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) See attachment "Indirect Cost" for explanation.					
TOTAL INDIRECT COSTS				\$ 163,960	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				\$ 330,007	
K. AMOUNT OF ANY REQUIRED COST-SHARING FROM NON-FEDERAL SOURCES				\$ -	
L. TOTAL COST OF PROJECT (J+K)				\$ 330,007	

**U.S. Department of Energy**  
**Budget Page**  
Year 4  
July 1, 2009 - June 30, 2010

ORGANIZATION Battelle, Pacific Northwest National Laboratory			Budget Page No: <u>5</u>		
PRINCIPAL INVESTIGATOR (PI)/PROJECT DIRECTOR (PD) Steven J. Ghan			Requested Duration: <u>12</u> (Months)		
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates List each separately with title. A.8 show number in bracket(s)			DOE Funded Person - mos	Funds Requested	Funds Granted
	CAL	ACAD	SUMR	by Applicant	by DOE
1. Ghan, Steven J - 64 - SCIENTIST/ENGINEER E	2.3			\$ 32,908	
2. Easter, Richard C - 63 - SCIENTIST/ENGINEER D	2.1			\$ 23,565	
3. Zaveri, Rahul A - 62 - SCIENTIST/ENGINEER C	2.1			\$ 19,550	
4. Liu, Xiaohong - 63 - SCIENTIST/ENGINEER D	6.6			\$ 75,409	
5. -	0.0			\$ -	
6. -	0.0			\$ -	
7. -	0.0			\$ -	
8. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)	0.0			\$ -	
9. ( ) TOTAL SENIOR PERSONNEL (1-8)	13.0			\$ 151,432	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES *	0.0			\$ -	
2. ( ) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)				\$ -	
3. ( ) GRADUATE STUDENTS *				\$ -	
4. ( ) UNDERGRADUATE STUDENTS *				\$ -	
5. (1) SECRETARIAL - CLERICAL				\$ 642	
6. (1) OTHER - Project Specialist				\$ 479	
TOTAL SALARIES AND WAGES (A+B)				\$ 152,553	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)			Included in Above		
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				\$ 152,553	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM)					
TOTAL PERMANENT EQUIPMENT				\$ -	
E. TRAVEL					
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				\$ 7,028	
2. FOREIGN				\$ -	
TOTAL TRAVEL				\$ 7,028	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)				\$ -	
2. TUITION & FEES				\$ -	
3. TRAINEE TRAVEL				\$ -	
4. OTHER (fully explain on justification page)				\$ -	
TOTAL PARTICIPANTS ( ) TOTAL COST				\$ -	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				\$ -	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				\$ 2,296	
3. CONSULTANT SERVICES				\$ -	
4. COMPUTER (ADP) SERVICES				\$ 4,154	
5. SUBCONTRACTS				\$ -	
6. OTHER				\$ -	
TOTAL OTHER DIRECT COSTS				\$ 6,450	
H. TOTAL DIRECT COSTS (ATHROUGH G)				\$ 166,032	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)			See attachment "Indirect Cost" for explanation.		
TOTAL INDIRECT COSTS				\$ 163,976	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				\$ 330,008	
K. AMOUNT OF ANY REQUIRED COST-SHARING FROM NON-FEDERAL SOURCES				\$ -	
L. TOTAL COST OF PROJECT (J+K)				\$ 330,008	

**U.S. Department of Energy**  
**Budget Page**  
Year 5  
July 1, 2010 - June 30, 2011

ORGANIZATION Battelle, Pacific Northwest National Laboratory			Budget Page No: <u>6</u>		
PRINCIPAL INVESTIGATOR (PI)/PROJECT DIRECTOR (PD) Steven J. Ghan			Requested Duration: <u>12</u> (Months)		
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates List each separately with title. A.8 show number in bracket(s)			DOE Funded Person - mos	Funds Requested	Funds Granted
	CAL	ACAD	SUMR	by Applicant	by DOE
1. Ghan, Steven J - 64 - SCIENTIST/ENGINEER E	2.2			\$ 33,009	
2. Easter, Richard C - 63 - SCIENTIST/ENGINEER D	1.9			\$ 22,544	
3. Zaveri, Rahul A - 62 - SCIENTIST/ENGINEER C	1.9			\$ 18,703	
4. Liu, Xiaohong - 63 - SCIENTIST/ENGINEER D	6.6			\$ 77,294	
5. -	0.0			\$ -	
6. -	0.0			\$ -	
7. -	0.0			\$ -	
8. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)	0.0			\$ -	
9. ( ) TOTAL SENIOR PERSONNEL (1-8)	12.7			\$ 151,550	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES *	0.0			\$ -	
2. ( ) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)				\$ -	
3. ( ) GRADUATE STUDENTS *				\$ -	
4. ( ) UNDERGRADUATE STUDENTS *				\$ -	
5. (1) SECRETARIAL - CLERICAL				\$ 564	
6. (1) OTHER - Project Specialist				\$ 393	
TOTAL SALARIES AND WAGES (A+B)				\$ 152,507	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)			Included in Above		
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				\$ 152,507	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM)					
TOTAL PERMANENT EQUIPMENT				\$ -	
E. TRAVEL					
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				\$ 7,204	
2. FOREIGN				\$ -	
TOTAL TRAVEL				\$ 7,204	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)				\$ -	
2. TUITION & FEES				\$ -	
3. TRAINEE TRAVEL				\$ -	
4. OTHER (fully explain on justification page)				\$ -	
TOTAL PARTICIPANTS ( ) TOTAL COST				\$ -	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				\$ -	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				\$ 2,353	
3. CONSULTANT SERVICES				\$ -	
4. COMPUTER (ADP) SERVICES				\$ 4,154	
5. SUBCONTRACTS				\$ -	
6. OTHER				\$ -	
TOTAL OTHER DIRECT COSTS				\$ 6,507	
H. TOTAL DIRECT COSTS (ATHROUGH G)				\$ 166,219	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) See attachment "Indirect Cost" for explanation.					
TOTAL INDIRECT COSTS				\$ 163,783	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				\$ 330,002	
K. AMOUNT OF ANY REQUIRED COST-SHARING FROM NON-FEDERAL SOURCES				\$ -	
L. TOTAL COST OF PROJECT (J+K)				\$ 330,002	

**INDIRECT COSTS  
PROPOSAL # 42333**

**ORGANIZATIONAL OVERHEAD**

ORGANIZATIONAL MANAGEMENT, SUPERVISION, AND ADMINISTRATIVE COSTS ARE INCLUDED HERE. ALSO INCLUDED ARE COSTS INCURRED BY TECHNICAL ORGANIZATIONS IN SUPPORT OF RESEARCH, AND EQUIPMENT WHICH WOULD BE IMPRACTICAL TO ALLOCATE TO INDIVIDUAL CONTRACTS. THIS COST CATEGORY INCLUDES: LABORATORY SUPPLIES, SMALL TOOLS, LAUNDRY, DECONTAMINATION/WASTE DISPOSAL, MAINTENANCE EXPENSES AND OTHER DEPARTMENTAL COSTS, AND EXPENSES ASSOCIATED WITH BATTELLE-OWNED EQUIPMENT WITH A FIRST COST OF LESS THAN \$50,000, SUCH AS DEPRECIATION, MAINTENANCE, TAXES, AND INSURANCE. THESE COSTS ARE ACCUMULATED IN AN INTERMEDIATE COST POOL AND ARE ALLOCATED TO COST OBJECTIVES AT A PREDETERMINED RATE PER DIRECT LABOR HOUR.

**PROGRAM DEVELOPMENT AND MANAGEMENT (PDM)**

PROGRAM DEVELOPMENT AND PROGRAM MANAGEMENT COSTS INCLUDE COSTS FOR BUSINESS DEVELOPMENT, PLANNING, AND MONITORING FOR A GROUP OF PROJECTS. COSTS ARE POOLED AND THEN APPLIED TO VALUE ADDED COSTS, LESS PDM COSTS, PLUS MATERIALS AND SUBCONTRACTS.

**GENERAL AND ADMINISTRATIVE EXPENSE (G&A)**

THE ALLOCATION BASE FOR G&A EXPENSES IS VALUE ADDED TO FINAL COST OBJECTIVES. THE VALUE-ADDED BASE INCLUDES: LABOR, TRAVEL, SERVICE AND EQUIPMENT CENTERS, ORGANIZATIONAL OVERHEAD, BUILDING AND UTILITY COST, AND OTHER DIRECT COSTS. IT EXCLUDES THE BASE COST FOR PROCUREMENT, SUBCONTRACTS, AND OTHER HANFORD CONTRACTOR SERVICES.

**INITIAL GRANT PERIOD, FROM 7/1/2006 THROUGH 6/30/2007**

	<u>FY2006</u> <u>RATE</u>	<u>RATE THIS</u> <u>PERIOD</u>	<u>BASE</u>	<u>INDIRECT</u> <u>COST</u>
<b>PROGRAM DEV AND MGMT (PDM)</b>	6.0%	6.0%	\$235,071	14,104
<b>ORGANIZATIONAL OVERHEAD:</b>			<u>BASE</u>	
Ops & Research Support	\$ 27.05	\$ 27.53	10 HOURS	\$ 275
Climate Physics	\$ 27.05	\$ 27.56	1292 HOURS	\$ 35,608
Atmospheric Chemistry & Meteorology	\$ 27.05	\$ 27.56	622 HOURS	\$ 17,131
Lab Technical Mgmt Cost	\$ 0.15	\$ 0.15	1924 HOURS	\$ 289
<b>TOTAL ORGANIZATIONAL OVERHEAD</b>				<b>\$ 53,302</b>
			<u>VALUE-ADDED BASE*</u>	
<b>GENERAL AND ADMINISTRATIVE COST</b>	33.0%	33.0%	\$221,500	\$ 73,095
<b>SERVICE ASSESSMENT</b>	2.4%	2.4%	BASE: \$322,270	\$ 7,734
<b>TOTAL INDIRECT COST</b>				<b>148,236</b>

**\*THE VALUE-ADDED BASE IS DERIVED BY ADDING THE FOLLOWING COST ELEMENTS:**

Direct Labor	\$ 142,031	Program Dev	\$ 14,104	Other Dir. Costs	\$ 4,154
Organizationa	53,302	Travel	6,527	Proc/Subcont. Svc. Chgs	1,382

**INDIRECT COSTS  
PROPOSAL # 42333**

**ORGANIZATIONAL OVERHEAD**

ORGANIZATIONAL MANAGEMENT, SUPERVISION, AND ADMINISTRATIVE COSTS ARE INCLUDED HERE. ALSO INCLUDED ARE COSTS INCURRED BY TECHNICAL ORGANIZATIONS IN SUPPORT OF RESEARCH, AND EQUIPMENT WHICH WOULD BE IMPRACTICAL TO ALLOCATE TO INDIVIDUAL CONTRACTS. THIS COST CATEGORY INCLUDES: LABORATORY SUPPLIES, SMALL TOOLS, LAUNDRY, DECONTAMINATION/WASTE DISPOSAL, MAINTENANCE EXPENSES AND OTHER DEPARTMENTAL COSTS, AND EXPENSES ASSOCIATED WITH BATTELLE-OWNED EQUIPMENT WITH A FIRST COST OF LESS THAN \$50,000, SUCH AS DEPRECIATION, MAINTENANCE, TAXES, AND INSURANCE. THESE COSTS ARE ACCUMULATED IN AN INTERMEDIATE COST POOL AND ARE ALLOCATED TO COST OBJECTIVES AT A PREDETERMINED RATE PER DIRECT LABOR HOUR.

**PROGRAM DEVELOPMENT AND MANAGEMENT (PDM)**

PROGRAM DEVELOPMENT AND PROGRAM MANAGEMENT COSTS INCLUDE COSTS FOR BUSINESS DEVELOPMENT, PLANNING, AND MONITORING FOR A GROUP OF PROJECTS. COSTS ARE POOLED AND THEN APPLIED TO VALUE ADDED COSTS, LESS PDM COSTS, PLUS MATERIALS AND SUBCONTRACTS.

**GENERAL AND ADMINISTRATIVE EXPENSE (G&A)**

THE ALLOCATION BASE FOR G&A EXPENSES IS VALUE ADDED TO FINAL COST OBJECTIVES. THE VALUE-ADDED BASE INCLUDES: LABOR, TRAVEL, SERVICE AND EQUIPMENT CENTERS, ORGANIZATIONAL OVERHEAD, BUILDING AND UTILITY COST, AND OTHER DIRECT COSTS. IT EXCLUDES THE BASE COST FOR PROCUREMENT, SUBCONTRACTS, AND OTHER HANFORD CONTRACTOR SERVICES.

**SECOND GRANT PERIOD, FROM 7/1/2007 THROUGH 6/30/2008**

	<u>FY2006</u> <u>RATE</u>	<u>RATE THIS</u> <u>PERIOD</u>	<u>BASE</u>	<u>INDIRECT</u> <u>COST</u>
<b>PROGRAM DEV AND MGMT (PDM)</b>	6.0%	6.0%	\$227,305	13,638
<b>ORGANIZATIONAL OVERHEAD:</b>			<u>BASE</u>	
Ops & Research Support	\$ 27.05	\$ 28.21	10 HOURS	\$ 282
Climate Physics	\$ 27.05	\$ 28.25	1300 HOURS	\$ 36,722
Atmospheric Chemistry & Meteorology	\$ 27.05	\$ 28.25	638 HOURS	\$ 18,030
Lab Technical Mgmt Cost	\$ 0.15	\$ 0.15	1948 HOURS	\$ 292
<b>TOTAL ORGANIZATIONAL OVERHEAD</b>				<b>\$ 55,326</b>
			<u>VALUE-ADDED BASE*</u>	
<b>GENERAL AND ADMINISTRATIVE COST</b>	33.0%	35.6%	\$228,335	\$ 81,327
<b>SERVICE ASSESSMENT</b>	2.4%	2.4%	BASE: \$322,270	\$ 7,734
<b>TOTAL INDIRECT COST</b>				<b>158,026</b>

\*THE VALUE-ADDED BASE IS DERIVED BY ADDING THE FOLLOWING COST ELEMENTS:

Direct Labor	\$ 147,748	Program Dev	\$ 13,638	Other Dir. Costs	\$ 4,154
Organizationa	55,326	Travel	6,690	Proc/Subcont. Svc. Chgs	779

**INDIRECT COSTS  
PROPOSAL # 42333**

**ORGANIZATIONAL OVERHEAD**

ORGANIZATIONAL MANAGEMENT, SUPERVISION, AND ADMINISTRATIVE COSTS ARE INCLUDED HERE. ALSO INCLUDED ARE COSTS INCURRED BY TECHNICAL ORGANIZATIONS IN SUPPORT OF RESEARCH, AND EQUIPMENT WHICH WOULD BE IMPRACTICAL TO ALLOCATE TO INDIVIDUAL CONTRACTS. THIS COST CATEGORY INCLUDES: LABORATORY SUPPLIES, SMALL TOOLS, LAUNDRY, DECONTAMINATION/WASTE DISPOSAL, MAINTENANCE EXPENSES AND OTHER DEPARTMENTAL COSTS, AND EXPENSES ASSOCIATED WITH BATTELLE-OWNED EQUIPMENT WITH A FIRST COST OF LESS THAN \$50,000, SUCH AS DEPRECIATION, MAINTENANCE, TAXES, AND INSURANCE. THESE COSTS ARE ACCUMULATED IN AN INTERMEDIATE COST POOL AND ARE ALLOCATED TO COST OBJECTIVES AT A PREDETERMINED RATE PER DIRECT LABOR HOUR.

**PROGRAM DEVELOPMENT AND MANAGEMENT (PDM)**

PROGRAM DEVELOPMENT AND PROGRAM MANAGEMENT COSTS INCLUDE COSTS FOR BUSINESS DEVELOPMENT, PLANNING, AND MONITORING FOR A GROUP OF PROJECTS. COSTS ARE POOLED AND THEN APPLIED TO VALUE ADDED COSTS, LESS PDM COSTS, PLUS MATERIALS AND SUBCONTRACTS.

**GENERAL AND ADMINISTRATIVE EXPENSE (G&A)**

THE ALLOCATION BASE FOR G&A EXPENSES IS VALUE ADDED TO FINAL COST OBJECTIVES. THE VALUE-ADDED BASE INCLUDES: LABOR, TRAVEL, SERVICE AND EQUIPMENT CENTERS, ORGANIZATIONAL OVERHEAD, BUILDING AND UTILITY COST, AND OTHER DIRECT COSTS. IT EXCLUDES THE BASE COST FOR PROCUREMENT, SUBCONTRACTS, AND OTHER HANFORD CONTRACTOR SERVICES.

**THIRD GRANT PERIOD, FROM 7/1/2008 THROUGH 6/30/2009**

	<u>FY2006</u> <u>RATE</u>	<u>RATE THIS</u> <u>PERIOD</u>	<u>BASE</u>	<u>INDIRECT</u> <u>COST</u>
<b>PROGRAM DEV AND MGMT (PDM)</b>	6.0%	6.0%	\$223,276	13,397
<b>ORGANIZATIONAL OVERHEAD:</b>			<u>BASE</u>	
Ops & Research Support	\$ 27.05	\$ 28.92	10 HOURS	\$ 289
Climate Physics	\$ 27.05	\$ 28.95	1307 HOURS	\$ 37,841
Atmospheric Chemistry & Meteorology	\$ 27.05	\$ 28.95	650 HOURS	\$ 18,804
Lab Technical Mgmt Cost	\$ 0.15	\$ 0.15	1967 HOURS	\$ 295
<b>TOTAL ORGANIZATIONAL OVERHEAD</b>				<b>\$ 57,229</b>
			<u>VALUE-ADDED BASE*</u>	
<b>GENERAL AND ADMINISTRATIVE COST</b>	33.0%	36.5%	\$234,519	\$ 85,599
<b>SERVICE ASSESSMENT</b>	2.4%	2.4%	BASE: \$322,272	\$ 7,735
<b>TOTAL INDIRECT COST</b>				<b>163,960</b>

\*THE VALUE-ADDED BASE IS DERIVED BY ADDING THE FOLLOWING COST ELEMENTS:

Direct Labor	\$ 152,796	Program Dev	\$ 13,397	Other Dir. Costs	\$ 4,154
Organizationa	57,229	Travel	6,857	Proc/Subcont. Svc. Chgs	86

**INDIRECT COSTS  
PROPOSAL # 42333**

**ORGANIZATIONAL OVERHEAD**

ORGANIZATIONAL MANAGEMENT, SUPERVISION, AND ADMINISTRATIVE COSTS ARE INCLUDED HERE. ALSO INCLUDED ARE COSTS INCURRED BY TECHNICAL ORGANIZATIONS IN SUPPORT OF RESEARCH, AND EQUIPMENT WHICH WOULD BE IMPRACTICAL TO ALLOCATE TO INDIVIDUAL CONTRACTS. THIS COST CATEGORY INCLUDES: LABORATORY SUPPLIES, SMALL TOOLS, LAUNDRY, DECONTAMINATION/WASTE DISPOSAL, MAINTENANCE EXPENSES AND OTHER DEPARTMENTAL COSTS, AND EXPENSES ASSOCIATED WITH BATTELLE-OWNED EQUIPMENT WITH A FIRST COST OF LESS THAN \$50,000, SUCH AS DEPRECIATION, MAINTENANCE, TAXES, AND INSURANCE. THESE COSTS ARE ACCUMULATED IN AN INTERMEDIATE COST POOL AND ARE ALLOCATED TO COST OBJECTIVES AT A PREDETERMINED RATE PER DIRECT LABOR HOUR.

**PROGRAM DEVELOPMENT AND MANAGEMENT (PDM)**

PROGRAM DEVELOPMENT AND PROGRAM MANAGEMENT COSTS INCLUDE COSTS FOR BUSINESS DEVELOPMENT, PLANNING, AND MONITORING FOR A GROUP OF PROJECTS. COSTS ARE POOLED AND THEN APPLIED TO VALUE ADDED COSTS, LESS PDM COSTS, PLUS MATERIALS AND SUBCONTRACTS.

**GENERAL AND ADMINISTRATIVE EXPENSE (G&A)**

THE ALLOCATION BASE FOR G&A EXPENSES IS VALUE ADDED TO FINAL COST OBJECTIVES. THE VALUE-ADDED BASE INCLUDES: LABOR, TRAVEL, SERVICE AND EQUIPMENT CENTERS, ORGANIZATIONAL OVERHEAD, BUILDING AND UTILITY COST, AND OTHER DIRECT COSTS. IT EXCLUDES THE BASE COST FOR PROCUREMENT, SUBCONTRACTS, AND OTHER HANFORD CONTRACTOR SERVICES.

**FOURTH GRANT PERIOD, FROM 7/1/2009 THROUGH 6/30/2010**

	<u>FY2006</u> <u>RATE</u>	<u>RATE THIS</u> <u>PERIOD</u>	<u>BASE</u>	<u>INDIRECT</u> <u>COST</u>
<b>PROGRAM DEV AND MGMT (PDM)</b>	6.0%	6.0%	\$223,291	13,397
<b>ORGANIZATIONAL OVERHEAD:</b>			<u>BASE</u>	
Ops & Research Support	\$ 27.05	\$ 29.64	10 HOURS	\$ 296
Climate Physics	\$ 27.05	\$ 29.68	1288 HOURS	\$ 38,225
Atmospheric Chemistry & Meteorology	\$ 27.05	\$ 29.68	622 HOURS	\$ 18,450
Lab Technical Mgmt Cost	\$ 0.15	\$ 0.15	1920 HOURS	\$ 288
<b>TOTAL ORGANIZATIONAL OVERHEAD</b>				\$ 57,259
			<u>VALUE-ADDED BASE*</u>	
<b>GENERAL AND ADMINISTRATIVE COST</b>	33.0%	36.5%	\$234,481	\$ 85,585
<b>SERVICE ASSESSMENT</b>	2.4%	2.4%	BASE: \$322,274	\$ 7,735
<b>TOTAL INDIRECT COST</b>				<b>163,976</b>

**\*THE VALUE-ADDED BASE IS DERIVED BY ADDING THE FOLLOWING COST ELEMENTS:**

Direct Labor	\$ 152,553	Program Dev	\$ 13,397	Other Dir. Costs	\$ 4,154
Organizationa	57,259	Travel	7,028	Proc/Subcont. Svc. Chgs	88

**INDIRECT COSTS  
PROPOSAL # 42333**

**ORGANIZATIONAL OVERHEAD**

ORGANIZATIONAL MANAGEMENT, SUPERVISION, AND ADMINISTRATIVE COSTS ARE INCLUDED HERE. ALSO INCLUDED ARE COSTS INCURRED BY TECHNICAL ORGANIZATIONS IN SUPPORT OF RESEARCH, AND EQUIPMENT WHICH WOULD BE IMPRACTICAL TO ALLOCATE TO INDIVIDUAL CONTRACTS. THIS COST CATEGORY INCLUDES: LABORATORY SUPPLIES, SMALL TOOLS, LAUNDRY, DECONTAMINATION/WASTE DISPOSAL, MAINTENANCE EXPENSES AND OTHER DEPARTMENTAL COSTS, AND EXPENSES ASSOCIATED WITH BATTELLE-OWNED EQUIPMENT WITH A FIRST COST OF LESS THAN \$50,000, SUCH AS DEPRECIATION, MAINTENANCE, TAXES, AND INSURANCE. THESE COSTS ARE ACCUMULATED IN AN INTERMEDIATE COST POOL AND ARE ALLOCATED TO COST OBJECTIVES AT A PREDETERMINED RATE PER DIRECT LABOR HOUR.

**PROGRAM DEVELOPMENT AND MANAGEMENT (PDM)**

PROGRAM DEVELOPMENT AND PROGRAM MANAGEMENT COSTS INCLUDE COSTS FOR BUSINESS DEVELOPMENT, PLANNING, AND MONITORING FOR A GROUP OF PROJECTS. COSTS ARE POOLED AND THEN APPLIED TO VALUE ADDED COSTS, LESS PDM COSTS, PLUS MATERIALS AND SUBCONTRACTS.

**GENERAL AND ADMINISTRATIVE EXPENSE (G&A)**

THE ALLOCATION BASE FOR G&A EXPENSES IS VALUE ADDED TO FINAL COST OBJECTIVES. THE VALUE-ADDED BASE INCLUDES: LABOR, TRAVEL, SERVICE AND EQUIPMENT CENTERS, ORGANIZATIONAL OVERHEAD, BUILDING AND UTILITY COST, AND OTHER DIRECT COSTS. IT EXCLUDES THE BASE COST FOR PROCUREMENT, SUBCONTRACTS, AND OTHER HANFORD CONTRACTOR SERVICES.

**FIFTH GRANT PERIOD, FROM 7/1/2010 THROUGH 6/30/2011**

	<u>FY2006</u> <u>RATE</u>	<u>RATE THIS</u> <u>PERIOD</u>	<u>BASE</u>	<u>INDIRECT</u> <u>COST</u>
<b>PROGRAM DEV AND MGMT (PDM)</b>	6.0%	6.0%	\$223,301	13,398
<b>ORGANIZATIONAL OVERHEAD:</b>			<u>BASE</u>	
Ops & Research Support	\$ 27.05	\$ 30.42	8 HOURS	\$ 243
Climate Physics	\$ 27.05	\$ 30.41	1281 HOURS	\$ 38,961
Atmospheric Chemistry & Meteorology	\$ 27.05	\$ 30.41	579 HOURS	\$ 17,598
Lab Technical Mgmt Cost	\$ 0.15	\$ 0.15	1868 HOURS	\$ 280
<b>TOTAL ORGANIZATIONAL OVERHEAD</b>				\$ 57,082
			<u>VALUE-ADDED BASE*</u>	
<b>GENERAL AND ADMINISTRATIVE COST</b>	33.0%	36.5%	\$234,437	\$ 85,569
<b>SERVICE ASSESSMENT</b>	2.4%	2.4%	BASE: \$322,269	\$ 7,734
<b>TOTAL INDIRECT COST</b>				<b>163,784</b>

**\*THE VALUE-ADDED BASE IS DERIVED BY ADDING THE FOLLOWING COST ELEMENTS:**

Direct Labor	\$ 152,507	Program Dev	\$ 13,398	Other Dir. Costs	\$ 4,154
Organizationa	57,082	Travel	7,204	Proc/Subcont. Svc. Chgs	91





# Face Page

**TITLE OF PROPOSED RESEARCH:**

A Scalable and Extensible Earth System Model for Climate Change Science

1. CATALOG OF FEDERAL DOMESTIC ASSISTANCE #  
81.049

2. CONGRESSIONAL DISTRICT:  
Applicant Organization's District: District 1 (NM)  
Project Site's District: District 10 (CA) for out NM for both

3A. I.R.S. ENTITY IDENTIFICATION OR SSN:  
85-0097942

3B. DUNS Number:  
007113228

4. AREA OF RESEARCH OR ANNOUNCEMENT TITLE/#:  
SciDAC2 LAB-06-04

5. HAS THIS RESEARCH PROPOSAL BEEN SUBMITTED  
TO ANY OTHER FEDERAL AGENCY?  
 YES  NO

PLEASE LIST \_\_\_\_\_

6. DOE/OER PROGRAM STAFF CONTACT (if known):  
Michael Strayer

7. TYPE OF APPLICATION:  
 New  Renewal  
 Continuation  Revision  
 Supplement

8. ORGANIZATION TYPE:  
 Local Govt.  State Govt.  
 Non-Profit  Hospital  
 Indian Tribal Govt.  Individual  
 Other  Inst. of Higher Educ.  
 For-Profit  
 Small Business  Disadvan. Business  
 Women-Owned  8(a)

9. CURRENT DOE AWARD # (IF APPLICABLE): \_\_\_\_\_

10. WILL THIS RESEARCH INVOLVE:  
10A. Human Subjects  No  If yes  
Exemption No. \_\_\_\_\_ or  
IRB Approval Date \_\_\_\_\_  
Assurance of Compliance No: \_\_\_\_\_  
10B. Vertebrate Animals  No  If yes  
IACUC Approval Date \_\_\_\_\_ or  
Animal Welfare Assurance No: \_\_\_\_\_

11. AMOUNT REQUESTED FROM DOE FOR ENTIRE  
PROJECT PERIOD \$ 1,642,695.00

12. DURATION OF ENTIRE PROJECT PERIOD:  
07/01/06 to 06/30/11  
MM/DD/YY MM/DD/YY

13. REQUESTED AWARD START DATE  
07/01/06  
MM/DD/YY

14. IS APPLICANT DELINQUENT ON ANY FEDERAL DEBT?  
 Yes (attach an explanation)  No

15. PRINCIPAL INVESTIGATOR/PROGRAM DIRECTOR  
NAME Mark Taylor  
TITLE Principal Member of the Technical Staff  
ADDRESS P.O. Box 5800, MS-1110  
Albuquerque, NM 87111  
PHONE NUMBER 505-284-1874

SIGNATURE OF PRINCIPAL INVESTIGATOR/ PROGRAM DIRECTOR  
(please type in full name if electronically submitted)  
Date 03/23/2006 Mark Taylor

PI/PD ASSURANCE: I agree to accept responsibility for the scientific conduct of the project and to provide the required progress reports if an award is made as a result of this submission. Willful provision of false information is a criminal offense. (U.S. Code, Title 18, Section 1001).

16. ORGANIZATION'S NAME Sandia National Laboratories  
ADDRESS P.O. Box 5800  
Albuquerque, NM 87175-1110

CERTIFYING REPRESENTATIVE'S  
NAME David E. Womble  
TITLE Acting Director of Center 1400  
PHONE NUMBER 505-845-7471

SIGNATURE OF ORGANIZATION'S CERTIFYING REPRESENTATIVE  
(please type in full name if electronically submitted)  
Date 03/23/2006

CERTIFICATION AND ACCEPTANCE: I certify that the statements herein are true and complete to the best of my knowledge, and accept the obligation to comply with DOE terms and conditions if an award is made as the result of this submission. A willfully false certification is a criminal offense. (U.S. Code, Title 18, Section 1001).

**NOTICE FOR HANDLING PROPOSALS**

This submission is to be used only for DOE evaluation purposes and this notice shall be affixed to any reproduction or abstract thereof. All Government and non-Government personnel handling this submission shall exercise extreme care to ensure that the information contained herein is not duplicated, used, or disclosed in whole or in part for any purpose other than evaluation without written permission except that if an award is made based on this submission, the terms of the award shall control disclosure and use. This notice does not limit the Government's right to use information contained in the submission if it is obtainable from another source without restriction. This is a Government notice, and shall not itself be construed to impose any liability upon the Government or Government personnel for any disclosure or use of data contained in this submission.

**PRIVACY ACT STATEMENT**

If applicable, you are requested, in accordance with 5 U.S.C., Sec. 562A, to voluntarily provide your Social Security Number (SSN). However, you will not be denied any right, benefit, or privilege provided by law because of a refusal to disclose your SSN. We request your SSN to aid in accurate identification, referral and review of applications for research/training support for efficient management of Office of Science grant/contract programs.

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**U.S. Department of Energy**  
**Budget Page**  
(See reverse for Instructions)

OMB Control No.  
1910-1400  
OMB Burden Disclosure  
Statement on Reverse

ORGANIZATION <b>Sandia National Laboratories</b>				Budget Page No: <u>1</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Mark Taylor</b>				Requested Duration: <u>3</u> (Months) FY2006 (July 2006 - September 2006)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)				DOE Funded	
				Person-mos.	
				CAL	ACAD
				SUMR	
				Funds Requested	
				by Applicant	
				Funds Granted	
				by DOE	
1.	Mark Taylor, Principal Member of Technical Staff	1.44			\$38,941
2.	Bill Spotz, Senior Member of Technical Staff	1.44			\$32,521
3.					
4.					
5.					
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE) TSM 110-119				
7.	( 2 ) TOTAL SENIOR PERSONNEL (1-6)	2.88			\$71,462
B. ( ) OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1.	( ) POST DOCTORAL ASSOCIATES				
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER				
TOTAL SALARIES AND WAGES (A+B)					\$71,462
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$71,462
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL				1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)	
				\$3,203	
				2. FOREIGN	
TOTAL TRAVEL					\$3,203
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					\$1,657
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					\$276
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					\$2,706
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS					\$4,639
H. TOTAL DIRECT COSTS (A THROUGH G)					\$79,304
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS					
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$79,304
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					\$79,304

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**U.S. Department of Energy**  
**Budget Page**  
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OMB Control No.  
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OMB Burden Disclosure  
Statement on Reverse

ORGANIZATION <b>Sandia National Laboratories</b>				Budget Page No: <u>2</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Mark Taylor</b>				Requested Duration: <u>12</u> (Months) FY2007 (October 2006 - September 2007)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)				DOE Funded	
				Person-mos.	
				Funds Requested	
				Funds Granted	
				by Applicant	
				by DOE	
1.	Mark Taylor, Principal Member of Technical Staff	5.40			\$151,972
2.	Bill Spatz, Senior Member of Technical Staff	5.40			\$126,918
3.					
4.					
5.					
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE) TSM 110-119				
7.	( 2 ) TOTAL SENIOR PERSONNEL (1-6)	10.80			\$278,890
B. ( ) OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1.	( ) POST DOCTORAL ASSOCIATES				
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER				
TOTAL SALARIES AND WAGES (A+B)				\$278,890	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				\$278,890	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL				1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS) \$9,596	
				2. FOREIGN	
TOTAL TRAVEL				\$9,596	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				\$6,697	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				\$1,116	
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES				\$10,862	
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				\$18,675	
H. TOTAL DIRECT COSTS (A THROUGH G)				\$307,161	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS					
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				\$307,161	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				\$307,161	

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OMB Control No.  
1910-1400  
OMB Burden Disclosure  
Statement on Reverse

ORGANIZATION <b>Sandia National Laboratories</b>				Budget Page No: <u>3</u>		
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Mark Taylor</b>				Requested Duration: <u>12</u> (Months) FY2008 (October 2007 - September 2008)		
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested by Applicant	
			CAL	ACAD	SUMR	Funds Granted by DOE
1.	Mark Taylor, Principal Member of Technical Staff		5.40			\$158,186
2.	Bill Spotz, Senior Member of Technical Staff		5.40			\$132,107
3.						
4.						
5.						
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE) TSM 110-119					
7.	( 2 ) TOTAL SENIOR PERSONNEL (1-6)		10.80			\$290,293
B. ( ) OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)						
1.	( ) POST DOCTORAL ASSOCIATES					
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3.	( ) GRADUATE STUDENTS					
4.	( ) UNDERGRADUATE STUDENTS					
5.	( ) SECRETARIAL - CLERICAL					
6.	( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)						\$290,293
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)						
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)						\$290,293
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)						
TOTAL PERMANENT EQUIPMENT						
E. TRAVEL			1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)		\$9,622	
			2. FOREIGN			
TOTAL TRAVEL					\$9,622	
F. TRAINEE/PARTICIPANT COSTS						
1. STIPENDS (Itemize levels, types + totals on budget justification page)						
2. TUITION & FEES						
3. TRAINEE TRAVEL						
4. OTHER (fully explain on justification page)						
TOTAL PARTICIPANTS ( ) TOTAL COST						
G. OTHER DIRECT COSTS						
1. MATERIALS AND SUPPLIES						\$6,697
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION						\$1,116
3. CONSULTANT SERVICES						
4. COMPUTER (ADPE) SERVICES						\$10,879
5. SUBCONTRACTS						
6. OTHER						
TOTAL OTHER DIRECT COSTS						\$18,692
H. TOTAL DIRECT COSTS (A THROUGH G)						\$318,607
I. INDIRECT COSTS (SPECIFY RATE AND BASE)						
TOTAL INDIRECT COSTS						
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)						\$318,607
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES						
L. TOTAL COST OF PROJECT (J+K)						\$318,607

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**Budget Page**  
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OMB Control No.  
1910-1400  
OMB Burden Disclosure  
Statement on Reverse

ORGANIZATION <b>Sandia National Laboratories</b>				Budget Page No: <u>4</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Mark Taylor</b>				Requested Duration: <u>12</u> (Months) FY2009 (October 2008 - September 2009)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested by Applicant
			CAL	ACAD	SUMR
1. Mark Taylor, Principal Member of Technical Staff			5.40		
2. Bill Spatz, Senior Member of Technical Staff			5.40		
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE) TSM 110-119					
7. ( 2 ) TOTAL SENIOR PERSONNEL (1-6)			10.80		\$300,586
B. ( ) OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)					\$300,586
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$300,586
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL			1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)		\$9,613
			2. FOREIGN		
TOTAL TRAVEL					\$9,613
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					\$6,697
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					\$1,116
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					\$10,874
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS					\$18,687
H. TOTAL DIRECT COSTS (A THROUGH G)					\$328,886
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS					
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$328,886
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					\$328,886

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**U.S. Department of Energy**  
**Budget Page**  
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OMB Control No.  
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OMB Burden Disclosure  
Statement on Reverse

ORGANIZATION <b>Sandia National Laboratories</b>				Budget Page No: <u>5</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Mark Taylor</b>				Requested Duration: <u>12</u> (Months) FY2010 (October 2009 - September 2010)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested by Applicant
			CAL	ACAD	SUMR
1. Mark Taylor, Principal Member of Technical Staff			5.40		
2. Bill Spotz, Senior Member of Technical Staff			5.40		
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE) TSM 110-119					
7. ( 2 ) TOTAL SENIOR PERSONNEL (1-6)			10.80		\$318,052
B. ( ) OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)					\$318,052
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$318,052
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL			1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)		\$9,587
			2. FOREIGN		
TOTAL TRAVEL					\$9,587
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					\$6,697
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					\$1,116
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					\$10,856
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS					\$18,669
H. TOTAL DIRECT COSTS (A THROUGH G)					\$346,308
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS					
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$346,308
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					\$346,308

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**Budget Page**  
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OMB Burden Disclosure  
Statement on Reverse

ORGANIZATION <b>Sandia National Laboratories</b>				Budget Page No: <u>6</u>		
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Mark Taylor</b>				Requested Duration: <u>9</u> (Months) FY2011 (October 2010 - June 2011)		
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested by Applicant	
			CAL	ACAD	SUMR	Funds Granted by DOE
1.	Mark Taylor, Principal Member of Technical Staff		3.96			\$131,890
2.	Bill Spotz, Senior Member of Technical Staff		3.96			\$110,146
3.						
4.						
5.						
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE) TSM 110-119					
7.	( 2 ) TOTAL SENIOR PERSONNEL (1-6)		7.92			\$242,036
B. ( ) OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)						
1.	( ) POST DOCTORAL ASSOCIATES					
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3.	( ) GRADUATE STUDENTS					
4.	( ) UNDERGRADUATE STUDENTS					
5.	( ) SECRETARIAL - CLERICAL					
6.	( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)						\$242,036
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)						
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)						\$242,036
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)						
TOTAL PERMANENT EQUIPMENT						
E. TRAVEL			1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)		\$6,391	
			2. FOREIGN			
TOTAL TRAVEL					\$6,391	
F. TRAINEE/PARTICIPANT COSTS						
1. STIPENDS (Itemize levels, types + totals on budget justification page)						
2. TUITION & FEES						
3. TRAINEE TRAVEL						
4. OTHER (fully explain on justification page)						
TOTAL PARTICIPANTS ( ) TOTAL COST						
G. OTHER DIRECT COSTS						
1. MATERIALS AND SUPPLIES						\$5,023
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION						\$837
3. CONSULTANT SERVICES						
4. COMPUTER (ADPE) SERVICES						\$8,142
5. SUBCONTRACTS						
6. OTHER						
TOTAL OTHER DIRECT COSTS						\$14,002
H. TOTAL DIRECT COSTS (A THROUGH G)						\$262,429
I. INDIRECT COSTS (SPECIFY RATE AND BASE)						
TOTAL INDIRECT COSTS						
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)						\$262,429
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES						
L. TOTAL COST OF PROJECT (J+K)						\$262,429

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U.S. Department of Energy
Budget Page
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OMB Control No.

1910-1400

OMB Burden Disclosure
Statement on Reverse

ORGANIZATION Sandia National Laboratorie:
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Mark Taylor
A. SENIOR PERSONNEL: P/PI, Co-PI's, Faculty and Other Senior Associates
1. Mark Taylor, Principal Member of Technical Staff
2. Bill Spatz, Senior Member of Technical Staff
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)
D. PERMANENT EQUIPMENT
E. TRAVEL
F. TRAINEE/PARTICIPANT COSTS
G. OTHER DIRECT COSTS
H. TOTAL DIRECT COSTS (A THROUGH G)
I. INDIRECT COSTS (SPECIFY RATE AND BASE)
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES
L. TOTAL COST OF PROJECT (J+K)





**Sandia National Laboratories**

Operated for the U.S. Department of Energy by  
**Sandia Corporation**

P.O. Box 5800  
Albuquerque, NM 87185-1384

Phone: (505)844-3653  
Fax: (505)844-7284  
Internet: [jscrook@sandia.gov](mailto:jscrook@sandia.gov)

**Jennifer S. Crooks**  
Controller

To whom it may concern:

We are providing the following financial-related information to assist you in your efforts in conducting business with Sandia National Laboratories. Sandia Corporation, a Lockheed Martin company, doing business as Sandia National Laboratories, functions as an M&O Contractor for the U.S. Department of Energy and is classified as an integrated contractor. As such, Sandia's books of account are fully integrated with those of DOE.

As a contractual requirement, Sandia adheres to the requirements of Cost Accounting Standards (CAS) and has filed a CAS disclosure statement, describing Sandia's accounting system and charging practices, with the DOE Contracting Officer. Sandia conducts its operations on a full-cost recovery basis and charges all direct costs and all allocable costs attributable to direct technical projects to those projects in a manner consistent with DOE and Sandia financial policy.

Sandia's specific overhead cost recovery rates and individual salary rates are proprietary information and are generally not released externally. However, because of its relationship with DOE, Sandia operations and accounting practices are fully auditable by the U. S. DOE Inspector General (DOE IG) on a regular basis, as well as by Sandia Corporation's Internal Audit Department. Sandia has established protocols for DOE IG audits of Sandia operations.

Questions regarding Sandia accounting practices or financial policy may be directed to me at (505) 844-3653 or to Ami Peterson, Sandia's CAS Advisor, at (505) 844-3085.

Sincerely,

A handwritten signature in cursive script, appearing to read "J. Crooks".

## BUDGET EXPLANATION

### **Key Sandia Personnel: Salaries and Wages**

- Mark A. Taylor, Principal Member of Technical Staff

Mark's technical contribution will be in the area of unstructured grid methods, dynamical cores for atmospheric general circulation models and software engineering for performance and scalability on parallel computers.

- William F. Spatz, Senior Member of Technical Staff

William's technical contribution will be in the area of numerical methods, multi-physics coupling and software development.

### **Equipment**

No equipment with a value of \$25,000 or greater will be purchased for this project.

### **Domestic Travel**

The anticipated travel costs will be used for domestic travel to relevant project-related conferences and workshops.

### **Foreign Travel**

No funds are requested for foreign travel at this time

### **Other direct Costs**

Materials and supplies are estimated to cover photocopying, laser printing facsimile and long distance telephone services connected with the projected work.

## 4 OTHER SUPPORT OF INVESTIGATORS

### 4.1 Oak Ridge National Laboratory

Institution	Name	Active or Pending	Funding Agency or Org.	Inclusive Dates of Project	Annual funding	Level of Effort %
ORNL	Drake, John B.	Active	DOE SciDAC1	7/1/2001-6/30/2006	\$4M	0.8
ORNL	Drake, John B.	Active	DOE/OBER	10/01/2004-09/30/2007	1.3M	0.2
ORNL	Erickson, David	Active	DOE SciDAC1	7/1/2001-6/30/2006	\$4M	0.5
ORNL	Erickson, David	Active	NASA	10/01/2004-09/30/2007	1.3M	0.2
ORNL	Hoffman, Forrest	Active	DOE/OBER	10/01/2004-09/30/2007	1.3M	0.2
ORNL	Hoffman, Forrest	Active	DOE SciDAC1	7/1/2001-6/30/2006	\$4M	0.5
ORNL	Post, W. M.	Active	DOE	1994-2006	\$648K	60
ORNL	Post, W. M.	Active	DOE	2004-2007	\$2M	20
ORNL	Post, W. M.	Active	DOE	2004-2006	\$250K	10
ORNL	Post, W. M.	Active	DOE	2002-2006	\$1.2M	5
ORNL	Post, W. M.	Active	ORNL-LDRD	2006-2007	\$200K	10
ORNL	Post, W. M.	Pending	DOE	2007-2009	\$200K	10
ORNL	Post, W. M.	Pending	DOE	2007-2009	\$650K	50
ORNL	Post, W. M.	Pending	DOE	2007-2009	\$500K	5
ORNL	Worley, Pat	Active	DOE SciDAC1	7/1/2001-6/30/2006	\$4M	0.5

### 4.2 Argonne National Laboratory

Institution	Name	Active or Pending	Funding Agency or Org.	Inclusive Dates of Project	Annual funding	Level of Effort
ANL	Jacob, Robert L.	Active	DOE	7/01 – 6/06	\$700K	.75
ANL	Jacob, Robert L.	Active	NSF-ITR	9/01 - 6/06	\$700K	.25
ANL	Jacob, Robert L.	Pending	DOE	7/06 – 6/11	\$320K	100
ANL	Jacob, Robert L.	Pending	DOE	7/06 – 6/11	\$400K	.25
ANL	Jacob, Robert L.	Pending	DOE	7/06 – 6/11	\$150K	.10

### 4.3 Brookhaven National Laboratory

Institution	Name	Active or Pending	Funding Agency or Org.	Inclusive Dates of Project	Annual funding	Level of Effort
BNL	McGraw, Robert	Active	DOE ARM	10/1/2005-9/30/2008	\$120K	0.2FTE
BNL	McGraw, Robert	Active	DOE ASP	10/1/2005-9/30/2008	\$113K	0.4
BNL	McGraw, Robert	Active	DOE ARM	10/1/2005-9/30/2008	\$600K	0.05
BNL	McGraw, Robert	Active	DOE ASP	10/1/2005-9/30/2008	\$450K	0.05
BNL	McGraw, Robert	This Proposal SAP	DOE SciDAC2	7/1/2006-6/30/2009	\$315K	0.2
BNL	Robert McGraw	Active	NASA	2/1/2006-1/31/2008	\$110K	0.1

#### 4.3 Los Alamos National Laboratory

Institution	Name	Active or Pending	Funding Agency or Org.	Inclusive Dates of Project	Annual funding	Level of Effort
LANL	Elliott, Scott	Active	DOE SciDAC1	7/1/2001-6/30/2006	989K	1.0
LANL	Elliott, Scott	This Proposal	DOE SciDAC2	7/1/2006-6/30/2011	990K	1.0
LANL	Jones, Philip	Active	DOE SciDAC1	7/1/2001-6/30/2006	\$989K	0.5
LANL	Jones, Philip	Active	DOE CCPP	10/1/2000-9/30/2008	\$2M	0.4
LANL	Jones, Philip	Active	DOE SciDAC1	7/1/2001-6/30/2006	\$217K	0.1
LANL	Jones, Philip	Pending	DOE SciDAC2	7/1/2006-6/30/2011	\$100K	0.1
LANL	Jones, Philip	This Proposal	DOE SciDAC2	7/1/2006-6/30/2011	\$990K	0.5
LANL	Lipscomb, W. H.	Active	DOE SciDAC1	7/1/2001-6/30/2006	989K	1.0
LANL	Lipscomb, W.H.	This Proposal	DOE SciDAC2	7/1/2006-6/30/2011	990K	1.0
LANL	Maltrud, Mathew	Active	DOE SciDAC1	7/1/2001-6/30/2006	\$989K	0.5
LANL	Maltrud, Mathew	Active	DOE OBER	10/1/2003-9/30/2006	\$263K	0.25
LANL	Maltrud, Mathew	Active	US Navy NOPP	10/1/2003-9/30/2006	\$80K	0.25
LANL	Maltrud, Mathew	Pending	DOE SciDAC2	7/1/2006-6/30/2011	\$100K	0.5
LANL	Maltrud, Mathew	This Proposal	DOE SciDAC2	7/1/2006-6/30/2011	\$990K	0.5

#### 4.4 Lawrence Berkeley National Laboratory

Institution	Name	Active or Pending	Funding Agency or Org.	Inclusive Dates of Project	Annual funding	Level of Effort
LBNL	Wehner, Michael	Active	DOE OBER	10/1/2005-9/30/2008	\$231K	0.75
LBNL	Wehner, Michael	Active	NASA	7/05-7/08	\$15K	0.05

#### 4.5 National Center for Atmospheric Research

Institution	Name	Active or Pending	Funding Agency or Org.	Inclusive Dates of Project	Annual funding	Level of Effort
NCAR	Lamarque, J-F.	Pending	DOE	07/2006-06/2011	\$33K	12
NCAR	Lamarque, J-F.	Active	DOE	05/2002-05/2007	\$2,412,300	8.4
NCAR	Lamarque, J-F.	Pending	NASA	11/2006-12/2008	\$595,296	2.4

#### 4.6 Pacific Northwest National Laboratory

Institution	Name	Active or Pending	Funding Agency or Org.	Inclusive Dates of Project	Annual funding	Level of Effort
PNNL	Easter, Richard	Active	DOE ASP	10/1/2004-9/30/2007	\$180K	0.22
PNNL	Easter, Richard	Active	DOE ASP	10/1/2004-9/30/2007	\$240K	0.03
PNNL	Easter, Richard	Active	DOE ASP	10/1/2004-9/30/2007	\$250K	0.22
PNNL	Easter, Richard	Active	DOE	9/30/2006	\$100K	0.1
PNNL	Easter, Richard	Active	DOD	10/2005 - 2/2006	\$50K	0.08
PNNL	Easter, Richard	This Proposal	DOE SciDAC2	7/1/2006-6/30/2011	\$4M	0.16
PNNL	Ghan, Steve	Active	DOE SciDAC1	7/1/2001-6/30/2006	\$4M	0.3
PNNL	Ghan, Steve	Active	DOE ARM	10/1/2005-9/30/2008	\$200K	0.3
PNNL	Ghan, Steve	Active	DOE ASP	10/1/2004-9/30/2007	\$250K	0.3
PNNL	Ghan, Steve	Active	DOE	-9/30/2006	\$100K	0.2
PNNL	Ghan, Steve	This Proposal	DOE SciDAC2	7/1/2006-6/30/2011	\$4M	0.2
PNNL	Liu, Xiaohong	Active	DOE ARM	10/1/2005-9/30/2008	\$200K	0.2
PNNL	Liu, Xiaohong	Active	DOE ASP	10/1/2004-9/30/2007	\$180K	0.2
PNNL	Liu, Xiaohong	Active	NSF	1/1/2006-10/31/2006	\$98K	0.3
PNNL	Liu, Xiaohong	This Proposal	DOE SciDAC2	7/1/2006-6/30/2011	\$4M	0.5

#### 4.7 Sandia National Laboratories

Institution	Name	Active or Pending	Funding Agency or Org.	Inclusive Dates of Project	Annual funding	Level of Effort
SNL	Spotz, William F.	Active	Sandia LDRD	10/1/03 – 9/30/06	\$205K	0.5
SNL	Spotz, William F.	Active	NNSA Accelerated Scientific Computing	2/17/06 – 9/30/06	\$75K	0.25
SNL	Spotz, William F.	Pending	SciDAC	7/1/2006-6/30/2011	\$6M	0.5
SNL	Spotz, William F.	Pending	University of British Columbia / Natural Sciences and Engineering Research Council of Canada	7/1/2006-6/30/2011	\$75K	0.25
SNL	Taylor, Mark	Pending	SciDAC	7/1/2006-6/30/2011	\$6M	0.45
SNL	Taylor, Mark	Pending	SciDAC	7/1/2006-6/30/2011	\$1.5M	.2
SNL	Taylor, Mark	Pending	SciDAC	7/1/2006-6/30/2011	\$3M	.25
SNL	Taylor, Mark	Pending	SciDAC	7/1/2006-6/30/2009	\$500K	.1

## 5 TASKS AND MILESTONES

### 5.1 Oak Ridge National Laboratory

The development of scalable implementations that effectively utilize the target platforms is a key focus of the Oak Ridge contribution to this project. Adapting and porting to the new Cray XT3 and later XT4 platforms will require substantial work in the atmosphere model. Introducing more granular parallel decompositions of the physics and chemistry, as well as improving scalability of the Finite Volume dynamical core through support of a generalization of the grid system will move the code from a 200 processor “sweet spot” to a 5K execution standard. All the improvements to scalability will be performed directly with development versions of the CCSM and CAM so that performance gains are immediately available to ongoing simulation projects.

The other efforts at Oak Ridge will address the biogeochemical aspects of the model development. In particular, we will play a key role in the delivery of the BGC inter-comparison project and the subsequent selection and implementation of the important processes in the Community Land Model, CLM. Evaluation of these processes and the resulting coupled carbon-climate model will be an important part of Oak Ridge’s contribution to the Integration and Evaluation tasks of the proposal.

Finally, Oak Ridge will be responsible for the management of the project along with production of progress reports and responsive interaction with the collaborating institutions and the OBER Climate Change Prediction Program.

Milestones Summary:

- Year 1: Definition of generalized grid systems for dynamical core and physics interfaces.
- Year 2: Biogeochemistry inter-comparison runs completed with supporting documentation
- Year 3: CCSM4 configuration with biogeochemistry optimized for five thousand processors.
- Year 4: Scalable design for CCSM5
- Year 5: New dynamical cores implemented and tested.

### 5.2 Argonne National Laboratory

The full peer-reviewable proposal is being submitted by Oak Ridge National Laboratory as the lead institution.

At Argonne, this project addresses several of the challenges involved in creating an Earth System Model based on the Community Climate System Model (CCSM). We will co-lead the creation of an integration and evaluation framework for CCSM based on a suite of unit and integration tests. This effort will require some refactoring of the current CCSM source code to make it more modular. Test code will be developed, in collaboration with other project members and CCSM working groups, for current physics within CCSM and new physics introduced to create an Earth System Model. We will create a more robust and easy to maintain version of the current integration test within CCSM, the single column atmosphere model. We will help create a sequential execution version of CCSM which will serve as the basis for extending integration testing throughout the CCSM component models.

The Model Coupling Toolkit (MCT) is the coupling software currently used in both the concurrent CCSM and the standalone atmosphere component, CAM. We will work to unify the use of MCT within CCSM and enhance its performance on platforms of interest. MCT is currently based on MPI1 and its two-sided message

passing model. With the increasing availability of MPI2, we will introduce a one-sided message passing model to MCT and explore how it can improve performance in the concurrent version of CCSM.

We will profile and optimize the load balance of CCSM in the concurrent model and also work to create alternate configurations of CCSM, such as sequential and hybrid execution, which are easier to load balance. We will assist with specific integration and evaluation efforts to bring in new biogeochemistry physics and dynamical cores into CCSM. Finally, we will help create a robust, flexible build system for CCSM which can easily support alternate configurations and multiple physics options.

Midway through this project, the next version of CCSM will be released and Argonne will be involved in system and integration testing for this important new version of the model.

Many of these milestones will be done in close collaboration with the National Center for Atmospheric Research.

Milestones Summary:

Year 1: Improved integration tests for CAM column physics. Use of MCT is being implemented and standardized for intercomponent communication within CAM. Extension of SCAM to CCSM CICE and CLM3 models.

Year 2: Integration and unit tests for current CAM physics and for CLM completed. Sequential version of CCSM. Improved build system for all configurations of CCSM. Begin incorporation of SCAM into ocean model.

Year 3: Perform integration and system tests for release of CCSM4. Release of MCT with one-sided message passing.

Year 4: Integration and unit tests for new chemistry and physics parameterizations introduced in CCSM4.

Year 5: Unit and integration tests for ocean and sea ice completed. Unit and integration test suite for full model available.

### **5.3 Brookhaven National Laboratory**

BNL will participate in the activities of this proposal through its SAP with SUNY-Stony Brook: “Statistical Approaches to Aerosol Dynamics for Climate Simulation”. Specifically, BNL will contribute to the proposed Earth Simulation Model by way of 3 tasks: (1) developing new capabilities for aerosol simulation using advanced statistical methods and improvements to the quadrature method of moments (QMOM); (2) leveraging of findings from its current DOE ASP and DOE ARM science programs related to aerosols and aerosol-cloud interactions - especially for development of new parameterizations suitable for use in the CCSM; and (3) supplying a new aerosol module based on the new methods [see description of this SAP in Sec. 3.1.3]. To successfully carry out these activities we will build on an already successful collaboration between the BNL Atmospheric Sciences Division, which will lead the science application work, and the Applied Mathematics and Statistics (AMS) Department at SUNY-SB, which will lead the mathematical development.

Activities during Year 1 will build on our previous collaborations, which achieved major advances of aerosol moment methods through a novel application of principal components analysis and through the use of quadrature, both for closure of the moment evolution equations and for estimation of aerosol physical and

optical properties directly from moments [see papers with AMS student C. Yoon listed under the McGraw biosketch heading of recent publications].

Activities during Year 2 will build on another important BNL-SUNY/AMS collaboration involving development of visual statistical classification and data mining software. This software has been successfully applied both to the classification of ambient aerosols (e.g. to classification of single-particle mass spectroscopic data taken during field campaigns in Houston and Korea) and to various medical applications. The linkage between modeling and measurement is well worth pursuing and we will determine during Year 2 whether the same algorithms, or similar ones, can be used to optimize how the aerosol is represented in climate models. For example, we will seek to optimized modal (class) partitioning, quadrature point assignment, and determine which multivariate compositional moments are best to track during the course of a simulation. Parameterizations for new particle formation, water uptake with changes in relative humidity, sea salt aerosol production flux, and for aerosol-cloud interactions and indirect effects, including drizzle formation, will be adapted to the model under Task 2. Year 3 will see the continuation of each these activities with major emphasis on preparing a new QMOM module for model integration in time for the following IPCC assessment (AR6).

#### **5.4 Los Alamos National Laboratory**

LANL will provide overall management of project, jointly with ORNL.

LANL will integrate new algorithms and new physics into the Parallel Ocean Program (POP), the ocean component of CCSM and work toward the transition to the hybrid vertical coordinate HYPOP. A particular focus will be the introduction of software infrastructure necessary for general, unstructured horizontal grids. We will create new diagnostics and quantitative metrics for ocean model evaluation. Finally, we will continue to optimize POP performance on advanced computer architectures.

LANL will also integrate and evaluate new algorithms for both ice sheets and sea ice within CCSM. The largest task will be the integration of the open-source Glimmer ice sheet model into CCSM. Further improvements of the ice sheet model will follow. We will integrate and evaluate snow parameterizations for the sea ice component of CCSM. Following the ocean model development, we will integrate an advanced horizontal grid infrastructure into both sea ice and ice sheet models and continue to optimize performance of the CICE model on advanced architectures.

LANL will continue to improve the ocean ecosystem and biogeochemical models for coupled carbon and sulfur cycle modeling. We will improve the trace gas module by adding new important trace gases and related processes for the coupled chemical climate. We will develop more quantitative methods for evaluating ocean ecosystem and biogeochemical models and use these methods to gain insight for improving the model's representation of ocean ecosystems.

Milestones Summary:

Year 1: Couple Glimmer ice sheet model as a CCSM component. Create design of new ocean model infrastructure for general horizontal grids and design for a comprehensive diagnostic module. Refine sulfur cycle and DMS mechanisms.

Year 2: Implement new grid infrastructure and new diagnostic module in ocean model. Implement new snow treatment in sea ice model. Add new trace gases to ocean biogeochemistry model and implement dust deposition.



Year 3: Perform necessary model testing of ocean and ice components for release of CCSM4. Participate in coupled carbon and chemistry simulations and analysis.

Year 4: Begin integration and evaluation of HYPOP model in CCSM. Extend new ocean grid infrastructure into sea ice model. Implement and test new dynamics scheme in ice sheet model.

Year 5: Implement and test alternative unstructured horizontal grids on ocean, sea ice, ice sheet models.

## **5.5 Lawrence Berkeley National Laboratory**

At Berkeley Lab, emphasis will be placed on development and testing of the biogeochemical aspects of the Earth System Model (ESM). Initial efforts will be focused on developing appropriate carbon cycle validation tools in partnership with PCMDI (Covey) and ORNL (Hoffman). Key to this effort is identifying appropriate observational datasets for comparison to model output. When the Kalnay data assimilation SAP produces a reanalysis, large scale model intercomparison and validation of the carbon cycle can begin in earnest. Additionally, the Kalnay SAP promises to produce better estimates of unconstrained biogeochemical model parameters. The effect of these parameter changes on the larger aspects of the simulated climate will be investigated and quantified.

We also have an interest in the bottom boundary layer of the ocean. This portion of the ocean circulation is important to many phenomena including near shore ocean biogeochemistry. We will implement a treatment of this boundary layer using the Imbedded Boundary Method (IBM) into a high resolution version of POP. Testing of the code will include examination of simulated upwelling and bottom boundary currents.

Year 1: Develop biogeochemical analysis tools using CDAT, including Taylor diagrams and performance portraits. Implement IBM into the one tenth degree resolution POP.

Year 2: Apply biogeochemical analysis tools to versions of the ESM with different land carbon models (CASA, CN, IBIS). Perform short high resolution POP/IBM simulations to quantify the effect of the bottom boundary layer parameterization.

Year 3: Incorporate the Kalnay carbon reanalysis into the biogeochemical analysis tools.

Year 4: Investigate the effect of optimal parameter estimation on the land component of the biogeochemical models.

Year 5: Assist in development of the land carbon model for the AR5 version of CCSM.

## **5.6 Lawrence Livermore National Laboratory**

We will continue our collaboration with our colleagues on this proposal at NCAR, PNNL, and BNL to implement atmospheric chemistry and aerosol capabilities into CCSM. We will focus on validating and refining the fast chemical mechanism we developed under our existing SciDAC project for use in millennial scale climate change simulations (such as IPCC simulations), for which performance has a high premium. We will extend our chemical mechanisms for simulating tropospheric ozone and sulfate aerosols to include interactions with the various aerosol modules we propose to implement, as well as the land and ocean biogeochemistry modules.

In our collaboration on aerosol capabilities for CCSM, we will focus on: (1) simulating the optical properties of the aerosols introduced into CCSM, (2) introducing the more detailed ‘sectional’ aerosol scheme which we have been developing in the off-line IMPACT code under the DOE ARM program, (3) collaborating on the implementation into CCSM of the other two aerosol schemes, the modal and moment methods, and (4) intercomparing and validating the different aerosol capabilities in CCSM.

The task of validating and understanding the behavior of the atmospheric chemistry and aerosol modules, and their interactions with each other and the biosphere, is a large and important task that will occupy a lot of our time. This is also the area in which we will collaborate most closely with the other groups within this collaboration in order to validate and characterize our modules as thoroughly as possible.

We will also participate in many aspects of software engineering, performance analysis, and optimization for CCSM. Much of this work will be under the aegis of this core proposal and will focus on the finite-volume dycore. The work that focuses on new parallel algorithms, very large processor count and next-generation architectures will be carried out under the *Performance Engineering for Next Generation Community Climate System Model* SAP.

We will continue to perform porting, maintenance, and routine optimization on supported platforms, with an initial focus on vector architectures and opteron clusters. This should be an ongoing activity throughout the life of the proposal. Major areas of code development will include support for a large number of tracers with FV, the idea being to add an additional decomposition direction over tracer index; this will result in a tracer decomposition that spans three dimensions. Decomposing the chemistry in 3-D by adding the vertical level will be undertaken as well. This effort will involve adding the requisite communications to connect the various domain decompositions.

We will also reassess the utility of both OpenMP and one-sided communications. On most platforms the gains have been modest in these areas, but due to evolving architectures (such as multi-core chips) regular reinvestigation is needed. We will also continue integration of the CAM version of FV with other implementations of the dycore and utilize the current efforts of S-J Lin and associates and implement support for the FV dycore on the cubed sphere grid.

#### **Atmospheric Chemistry Milestones for LLNL:**

Year 1: Validate fast mechanism for altered emission scenarios (pre-industrial & 2100).

Year 2: Incorporate feedbacks between atmospheric chemistry and biosphere into CCSM.

Year 3: Validate transient simulation from pre-industrial to 2100 using emissions prescribed for IPCC AR5.

Year 4: Evaluate sensitivity of climate to feedbacks between atmospheric chemistry, aerosols, and biosphere.

Year 5: Evaluate the performance and climate change implications of atmospheric chemistry and aerosols in IPCC AR5 simulations.

#### **Aerosol Milestones for LLNL:**

Year 1: Test and improve sectional scheme in stand alone chemistry/aerosol model in collaboration with DOE-ARM.

Year 2: Validate modal aerosol simulations in CCSM with those in stand alone chemistry/aerosol model.

Year 3: Develop parameterization of optical properties for use in modal and sectional schemes.

Year 4: Implement sectional scheme into next generation CCSM.

Year 5: Validate sectional scheme in next generation CCSM.

#### **Model Performance Milestones for LLNL:**

Year 1: Implement 3-D data decomposition for tracers (tracer index) and chemistry (vertical level)

Year 2: Reassess use of OpenMP and one-sided communications.

Integrate CAM-FV with other FV implementations.

Year 3: Implement support for cubed sphere grid in FV dycore.

Year 4: Determine optimal configuration parameters for AR5 simulations.

Year 5: Reassess configuration parameters for architectures undertaking biogeochemistry / atmospheric chemistry/ aerosol sensitivity calculations.

## **5.7 National Center for Atmospheric Research (NCAR)**

NCAR will be responsible for three basic tasks:

- 1) Oversight and coordination of the integration and evaluation effort;
- 2) Oversight and coordination of new software frameworks for CCSM4; and
- 3) Coordination of the development of atmospheric chemistry for CCSM4.

At NCAR, we will coordinate the creation of the necessary software to implement an Earth System Model based on the Community Climate System Model that will have the capability of running as a single-executable sequential system, a single-executable concurrent system and a multiple-executable concurrent system (the current functionality). All of the current CCSM functionality, including the communication of biogeochemical fluxes and states between components and the ability to seamlessly switch a prescribed forcing model for an active model at compile time, will be incorporated into the new modes of running the system.

Creating this new functionality in CCSM will result in increased portability, extensibility, code-reusability and performance. It will also permit the creation of the next generation integration and evaluation framework for CCSM. We will co-lead in the construction of this framework by first extending the single column atmosphere model (SCAM) to all CCSM components. As part of this work we will coordinate and participate in the development of interface standards that will generate flexible environments for running both CCSM and CCSM/SCAM with a wide variety of interactive or “data” components and boundary conditions.

The current CCSM build system can only build the full models in an MPMD configuration. The creation of a sequential CCSM and new unit and integration tests will require the creation of a more flexible build system. We will coordinate and participate in the extension of the CCSM build/run scripts to create this new flexibility.

We will also coordinate and help carry out improvements to the CCSM software infrastructure related to the incorporation of new terrestrial and ocean biogeochemistry. As part of this effort, we will also help carry out necessary model simulations to validate the addition of biogeochemistry to CCSM components. Finally, we will coordinate the performance optimization of component biogeochemistry across a variety of architectures.

Midway through this project, the next version of CCSM will be released. NCAR will coordinate the testing and control simulations associated with the CCSM4 release.

### **Milestone summary for software engineering:**

Year 1: Replace stand-alone CAM sea-ice and CAM ocean components with CCSM CICE and CCSM docn7 within CAM where all components will be on the same grid. Coordinate the incorporation of SCAM into CCSM CICE and CCSM CLM running in “CAM”.

Year 2: Create a sequential CCSM with the ability for the ocean and sea-ice components to run on different grids from the atmospheric and land components. Extend CCSM build/run system to support both sequential and concurrent modes. Coordinate the incorporation of SCAM into CCSM POP.

Year 3: Coordinate integration, unit, system and performance tests for release of CCSM4. Coordinate the release of CCSM4. Determine optimal CCSM configurations (i.e. sequential or concurrent) for particular experimental scenarios. This will involve the validation of new terrestrial and ocean biogeochemistry in the sequential system. Coordinate control simulations associated with the CCSM4 release.

Year 4: Coordinate production runs that will be carried out with CCSM4. Start creating a “hybrid” CCSM with the ability for some components to run sequentially whereas others run concurrently.

Year 5: Coordinate and help finish the creation of a “hybrid” CCSM.

### **Milestone summary for chemistry and aerosols:**

Years 1-2:

- 1) Integrate and test the modal aerosol package MIRAGE from S. Ghan (PNNL) in CAM3. This aerosol package will initially be coupled to the full gas-phase chemistry in CAM3 developed under SciDAC-1.
- 2) Integrate and test the fast mechanism from P. Cameron-Smith (LLNL) in CAM3. The testing procedure will include a comparison to the simulation with the full chemistry mechanism for snapshot simulations under present, pre-industrial and future emission scenarios.

Years 3-4:

- 1) Similar work to tasks in years 1-2 will be performed with the aerosol package from the McGraw SAP, in funded.
- 2) Collaborate on the analysis of the present-day simulations (aerosols and gas-phase); this includes comparison with available data. For this purpose we are developing a set of tools for the comparison of model results against surface, airborne and satellite measurements. This will be expanded to include aerosol size distribution measurements.

Years 3-5:

- 1) Collaborate with the scientists at LLNL and PNNL on the setup, performance and analysis of the pre-industrial to present-day simulation (extension of Lamarque et al, 2005). This includes the analysis of the feedbacks between climate and atmospheric chemistry, including aerosols and their impact on cloud droplet number. These simulations will support the work of this team to the IPCC AR5.

## **5.8 Pacific Northwest National Laboratory**

At PNNL, this project will provide an integrated and validated package of aerosol properties and processes for the CCSM. During year 1, we will port the modal representation of the aerosol in the PNNL version of CAM2 to a branch of CAM3.x. We will introduce prognostic number concentration for each of seven different aerosol modes, and add treatments of the processes that influence number concentration. We will also define size distributions of the primary particle emissions so that emissions of number and mass for each primary particle can be determined, introduce treatments of water uptake and optical properties for internal mixtures of aerosol, and add a treatment of nucleation scavenging consistent with the treatment of droplet nucleation.

During year 2, we will work with NCAR and LLNL staff to evaluate the simulated aerosol distribution and its radiative signature, and to refine and simplify the aerosol package as appropriate. We will then present the aerosol simulation to the CCSM chemistry-climate working group for approval, and upon approval merge the PNNL aerosol branch to the developmental trunk of CAM.

During year 3 we will use the new aerosol treatment to estimate direct and indirect radiative and climatic effects of anthropogenic aerosol.

During year 4 we will update the treatment of secondary organic aerosol and of new particle formation using results from the DOE Atmospheric Science Program.

During year 5 we will support the application of the quadrature method of moments aerosol treatment to the CCSM.

Milestones Summary:

Year 1: Apply modal treatment of aerosol to CCSM.

Year 2: Evaluate and refine treatment, then merge on to developmental branch.

Year 3: Simulate radiative and climatic impact of aerosol.

Year 4: Update the treatment of secondary organic aerosol and new particle formation.

Year 5: Begin application of quadrature method of moments aerosol treatment.

## **5.9 Sandia National Laboratories**

A key focus of this proposal is the integration and evaluation of new numerical methods and model improvements in CCSM. Motivated by the need for much increased scalability in future versions of CCSM, one component of this proposal will focus on dynamical cores for CAM. Current dynamical cores based on latitude-longitude grids have inherent scalability limitations on parallel computers and replacements must be available within the next 5 years. We will be concentrating our efforts on proven cubed-sphere dynamical cores that have undergone significant development in the last ten years. Sandia staff has played a significant role in these efforts, documented in over 20 publications on dynamical cores.

At Sandia, we will first be working with the other laboratories on the modifications necessary to allow CAM to support more general grids such as those based on the cubed-sphere and icosahedral discretizations of the sphere. Concurrently, we will be continuing our collaboration with the developers of NCAR's HOMME by performing the integration of HOMME into CAM. The HOMME software package provides the necessary parallel and numerical operators for supporting cubed-sphere methods on tens of thousands of processors. We will also be working on the integration of a FV dycore, either directly from GFDL, or within the HOMME framework. Finally, promising new dycores currently being developed by University SciDAC awards and possible SAPs will be considered for integration in the later years of this effort.

Experience with CCSM has shown that validating an established dynamical core in a system as complex as CCSM requires a considerable amount of effort. Thus we expect to spend the bulk of this project on the evaluation and tuning on a small set of closely related dynamical cores with capabilities most needed for CAM. Initial efforts will focus solely on the lower order, locally conservative FV method and its discontinuous Galerkin (DG) generalization. The first goal will be to maintain, in CAM, the proven scalability and performance that these dycores achieve outside of CAM. The second goal will be the proper tuning of specific dycore components for use within CAM, since these components will have unforeseen interactions with the many physical models in CAM. It is anticipated that this will require some algorithmic modifications. We will also use the DG method to determine if 4<sup>th</sup> order accurate (or higher) methods have an advantage over 2<sup>nd</sup> order accurate methods. The five year goal of a validated, highly scalable cubed-sphere dycore in CAM will be achieved through close collaboration with the larger effort focused on model evaluation within CCSM made possible by this proposal.

### **Tasks and Milestones for Sandia National Laboratories:**

Years 1-2: Assist with the continued restructuring of CAM to support new dynamical cores and increase parallel scalability.

Years 1-2: Integration of cubed-sphere dycores into CAM. This work will include HOMME and/or a FV dycore.

Years 2-3: Evaluate the performance and scalability of a select subset of locally conservative, cubed-sphere dynamical cores in CAM. Tune and optimize dycore specific features such as time stepping methods and solvers.

Years 3-5: Use the evaluation techniques and experience developed by the entire SciDAC team to complete the integration of a highly scalable cubed-sphere version of CAM. Perform simulations of increasingly sophisticated model problems to evaluate and tune dycore specific components and their interactions with other physical models in CAM.

Year 4-5: Perform integration and evaluation of promising new dynamical cores developed by University SciDAC and SAPs.

## 6 RESUMES

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### EDUCATION & RESEARCH EXPERIENCE

- 10/02-present    Scientist, Lawrence Livermore National Laboratory, Livermore, CA  
(leading the LLNL atmospheric chemistry contribution to the DOE SciDAC program; PI of the LLNL Asian aerosol combined experimental and modeling project; PI of the LLNL project to add reactive chemistry and aerosols to the NARAC operational emergency response code)
- 7/00-9/02        Post-Doc, with Doug Rotman, Lawrence Livermore National Laboratory, Livermore, CA  
(Application of the IMPACT atmospheric chemistry model to chemical and aerosol distributions. Improvement of mass-conservation and photolysis schemes)
- 7/98-6/00        Post-Doc, with Daniel Jacob, Harvard University, Cambridge, MA  
(Developed an integrated atmospheric chemistry and general circulation model)
- 9/94-6/98        Ph.D., Physics, with Fred Taylor, Oxford University, United Kingdom  
(Radiative transfer analysis of Jovian clouds using the NASA Galileo spacecraft)
- 2/92-2/94        M.Sc, Physics, with Dan Walls, Auckland University, New Zealand  
(Theoretical quantum optics: quantum non-demolition measurements)

### HONORS

- 2001    LLNL Energy and Environment Program Award  
1994    Commonwealth Scholarship to UK  
1994    Shirlcliffe Fellowship  
1994    Univ. of Auckland Doctoral scholarship  
1993    Univ. of Auckland Fowlds Memorial Prize (Top in Science Faculty)  
1992    Univ. of Auckland Masters graduate scholarship  
1991    Univ. of Auckland Senior Prize for Physics

### SELECTED PUBLICATIONS & PRESENTATIONS

“Assessing future nitrogen deposition and carbon cycle feedback using a multi-model approach. Part 1: Analysis of nitrogen deposition”, J.-F. Lamarque, J. Kiehl, G. Brasseur, T. Butler, **P. Cameron-Smith**, W. D. Collins, W. J. Collins, C. Granier, D. Hauglustaine,

P. Hess, E. Holland, L. Horowitz, M. Lawrence, D. McKenna, P. Merilees, M. Prather, P. Rasch, D. Rotman, D. Schindell, and P. Thornton, *J. Geophys. Res.*, Vol. 110, No. D19, D19303, doi:10.1029/2005JD005825, 05 October 2005.

“Impact of Long-Range Dust Transport on Northern California in Spring 2002”, P. Cameron-Smith, D. Bergmann, C. Chuang, G. Bench, S. Cliff, P. Kelly, K. Perry, A. VanCuren, AMS ASAAQ2005 conference [talk], 2005.

“IMPACT, the LLNL 3-D global atmospheric chemical transport model for the combined troposphere and stratosphere: Model description and analysis of ozone and other trace gases”, Rotman, D. A.; Atherton, C. S.; Bergmann, D. J.; Cameron-Smith, P. J.; Chuang, C. C.; Connell, P. S.; Dignon, J. E.; Franz, A.; Grant, K. E.; Kinnison, D. E.; Molenkamp, C. R.; Proctor, D. D.; Tannahill, J. R.; *J. Geophys. Res.*, Vol. 109, No. D4, D04303 10.1029/2002JD003155, 18 February 2004.

**WILLIAM D. COLLINS**  
**National Center for Atmospheric Research**

**PROFESSIONAL PREPARATION:**

1988 Ph.D., Astronomy and Astrophysics, University of Chicago  
1984 M.S., Astronomy and Astrophysics, University of Chicago  
1984 B.A., Physics (cum laude) Princeton University

**APPOINTMENTS:**

2003–2005 CCSMSSC Chair, National Center for Atmospheric Research  
2001–present, Adjoint Professor, PAOS Program, University of Colorado  
2001–present Scientist III, National Center for Atmospheric Research  
1997–2001 Scientist II, National Center for Atmospheric Research

**RECENT PUBLICATIONS RELATED TO PROPOSED PROJECT**

Meehl, G. A., W. d. Collins, B. A. Boville, J. T. Kiehl, T. M. I., Wigley, and J. M. Arblaster, 2000: “Response of the NCAR Climate System Model to Increased Co<sub>2</sub> and the Role of Physical Processes,” *J. Climate*, 13, 1879-1898.

Collins, W. D., 2001: “Effects of Enhanced Shortwave Absorption on Coupled Simulations of the Tropical Climate System,” *J. Climate*, 14, 1147-1165.

Collins, W. D., P. J. Rasch, B. E. Eaton, B. V. Khatatov, J.-F. Lamarque, and C. S. Zender, 2001: “Simulating Aerosols Using Chemical Transport Model with Assimilation of Satellite Aerosol Retrievals: Methodology for INDOEX,” *J. Geophys. Res.* 106, 7313-7336.

Collins, W. D., 2001: “Parameterization of Generalized Cloud Overlap for Radiative Calculations in General Circulation Models,” *J. Atmos. Sci.*, 58, 3224-3242.

Collins, W. D., J. K. Hackney, and D. P. Edwards, 2002: “An Updated Parameterization for Infrared Emission and Adsorption by Water Vapor in the National Center for Atmospheric Research Community Atmosphere Model,” *J. Geophys. Res.*, 107, Article no. 4664, DOI: 10.1029/2001JD001365.

**SYNERGISTIC ACTIVITIES**

Chair, AMS Committee on Atmospheric Radiation, 2001-present  
Co-Chair, NCAR Atmospheric Model Working Group, 2001-2003  
Chair, NCAR/CCSM Scientific Steering Committee, 2003-2005  
Chair, Gordon Research Conference on Radiation and Climate, 2007.



**Anthony Craig**  
**National Center for Atmospheric Research**  
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**EDUCATION:**

1991 M. S., Physical Oceanography, University of Washington, Seattle, WA  
1987 M.S., Aeronautical Engineering, Massachusetts Institute of Technology, Cambridge, MA  
1985 B.S., Aerospace Engineering, University of Colorado, Boulder, CO

**PROFESSIONAL EXPERIENCE**

2004-present Software Engineer, National Center for Atmospheric Research  
2001-2004 Software Engineer IV, National Center for Atmospheric Research  
1992-2001 Software Engineer III, National Center for Atmospheric Research  
1989-1991 Research Assistant, NOAA Pacific Marine Environmental Laboratory, Seattle, WA  
1987-1988 Senior Engineer, Boeing Commercial Airplanes, Seattle, WA  
1985-1987 Research Assistant, Massachusetts Institute of Technology, Cambridge, MA

**RELATED EXPERIENCE**

2003-2004 Member, CCSM Scientific Steering Committee  
2003-2004 Member, NCAR Software Engineering Committee  
2001-2002 Member, NCAR Supercomputer RFP Committee  
2001-2003 Co-Chair, CCSM Software Engineering Working Group  
2002 Invited Speaker, Computing in the Atmospheric Sciences, Annecy, France  
2003 Invited Speaker, DoD HPC Climate Meeting, Austin, TX  
2002 Invited Speaker, DOE Conference on High Speed Computing, Salishan, OR

**PUBLICATIONS:**

P. Craig, R. Jacob, B. Kauffman, T. Bettge, J. Larson, E. Ong, C. Ding, Y. He, 2005: CPL6: "The New Extensible, High Performance Parallel Coupler for the Community Climate System Model," The International Journal for High Performance Computing Applications, 19, No. 3, 309-328.

Gent, P. R., A. P. Craig, C. M. Bitz, and J. W. Weatherly, 2001: "Parameterization Improvements in an Eddy-Permitting Ocean Model for Climate." Journal of Climate, 15, 1447-1459.

Washington, W. M., J. W. Weatherly, G. A., Meehl, A. J. Semtner, Jr., T. W. Bettge, A. P. Craig, W. G. Strand, Jr., J. M. Arblaster, V. B. Waylkand, R. Jamesx, Y. Zhang, 2000: "Parallel Climate Model (PCM) Control and Transient Simulations Climate Dynamics, 16. issue 10/11, 755-774.

Meehl, G. A., P. Gent, J. M. Arblaster, B. Otto-Bliesner, E. Brady, and A. Craig, 2000: "Factors that Affect Amplitude of El Nino in Global Coupled Climate Models," Climate Dynamic, 17, issue 7, 515-526.

Craig, A. P., L. Bullister, D. E. Harrison, R. M. Chervin, and A. J. Semtner, Jr., 1998: "A Comparison of Temperature, Salinity, and Chlorofluorocarbon with Results from a One Degree Resoltuion Three-Dimensional Global Ocean Model," Journal of Geophysical Research, 103, C1.

**John B. Drake**  
**Climate Dynamics**  
**Oak Ridge National Laboratory**  
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## EDUCATION

1991 Ph.D, Mathematics, University of Tennessee  
1979 M.S., Mathematics, Purdue University  
1977 B. S., Mathematics, University of Kentucky

## APPOINTMENTS

1999 – present Climate Dynamics Group (leader), Computer Science and Mathematics Division, Oak Ridge National Laboratory  
1984 – 1999 Mathematics Group, Computer Science and Mathematics Division, Oak Ridge National Laboratory  
1979 – 1984 Engineering Mechanics Section, Technical Applications Department, Computer Science Division, Lockheed Martin Energy Systems

## PUBLICATIONS

“A Standard Test Set for Numerical Approximations to the Shallow Water Equations on the Sphere,” D.L. Williamson, J.B. Drake, J.J. Hack, R. Jakob, and P.N. Swarztrauber, *J. Comp. Phys.* Vol. 102 (1992), pp. 211-224.

“Design and Performance of a Scalable Parallel Community Climate Model,” J.B. Drake, I.T. Foster, J.G. Michalakes, B. Toonen, and P.H. Worley, *Parallel Computing*, Vol. 21 (1995), pp. 1571-1591.

“Parallel Algorithms for Semi-Lagrangian Transport in Global Atmospheric Circulation Models,” J.B. Drake, I.T. Foster, J.G. Michalakes, and P.H. Worley, in *Parallel Processing for Scientific Computing*, SIAM, pp. 119-124, February 1995.

“The Cartesian Method for Solving Partial Differential Equations in Spherical Geometry,” P.N. Swarztrauber, D.L. Williamson, J.B. Drake, *Dynamics of Oceans and Atmospheres*, Vol. 27 (1997), pp. 6779-706.

“Performance Tuning and Evaluation of a Parallel Community Climate Model,” J.B. Drake, S. Hammond, R. James, and P.W. Worley, in *Proc. of IEEE SC99*, Portland, OR, November 1999.

“Statistical Downscaling of the United States Regional Climate from Transient GCM Scenarios,” W.M. Putman, J.B. Drake, and G. Ostrouchov, in *Proc. of AMS 12th Conf. on Applied Climatology*, May 2000.

“A Global Semi-Lagrangian Spectral Model for the Shallow Water Equations with Variable Resolution,” D.X. Guo and J.B. Drake, *J. Comp. Phys.*, Vol. 206 (2005), pp. 559-577.

“Overview of the Software Design and Parallel Algorithms of the CCSM,” J.B. Drake, P.W. Jones, G.R. Carr, *Int. J. High Perf. Comput. Appl.*, to appear 2005

“Software Design for Performance Portability in the Community Atmosphere Model,” P.H. Worley, J.B. Drake, *Int. J. High Perf. Comput. Appl.*, to appear 2005

## SYNERGISTIC ACTIVITIES

Organizing committee (and host) of PDE's on the Sphere workshop series, 1991-present.  
Organizing committee SIAM Computational Science and Engineering conference, 2003.  
Member CCSM Advisory Board, 2003-present.  
Member DOE Climate Change Prediction Program Advisory Committee, 2003-present.  
Guest editor, International Journal on High Performance Computing and Applications.

#### Collaborators & Other Affiliations

As PI of the SciDAC CCSM Consortium project, my collaborators include researchers in the NCAR Climate Global Dynamics Division and the Department of Energy Laboratories of Los Alamos National Laboratory, Argonne National Laboratory, Lawrence Livermore National Laboratory, Berkeley National Laboratory and Pacific Northwest National Laboratory. I have no other affiliations than Oak Ridge National Laboratory which is managed by the U.T. - Battelle Corporation.

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**Climate Dynamics**  
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## **EDUCATION**

- 1987 Ph.D. (Chemical Oceanography/Atmospheric Chemistry)  
Graduate School of Oceanography  
University of Rhode Island  
Narragansett, Rhode Island
- 1982 B. S. (Chemistry)  
The College of William and Mary  
Williamsburg, Virginia

## **APPOINTMENTS**

- 2000 - present Senior Research Staff Member  
Director, Climate and Carbon Research Institute  
Computer Science and Mathematics Division  
Oak Ridge National Laboratory  
Oak Ridge, Tennessee
- 2003 - present Adjunct Professor  
Division of Earth and Ocean Sciences  
Nicholas School of the Environment and Earth Sciences  
Duke University  
Durham, North Carolina
- 1990 - 1999 Scientist  
National Center for Atmospheric Research  
Boulder, Colorado
- 1987 - 1990 Post-doctoral Research Fellow  
Scripps Institution of Oceanography  
University of California, San Diego  
La Jolla, California

## **PUBLICATIONS**

- Erickson, D. J. III, 'Variations in the global air-sea transfer velocity field of CO<sub>2</sub>', Global Biogeochem. Cycles, 3, 37-41, 1989.
- Erickson, D. J. III, 'A stability dependent theory for air-sea gas exchange', J. Geophys. Res., 98, 8471-8488, 1993.
- Erickson, D. J. III, P. J. Rasch, P. P. Tans, P. Friedlingstein, P. Ciais, E. Maier-Reimer, K. Kurz, C. A. Fischer and S. Walters,  
"The seasonal cycle of atmospheric CO<sub>2</sub>: A study based on the NCAR Community Climate Model (CCM2)," J. Geophys. Res., 101, 15079-15097, 1996.
- Meehl, G. A., W. Washington, D. J. Erickson III, B. P. Briegleb and P. Jaumann, "Climate change from increased CO<sub>2</sub> and the direct and indirect effects of sulfate aerosols," Geophys. Res. Lett., 23, 3755-3758, 1996.
- Erickson, D. J. III, R. Zepp and E. Atlas, "Ozone depletion and the air-sea exchange of greenhouse and climate reactive gases," Chemosphere - Global Change Science, 137-149, 2000.

**Scott Elliott**  
**CCS Division, COSIM Team**  
**Los Alamos National Laboratory**  
[sme@lanl.gov](mailto:sme@lanl.gov)

**SELECTED PROFESSIONAL EXPERIENCE AND EDUCATION**

2004-present Extensive visitation/collaboration with the Computer Science Division, Climate Group, ORNL.  
2002-present Biogeochemistry specialist; Climate Ocean Sea Ice Modeling (COSIM), LANL.  
2000-present Visiting Scientist, Community Climate System Model (CCSM) group, NCAR, Boulder, CO.  
1993-present Technical Staff Member, EES and CCS Divisions, Los Alamos National Laboratory.  
1992-1993 University of California INCOR Fellow; IGPP, Los Alamos National Laboratory.  
1989-1991 Research Scientist, Department of Atmospheric Sciences, UCLA.  
1986-1988 Post-doctoral Research in Atmospheric and Marine Chemistry; University of California Irvine.  
1984-1986 Visiting Scientist, Atmospheric Chemistry Division, the KFA at Julich, (former) West Germany.  
1975-1984 B.S. and Ph.D. in Physical Chemistry; University of California (San Diego, Irvine campuses).

**SELECTED RECENT PUBLICATIONS**

Elliott, S., "Marine Systems Simulation in the Anthropocene," *The Scientific World*, submitted, 2005.

Elliott, S., S. Chu, and D. J. Erickson, "TRACEGAS\_MOD: Processing for Low Concentration Volatiles in the Community Climate System Model Ocean," *Environmental Modeling & Software*, submitted, 2005.

Elliott, S., S. Chu, and D. J. Erickson, "Contours of Simulated Marine Dimethyl Sulfide Distributions Under Variation in a Gabcic Mechanism," *Environmental Modeling & Software*, in press, 2005.

Chu, S., S. Elliott, M. Maltrud, and A. McPherson, "Animation of Global Marine Chlorophyll Distributions from Fine Grid Biogeochemistry/Transport Modeling," *ESEC Volume 2, FiatLux: Chapter 9*, 2004.

Chu, S., S. Elliott, M. Maltrud, and F. Chai, "Iron Patch Enrichments in the Southern Ocean of a Global Eddy Permitting General Circulation Model," *ESEC Volume 2, FiatLux: Chapter 8*, 2004.

**INEZ Y. FUNG**  
**Berkeley Atmospheric Sciences Center**  
**University of California, Berkeley**  
**Berkeley, CA 94720-4767**  
**Telephone: (510) 643 9367 FAX: (510) 643 9377**  
**Email: [ifung@berkeley.edu](mailto:ifung@berkeley.edu)**

**Education:**

1971: S.B. (Applied Mathematics), Massachusetts Institute of Technology

1977: Sc.D. (Meteorology), Massachusetts Institute of Technology

**Professional Employment:**

1998-: University of California, Berkeley

Professor, Department of Earth and Planetary Science,

Department of Environmental Science, Policy and Management

Richard and Rhoda Goldman Distinguished Professor for the Physical Sciences, 1997-2002

1998-2005: Director, Berkeley Atmospheric Sciences Center

2005-: Director, Berkeley Institute of the Environment

**Synergistic Activities Relevant to this Proposal**

2000-2004: Member, Scientific Steering Committee, US Interagency Carbon Cycle Program; 1998-2004 co-Chair (with S.C. Doney), Biogeochemistry Working Group (BGC WG), NCAR Community Climate System Model; 2005-co-Lead (with J. Randerson), Diagnostic Team for CCSM BGC WG; 2006: Organizer, Summer Graduate Workshop on Carbon Data Assimilation (at Mathematical Sciences Research Institute, Berkeley, CA).

**Selected Publications:**

Fung, I., S.C. Doney, K. Lindsay, and J. John (2005). Evolution of carbon sinks in a changing climate. Proc. Nat. Acad. Sci. (USA), 102, 11201-11206.

Doney, S.C., K. Lindsay, I. Fung and J. John (2005). Natural Variability in a Stable, 1000 Year Global Coupled Climate-Carbon Cycle Simulation. J Climate, in press.

Friedlingstein, P., P. Cox, R. Betts, L. Bopp, W. von Bloh, V. Brovkin, S. Doney, M. Eby, I. Fung, B. Govindasamy, J. John, C. Jones, F. Joos, T. Kato, M. Kawamiya, W. Knorr, K. Lindsay, H. D. Matthews, T. Raddatz, P. Rayner, C. Reick, E. Roeckner, K.-G. Schnitzler, R. Schnur, K. Strassmann, S. Thompson, A. J. Weaver, C. Yoshikawa, and N. Zeng. Climate-carbon cycle feedback analysis, results from the C<sup>4</sup>MIP model intercomparison. J. Climate (in press).

Lee, J.-E., R. Oliviera, T. Dawson and I. Fung (2005). Root functioning modifies seasonal climate. Proc. Nat. Acad. Sci.(USA), 102, 17576-17581.

Angert, A., Sebastien Biraud, Celine Bonfils, Cara Henning, Wolfgang Buermann, Jorge Pinzon, Compton Tucker, Inez Fung (2005). Drier summers cancel out the CO<sub>2</sub> uptake enhancement induced by warmer springs. Proc. Nat. Acad. Sci. (USA), 102, 10823-10827.

**PETER ROBERT GENT**  
**National Center for Atmospheric Research**

**Academic Experience**

1967–1970	First Class Honours Degree in Mathematics, University of Bristol.
1970–1971	M.Sc. (with Commendation) in Fluid Dynamics, Department of Mathematics, University of Bristol.
Dec. 1971–1973	Ph.D. in Fluid Dynamics; Department of Mathematics, University of Bristol, with supervisor Dr. P. G. Drazin. Thesis Title, “Baroclinic Instability of Slowly Varying Flows.”
Oct. 1973–June 1976	Research Fellow in the Department of Oceanography, University of Southampton.
Sept. 1976–June 1979	Visiting Scientist to the Oceanography Project, National Center for Atmospheric Research, Boulder, Colorado.
July 1979–June 1983	Scientist II with the Oceanography Section, National Center for Atmospheric Research, Boulder, Colorado.
July 1983–June 1990	Scientist III with the Oceanography Section, National Center for Atmospheric Research, Boulder, Colorado.
July 1990–Present	Senior Scientist with the Oceanography Section, National Center for Atmospheric Research, Boulder, Colorado.
Jan. 1994–June 2005	Head of the Oceanography Section, CGD, National Center for Atmospheric Research, Boulder, Colorado.
Sept.–Oct. 1996	Visiting Scientist at the Isaac Newton Institute for Mathematical Sciences at the University of Cambridge, England.
Jan.–Feb. 2003	Distinguished Frohlich Visiting Scholar at the CSIRO Division of Oceanography, Hobart, Australia.
July 2005–Present	Chairman of the Science Steering Committee of the Community Climate System Model.

**Recent Refereed Publications**

Danabasoglu, G., J. C. McWilliams, and P. R. Gent, 1994: The role of mesoscale tracer transports in the global ocean circulation. *Science*, 264, 1123–1126.

Gent, P. R., J. Willebrand, T. J. McDougall, and J. C. McWilliams, 1995: Parameterizing eddy-induced tracer transports in ocean circulation models. *J. Phys. Oceanogr.*, 25, 463–474.

Gent, P. R., and J. C. McWilliams, 1996: Eliassen-Palm fluxes and the momentum equation in non-eddy-resolving ocean circulation models. *J. Phys. Oceanogr.*, 26, 2539-2546. Boville, B. A., and P. R. Gent, 1998: The NCAR climate system model, version one. *J. Climate*, 11, 1115-1130.

Gent, P. R., F. O. Bryan, G. Danabasoglu, S. C. Doney, W. R. Holland, W. G. Large and J. C. McWilliams, 1998: The NCAR climate system model global ocean component. *J. Climate*, 11, 1287-1306.

Large, W. G., and P. R. Gent, 1999: Validation of vertical mixing in an equatorial ocean model using large eddy simulations and observations. *J. Phys. Oceanogr.*, 29, 449464.

- Wainer, I., P. R. Gent and G. Goni, 2000: Annual cycle of the Brazil-Malvinas confluence region in the National Center for Atmospheric Research Climate System Model. *J. Geophys. Res.*, 105, 26,167-26,177.
- Gent, P. R., W. G. Large and F. O. Bryan, 2001: What sets the mean transport through Drake Passage? *J. Geophys. Res.*, 106, 2693-2712.
- Large, W. G., G. Danabasoglu, J. C. McWilliams, P. R. Gent and F. O. Bryan, 2001: Equatorial circulation of a global ocean climate model with anisotropic horizontal viscosity. *J. Phys. Oceanogr.*, 31, 518-536.
- Gent, P. R., 2001: Will the North Atlantic Ocean thermohaline circulation weaken during the 21st century? *Geophys. Res. Lett.*, 28, 1023-1026.
- Meehl, G. A., P. R. Gent, J. M. Arblaster, B. Otto-Bliesner, E. Brady and A. Craig, 2001: Factors that affect the amplitude of El Nino in global coupled climate models. *Clim. Dyn.*, 17, 515-526.
- Gent, P. R., 2001: Parameterizing eddies in ocean climate models. Proceedings of the IUTAM Symposium on Advances in Mathematical Modelling of Atmosphere and Ocean Dynamics, 19-30, Kluwer Academic Publishers, Dordrecht.
- Gent, P. R., A. P. Craig, C. M. Bitz and J. W. Weatherly, 2002: Parameterization improvements in an eddy-permitting ocean model for climate. *J. Climate*, 15, 1447-1459.
- Kiehl, J. T. and P. R. Gent, 2004. The Community Climate System Model, version 2. *J. Climate*, 17, 3666–3682.
- Gent, P. R. and G. Danabasoglu, 2004. Heat uptake and the thermohaline circulation in the Community Climate System Model, version 2. *J. Climate*, 17, 4058–4069.
- Smith, R. D. and P. R. Gent, 2004. Anisotropic Gent-McWilliams parameterization for ocean models. *J. Phys. Oceanogr.*, 34, 2541–2564. July 2005



**Steven J. Ghan**  
**Pacific Northwest National Laboratory**

**Primary Research Interests:**

Cloud-aerosol interactions, cloud microphysics parameterization, aerosol-climate interactions, chemistry-climate interactions, global and regional climate modeling, subgrid orography parameterization

**Career Highlights:**

- Ph.D. in Meteorology, Massachusetts Institute of Technology, 1988.
- Atmospheric Scientist, Lawrence Livermore National Laboratory, 1984 – 1990.
- Atmospheric Scientist, Pacific Northwest National Laboratory, 1990 – present.
- Affiliate Professor, University of Washington, 1994 – 2005.
- Principal Investigator:
  - DOE Atmospheric Radiation Measurement program, 1991 – present
  - NASA Aerosol Interdisciplinary Science Program, 1993 – 1997
  - NASA EOS Interdisciplinary Science program, 1997 – 2003
  - DOE Climate Change Prediction Program, 1999 – 2001
  - DOE Atmospheric Science Program, 2004 – present
- Co-Investigator, DOE Scientific Discovery through Advanced Computing: Climate Change Prediction Program, 2001 - present
- Showed that cloud microphysics parameterizations developed for cloud-resolving models can be easily adapted for stratiform clouds in GCMs.
- Developed an aerosol activation parameterization based on Kohler theory and log-normal aerosol size distribution.
- Introduced droplet number as a prognostic variable in a global model.
- Co-developed a parameterization of the subgrid influence of orography on clouds, precipitation, and land surface processes.
- Used the orography parameterization in a regional model to estimate a 30-70% reduction in Cascade snowpack in response to doubled CO<sub>2</sub>.
- Applied the orography parameterization to a global circulation model.
- Contributing author, *Climate Change 1995*, Contribution of Working Group I to the Second Assessment Report of the Intergovernmental Panel on Climate Change.
- Contributing author, Chapters 5 and 6, *Climate Change 2001: The Scientific Basis*, Contribution of Working Group I to the Third Assessment Report of the Intergovernmental Panel on Climate Change.
- Steering committee, DOE Atmospheric Radiation Measurement Cloud Parameterization and Modeling working group, 1999 – 2004.
- Advisory panel, NSF Climate Process Team, 2003 – present.
- Leadership Team, DOE Atmospheric Science Program, 2004 – present
- Science Steering Committee, DOE Atmospheric Science Program, 2005 – present.
- Scientific Steering Committee, NCAR Community Climate System Model, 2006 – present.

## Journal Publications (of 69):

- Ghan, S. J., L. R. Leung, R. C. Easter, and H. Abdul-Razzak, 1997: Prediction of droplet number in a general circulation model. *J. Geophys. Res.*, *102*, 21,777-21,794.
- Abdul-Razzak, H., and S. J. Ghan, 2000: A parameterization of aerosol activation. Part 2: Multiple aerosol types. *J. Geophys. Res.*, *105*, 6837-6844.
- Ghan, S., N. Laulainen, R. Easter, R. Wagener, S. Nemesure, E. Chapman, Y. Zhang, and R. Leung, 2001: Evaluation of aerosol direct radiative forcing in MIRAGE, *J. Geophys. Res.*, *106*, 5295-5316.
- Ghan, S. J., R. C. Easter, J. Hudson, and F.-M. Breon, 2001: Evaluation of aerosol indirect radiative forcing in MIRAGE, *J. Geophys. Res.*, *106*, 5317-5334.
- Ghan, S. J., R. C. Easter, E. Chapman, H. Abdul-Razzak, Y. Zhang, R. Leung, N. Laulainen, R. Saylor and R. Zaveri, 2001: A physically-based estimate of radiative forcing by anthropogenic sulfate aerosol, *J. Geophys. Res.*, *106*, 5279-5294.
- Ghan, S. J., X. Bian, A. G. Hunt, and A. Coleman, 2002: The thermodynamic influence of subgrid orography in a global climate model, *Climate Dynamics*, *20*, 31-44, DOI: 10.1007/s00382-002-0257-5.
- Zhang, Y., R.C. Easter, S. J. Ghan, and H. Abdul-Razzak, 2002: Impact of aerosol size representation on modeling aerosol-cloud interactions, *J. Geophys. Res.*, *107*, 4558, 10.1029/2001JD001549.
- Easter, R. C., S. J. Ghan, Y. Zhang, R. D. Saylor, E. G. Chapman, N. S. Laulainen, H. Abdul-Razzak, L. R. Leung, X. Bian and R. A. Zaveri, 2004: MIRAGE: Model description and evaluation of aerosols and trace gases, *J. Geophys. Res.*, *109*, doi: 10.1029/2004JD004571.
- Ghan, S. J., and T. Shippert, 2005: Load balancing and scalability of a subgrid orography scheme in a global climate model. *Int. J. High Performance Comput. Appl.*, *19*, 237-245.
- Ghan, S. J., T. Shippert, and J. Fox, 2005: Physically-based global downscaling: Regional evaluation. *J. Climate*, in press.
- Ghan, S. J., and T. Shippert, 2005: Physically-based global downscaling: Climate change projections for a full century. *J. Climate*, in press.
- Kinne, S., M. Schulz, C. Textor, S. Guibert, Y. Balkanski, S. Bauer, T. Berntsen, T. Berglen, O. Boucher, M. Chin, W. Collins, F. Dentener, T. Diehl, R. Easter, H. Feichter, D. Fillmore, S. Ghan, P. Ginoux, S. Gong, A. Grini, J. Hendricks, M. Herzog, L. Horowitz, I. Isaksen, T. Iversen, A. Jones, S. Kloster, D. Koch, M. Krool, A. Lauer, J. F. Lamarque, G. Lesins, X. Liu, U. Lohmann, V. Montanaro, G. Myhre, J. Penner, G. Pitari, S. Reddy, D. Roberts, O. Seland, P. Stier, T. Takemura, X. Tie, 2005: An AeroCom initial assessment – optical properties in aerosol component modules of global models. *Atmos. Chem. & Phys. Discuss*, *5*, 8285–8330.

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**Education**

University of Texas at Austin, B.Sc. Physics, 1990  
University of Texas at Austin, B.Sc. Mathematics, 1990  
University of Wisconsin-Madison, Ph.D. Atmospheric Science, 1997

**Professional Experience**

Computational Scientist, Mathematics and Computer Science Division, 2005 —  
Assistant Computational Scientist, Argonne National Laboratory, 2000-2005  
Research Associate, Department of the Geophysical Sciences, University of Chicago, 1999-2000  
Research Associate, Space Science and Engineering Center, University of Wisconsin, 1998-1999  
Research Assistant, Space Science and Engineering Center, University of Wisconsin, 1991-1997

**Honors and Awards**

American Meteorological Society/Cray Research Graduate Fellowship, 1991

**Collaborations and Other Affiliations**

Fellow, Computation Institute, University of Chicago/Argonne, 2001—  
Honorary Fellow, Center for Climatic Research, University of Wisconsin, 2000 —

**Memberships**

American Geophysical Union

**Areas of Technical Specialization**

Dr. Jacob's scientific interests are in the area of low frequency variability in the climate system, paleoclimate, ocean modeling and the software engineering of climate models.

**Recent Publications**

Jacob, R., J. Larson, and E. Ong, 2005: "MxN Communication and Parallel Interpolation in CCSM3 Using the Model Coupling Toolkit". *Int. J. High Perf. Comp. App.* **19(3)**, 293-307.

Larson, J., R. Jacob, and E. Ong, 2005: "The Model Coupling Toolkit: A New Fortran90 Toolkit for Building Multi-Physics Parallel Coupled Models", *Int. J. High Perf. Comp. App.*, **19(3)**, 277-292.

Craig, T., R. Jacob, B. Kauffman, T. Bettge, J. Larson, E. Ong, C. Ding, H. Ye: 2005: "Cpl6: The New Extensible High-Performance Parallel Coupler for the Community Climate System Model", *Int. J. High Perf. Comp. App.*, **19(3)**, 309-327.

Gallimore, R., J. E. Kutzbach, R. L. Jacob, 2005: "Coupled Atmosphere-Ocean-Vegetation Simulations for Modern and Mid-Holocene Climates: Role of Extratropical Vegetation Cover Feedbacks", *Climate Dynamics*, **25**, 755-756, doi: 10.1007/s00382-005-0054-z.

Notaro, M., Z. Liu, R. Gallimore, S. J. Vavrus, J. E. Kutzbach, I. C. Prentice, R. L. Jacob, 2005: "Simulated and Observed Pre-Industrial to Modern Vegetation and Climate Changes", *J. Climate*, **18**, 3650-3671

C. Poulsen and R. Jacob 2004: "Factors that inhibit Snowball Earth simulation", *Paleoceanography*, **19**, PA4021, doi:10.1029/2004PA001056.

J. Lewis, M. Eby, A. Weaver, S. Johnson, R. Jacob 2004: "Global glaciation in the Neoproterozoic: Reconciling previous modeling results?", *Geophys. Res. Lett.*, 31(8), L08201.

**Philip W. Jones**  
**Theoretical Fluid Dynamics Group**  
**Los Alamos National Laboratory**  
**T-3, MS B216, PO Box 1663**  
**Los Alamos, NM 87545-1663**  
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## **PROFESSIONAL EXPERIENCE**

2003 – present: Project Leader, Climate, Ocean and Sea Ice Modeling, Los Alamos National Laboratory  
1993 – present : Technical Staff Member, Theoretical Division (T-3), Los Alamos National Laboratory  
1991 – 1993: Postdoctoral Research Assoc., Earth and Environmental Sciences Division, Los Alamos National Laboratory

## **EDUCATION**

Ph.D. 1991, Astrophysical, Planetary and Atmospheric Sciences, University of Colorado, Boulder, CO  
B.S. 1985, Physics and Mathematics with distinction, Iowa State University, Ames, IA

## **TECHNICAL ACTIVITIES**

Project leader for Climate, Ocean and Sea Ice Modeling project at LANL, managing model development of the POP, HYPOP, and CICE models and applications of these models to climate and ocean problems.

Lead software developer for the Parallel Ocean Program (POP) and Hybrid Coordinate Parallel Ocean Program (HYPOP). Responsible for computational performance of models, software engineering, documentation and user support.

Developer of Spherical Coordinate Remapping and Interpolation Package (SCRIP), providing conservative and other regridding methods to the coupled climate community. Also responsible for incorporating this functionality within Earth System Modeling Framework (ESMF).

## **HONORS AND AWARDS**

LANL Teamwork Award, 2001.

## **PROFESSIONAL MEMBERSHIPS**

Member, American Geophysical Union  
Member, American Meteorological Society

## **EDITORIALS AND COMMITTEES**

Guest editor: International Journal of High Performance Computing and Application, special issue on the Community Climate System Model.

Review committee: 2005 Lehman review of Oak Ridge National Lab. Leadership Computing Facility

DOE Climate Change Prediction Program Advisory Committee, 2004-present

## **SELECTED RELEVANT PUBLICATIONS**

Drake, J.B., P.W. Jones, G.R. Carr Jr., 2005, Overview of the Software Design of the Community Climate System Model, *Int. Journ. High Perf. Comput. Application*, **19**, 177-186.

- Kerbyson, D.J. and P.W. Jones, 2005, A Performance Model of the Parallel Ocean Program, *Int. Journ. High Perf. Comput. Application*, **19**, 261-276.
- Jones, P.W., Worley, P.H., Yoshida, Y., White, J.B. III, Levesque, J., 2005: Practical Performance Portability in the Parallel Ocean Program (POP), *Concurrency Comput. Prac. Exper.*, **17**, 1317.
- Randall, D.A., Ringler, T.D., Heikes, R.P., Jones, P. and Baumgardner, J., 2002: Climate Modeling with Spherical Geodesic Grids, *Computing in Science Eng.*, **4**, 32-41.
- Jones, P.W., 1999: First- and Second-order Conservative Remapping Schemes for Grids in Spherical Coordinates, *Mon. Weath. Rev.*, **127**, 2204-2210.
- Jones, P.W., Malone, R.C. and Lai, C.A., 1998: The Los Alamos Coupled Model, *Proceedings of the Second International Workshop on Software Engineering and Code Design in Parallel Meteorological and Oceanographic Applications*, ed. M. O'Keefe and C. Kerr, NASA Publication GSFC/CP-1998-206860.
- Jones, P.W., 1998: The Los Alamos Parallel Ocean Program (POP) and Coupled Model on MPP and Clustered SMP Computers, *Making its Mark: Proceedings of the 7th ECMWF Workshop on the Use of Parallel Processors in Meteorology*, ed. G. R. Hoffmann and N. Kreitz (Singapore: World Scientific Publishing).
- Hayashi, Y., Golder, D.G. and Jones, P.W., 1997: Tropical Gravity Waves Simulated by High-Resolution SKYHI General Circulation Models, *J. Meteor. Soc. Japan*, **75**, 1125-1139.
- Jones, P.W., Hamilton, K.P. and Wilson, R.J., 1996: A Very High-Resolution General Circulation Model Simulation of the Global Circulation in Austral Winter, *J. Atm. Sci.*, **54**, 1107-1116.
- Jones, P.W., Kerr, C.L. and Hemler, R.S., 1995: Practical Considerations in Development of a Parallel SKYHI General Circulation Model, *Parallel Computing*, **21**, 1677-1694.

**Jean-François Lamarque**  
**National Center for Atmospheric Research**  
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**Boulder, CO 80307**  
**email: lamar@ucar.edu**

## Education

Catholic University of Louvain, 1987, Licence en Sciences Physiques (highest honors).  
Catholic University of Louvain, 1988, Maîtrise en Sciences Physiques (highest honors).  
Catholic University of Louvain, 2003, Doctorat en Sciences Physiques (highest honors).

## Positions Held

2004-Present *Scientist II*, National Center for Atmospheric Research, Boulder, CO  
2002-2004 *Scientist I*, National Center for Atmospheric Research, Boulder, CO  
1997-2002 *Project Scientist I (research area: data assimilation)*, National Center for Atmospheric Research, Boulder, CO  
1995-1997 *Visiting Scientist (research area: stratosphere-troposphere exchange)*, National Center for Atmospheric Research, Boulder, CO  
1993-1995 *Postdoctoral fellow, Advanced Study Program*, National Center for Atmospheric Research, Boulder, CO  
1990-1993 *Graduate Research Assistant, Advanced Study Program*, National Center for Atmospheric Research, Boulder, CO  
1987-1990 *Research Assistant*, Catholic University of Louvain, Belgium

## Five Publications related to this proposal

1. Gauss, M., G. Myhre, I. S. A. Isaksen, W. J. Collins, F. J. Dentener, K. Ellingsen, L. K. Gohar, V. Grewe, D. A. Hauglustaine, D. Iachetti, J.-F. Lamarque, E. Mancini, L. J. Mickley, G. Pitari, M. J. Prather, J. A. Pyle, M. G. Sanderson, K. P. Shine, D. S. Stevenson, K. Sudo, S. Szopa, O. Wild, G. Zeng, Radiative forcing since preindustrial times due to ozone change in the troposphere and the lower stratosphere. *Atmos. Chem. Phys.*, 6, 575-599, 2006.
2. Stevenson, D.S., F.J. Dentener, M.G. Schultz, K. Ellingsen, T. P.C. van Noije, O. Wild, G. Zeng, M. Amann, C.S. Atherton, N. Bell, D.J. Bergmann, I. Bey, T. Butler, J. Cofala, W.J. Collins, R.G. Derwent, R.M. Doherty, J. Drevet, H.J. Eskes, A.M. Fiore, M. Gauss, D.A. Hauglustaine, L.W. Horowitz, I.S.A. Isaksen, M.C. Krol, J.-F. Lamarque, M.G. Lawrence, V. Montanaro, J.-F. Müller, G. Pitari, M.J. Prather, J.A. Pyle, S. Rast, J.M. Rodriguez, M.G. Sanderson, N.H. Savage, D.T. Shindell, S.E. Strahan, K. Sudo, and S. Szopa, Multi-model ensemble simulations of present-day and near-future tropospheric ozone. Accepted for publication in *J. Geophys. Res.*, 2005.
3. Lamarque, J.-F., J. T. Kiehl, P. G. Hess, W. D. Collins, L. K. Emmons, P. Ginoux, C. Luo, and X. X. Tie, Response of a coupled chemistry-climate model to changes in aerosol emissions: Global impact on the hydrological cycle and the tropospheric burdens of OH, ozone and NO<sub>x</sub>. *Geophys. Res. Lett.*, Vol. 32, No. 16, L16809, 2005.
4. Lamarque, J.-F., J. Kiehl, G. Brasseur, T. Butler, P. Cameron-Smith, W. D. Collins, W. J. Collins, C. Granier, D. Hauglustaine, P. Hess, E. Holland, L. Horowitz, M. Lawrence, D. McKenna, P. Merilees, M. Prather, P. Rasch, D. Rotman, D. Shindell and P. Thornton, Assessing future nitrogen deposition and carbon cycle feedback using a multi-model approach. Analysis of nitrogen deposition. *J. Geophys. Res.*, 110, D19303, doi:10.1029/2005JD005825, 2005.
5. Lamarque, J.-F., P. Hess, L. Emmons, L. Buja, W. Washington and C. Granier, Tropospheric ozone evolution between 1890 and 1990. *J. Geophys. Res.*, 110, No. D8, D08304, doi:10.1029/2004JD005537, 2005.

**William H. Lipscomb**  
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**EDUCATION**

1998 Ph.D., Atmospheric Sciences, University of Washington, Seattle, WA  
1990 M.A., Physics and Philosophy, Oxford University, Oxford, England  
1987 B.S., Physics, Duke University, Durham, NC

**EMPLOYMENT**

2001-present Technical staff member, Los Alamos National Laboratory, Theoretical Division,  
Fluid Dynamics Group

1998-2001 Postdoctoral research associate, Los Alamos National Laboratory

1992-1998 Ph.D. candidate, Department of Atmospheric Sciences, University of Washington

1991-1992 Research assistant, National Research Council, Board on Environmental Studies and Toxicology

**SELECTED PUBLICATIONS**

Lipscomb, W.H., E. C. Hunke, W. Maslowski, and J. Jakacki, "Improving Ridging Schemes for High-Resolution Sea Ice Models," J. Geophys. Res., accepted, 2006.

Lipscomb, W. H., and T. D. Ringer, "An Incremental Remapping Transport Scheme on a Spherical Geodesic Grid," Mon. Wea. Rev., 133, 2335-2350, 2005.

Lipscomb, W. H., and E. C. Hunke, "Modeling Sea Ice Transport Using Incremental Remapping," Mon. Wea. Rev., 132, 1341-1354, 2004.

Hunke, E. C., and W. H. Lipscomb, "CICE: The Los Alamos Sea Ice Model, Documentation and Software, version 3.1," Technical Report LA-CC-98-16, Los Alamos National Laboratory, Los Alamos, NM, 2004.

Maslowski, W., and W. H. Lipscomb, "High-Resolution Simulations of Arctic Sea Ice During 1979-1993," Polar Research, 22, 67-74, 2003.

Lipscomb, W. H., "Remapping the Thickness Distribution in Sea Ice Models," J. Geophys. Res., 106, 13,989-14,000, 2001.

Bitz, C. M., and W. H. Lipscomb, "An Energy-Conserving Thermodynamic Model of Sea Ice, J. Geophys. Res., 104, 15,669-15,677, 1999.

**HONORS AND AWARDS**

Editor's Award, Journal of Climate, American Meteorological Society, 2003.  
NASA Global Change Fellow, 1994-1996  
National Science Foundation Graduate Fellow, 1992-1994.  
Achievement Rewards for College Scientists (ARCS) Fellow, 1992-1995.  
Rhodes Scholar, Oxford University, 1987-1990.

**Mathew E. Maltrud**  
**Fluid Dynamics Group (T-3), MS B216**  
**Los Alamos National Laboratory**  
**Los Alamos, NM 87545**  
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### **CURRENT POSITION**

Technical Staff Member in the Theoretical Division at Los Alamos National Laboratory. Member of LANL's Climate, Ocean and Sea Ice Modeling (COSIM) project.

### **RESEARCH INTERESTS**

High resolution ocean and climate modeling with emphasis on model/data comparison.  
Representation of water mass formation and transport processes in ocean models.  
Marine ecosystem and biogeochemical simulations within ocean and climate models.  
High performance computing issues related to ocean and climate modeling.

### **EDUCATION**

March, 1992 Ph.D. in Oceanography from Scripps Institution of Oceanography/University of California, San Diego.  
June 1984 B.S. degree in Applied Physics (with Highest Honors) from University of California, Davis.

### **SELECTED PUBLICATIONS**

S. Peacock and M. E. Maltrud, "Transit-time distributions in a global ocean model", *Journal of Physical Oceanography*, in press.

S. Peacock, M. Maltrud and R. Bleck, "Putting models to the data test: A case study using Indian Ocean CFC-11 data", *Ocean Modelling*, 9, pp. 1-22, 2005.

M. E. Maltrud and J. L. McClean, "An eddy resolving global 1/10 degrees ocean simulation", *Ocean Modelling*, 8, pp. 31-54, 2005.

D. J. McGillicuddy, L. A. Anderson, S.C Doney, and M. E. Maltrud, "Eddy-driven sources and sinks of nutrients in the upper ocean: results from a 0.1 degree resolution model of the North Atlantic", *Global Biogeochemical Cycles*, 17, pp. 1035-1054, 2003.

A. M. Treguier, N. G. Hogg, M. Maltrud, K. Speer, and V. Thierry, "On the origin of deep zonal flows in the Brazil Basin", *Journal of Physical Oceanography*, 33, pp. 580-599, 2003.

S. Chu, S. M. Elliott, and M. E. Maltrud, "Global eddy permitting simulations of surface ocean nitrogen, iron, sulfur cycling", *Chemosphere*, 50, pp. 223-235, 2003.



**Robert L. McGraw**  
**Atmospheric Sciences Division**  
**Brookhaven National Laboratory**  
**Upton, NY 11973**  
**e-mail: [rlm@bnl.gov](mailto:rlm@bnl.gov)**

**EDUCATION**

1979 Ph.D. Physical Chemistry, University of Chicago.  
1974 M.S. Chemistry, University of Chicago.  
1972 B.S. Chemistry, Drexel University, Philadelphia, PA

**EMPLOYMENT**

2005 - Deputy Division Head, Atmospheric Sciences Division, Brookhaven National Laboratory  
2003 - Senior Scientist, Brookhaven National Laboratory  
1998 -2003 Member Brookhaven Council (Council Secretary 2001-2003)  
1993 -2003 Scientist, Brookhaven National Laboratory  
(Tenured from 1995)  
1985 -1993 Member Technical Staff, Rockwell International Science Center,  
Thousand Oaks, CA  
1990 -1993 Member Scientific Advisory Board, Rockwell International North American Aircraft Division (now part  
of Boeing)  
1983 -1985 Associate Scientist, Brookhaven National Laboratory  
1981 -1983 Assistant Scientist, Brookhaven National Laboratory  
1977 -1981 Postdoctoral Research Associate, Chemistry Department, University of California  
Los Angeles

**RESEARCH ACTIVITIES/INTERESTS**

Atmospheric aerosol microphysics and simulation methods; Homogeneous and heterogeneous nucleation of supercooled vapors and vapor mixtures as mechanisms for gas-to-particle conversion; Cloud microphysics and precipitation; Nucleation in condensed phase systems; Statistical physics and computational modeling of light propagation and scattering in materials for nonlinear optics applications.

**JOURNAL PUBLICATIONS (Five Recent Publications)**

McGraw, R., and Liu, Y. (2006), Brownian drift-diffusion model for evolution of droplet size distributions in turbulent clouds, *Geophys. Res. Lett.*, 33, L03802, doi:10.1029/2005GL023545.

Liu, Y., Daum, P. H., McGraw, R., and Wood R. (2006), Parameterization of the autoconversion process. Part II: Generalization of Sundqvist-type parameterizations, *J. Atmos. Sci.*, in press.

Liu, Y., Daum, P. H. and McGraw, R. (2005), Size truncation effect, threshold behavior, and a new type of autoconversion parameterization, *Geophysical Research Letters*, 32, L11811, doi:10.1029/2005GL022636.

Yoon, C., and McGraw, R. (2004) Representation of generally-mixed multivariate aerosols by the quadrature method of moments: I. Statistical foundation. *J. Aerosol Sci.* 35, 561-576 (2004).

Yoon, C., and McGraw, R., (2004) Representation of generally-mixed multivariate aerosols by the quadrature method of moments. II Aerosol dynamics, *J. Aerosol Sci.* 35, 577-598 (2004).

**Arthur A. Mirin**  
**Center for Applied Scientific Computing, L-591**  
**Lawrence Livermore National Laboratory**  
**Livermore, CA 94551**  
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**Research Interests**

- Scientific computing
- High-performance computing
- Climate and atmospheric modeling
- Numerical hydrodynamics

**Education**

Ph.D. Mathematics, University of California at Berkeley, June 1974

A.B. Mathematics, University of California at Berkeley, June 1969

**Professional Experience**

- 11/03–present Leader, Scientific Computing Group, Center for Applied Scientific Computing, Lawrence Livermore National Laboratory (LLNL), Livermore, CA
- 5/96–10/03 Computational Physicist, Center for Applied Scientific Computing, LLNL
- 1985–4/96 Leader, Computational Physics Group, National Energy Research Supercomputer Center, LLNL
- 1974–1984 Computational Physicist, National Energy Research Supercomputer Center, LLNL
- 1970–1974 Mathematical Programmer, Magnetic Fusion Energy Division, LLNL
- 1969–1970 Mathematical Programmer, Computation Division, LLNL
- 1975–1986 Lecturer, Department of Applied Science, University of California, Davis/Livermore

**Honors and Organizations**

- Gordon Bell Award for Best Performance, 1999 (coordinated the simulation that won this honor)
- Lawrence Livermore National Laboratory FY2000 Science and Technology Award
- Society for Industrial and Applied Mathematics
- American Physical Society
- American Geophysical Union
- Phi Beta Kappa academic honor society

**Selected Publications and Presentations**

Mirin, A.A., P.H. Worley, W.B. Sawyer, L. Oliker, D. Parks and M.F. Wehner, “Performance Intercomparison of Community Atmosphere Model on High-End Computing Platforms,” Twelfth SIAM Conference on Parallel Processing for Scientific Computing, San Francisco (2006). UCRL-ABS-215859.

Mirin, A.A. and W.B. Sawyer, “A Scalable Implementation of a Finite-Volume Dynamical Core in the Community Atmospheric Model,” *Int’l. Jour. High Performance Computing Applications*, 19, No. 3 (2005), 203. UCRL-JRNL-206816.

Bala, G., K. Caldeira, A. Mirin, M. Wickett and C. Delire, “Multi-century Changes to Global Climate and Carbon Cycle: Results from a Coupled Climate and Carbon Cycle Model,” *Journal of Climate* 18, No. 31 (2005), 4531. UCRL-JRNL-209851.

Oliker, L., J. Carter, M. Wehner, A. Canning, S. Ethier, G. Bala, A. Mirin, D. Parks, P. Worley, S. Kitawaki and Y. Tsuda, "Leading Computational Methods on Scalar and Vector HEC Platforms," Proc. Supercomputing 2005 Conference, Seattle (2005). UCRL-CONF-212184.

Wehner, M, L. Oliker, A. Mirin, P. Worley and D. Parks, "Towards a Direct Simulation of Human Induced Changes in the Hurricane Cycle," Supercomputing 2005 Conference, Seattle (2005). UCRL-POST-216579

Bala, G., K. Caldeira, A. Mirin, M. Wickett and C. Delire, "Direct Physical Effects of CO<sub>2</sub>-Fertilization on Global Climate," American Geophysical Union Meeting, San Francisco (2005), poster B21B-1028. UCRL-POST-217229.

Govindasamy, B., S. Thompson, A. Mirin, M. Wickett, K. Caldeira and C. Delire, "Increase of Carbon Cycle Feedback with Climate Sensitivity: Results from a Coupled Climate and Carbon Cycle Model," *Tellus*, 57B (2005), 153. UCRL-JRNL-203401.

Thompson, S.L., B. Govindasamy, A. Mirin, K. Caldeira, C. Delire, J. Miolovich, M. Wickett and D. Erickson, "Quantifying the Effects of CO<sub>2</sub> Fertilized Vegetation on Future Global Climate and Carbon Dynamics," *Geophys. Res. Lett.*, 31, No. 23 (2004), L23211. UCRL-JRNL-207218.

Mirin, A.A. and W.B. Sawyer, "Performance of an Advanced Atmospheric Dynamical Core," *Eleventh SIAM Conference on Parallel Processing for Scientific Computing*, San Francisco, CA., Feb. 25-27, 2004. UCRL-PRES-202424.

Sawyer, W.B. and A.A. Mirin, "A Scalable Implementation of a Finite-Volume Dynamical Core in the Community Atmospheric Model," *Proc. Sixteenth IASTED Int'l. Conf. on Parallel and Distributed Computing and Systems*, Cambridge, MA, Nov. 9-11, 2004. UCRL-PROC-204955.

Sawyer, W.B. and A.A. Mirin, "The Implementation of the Finite-Volume Dynamical Core in the Community Atmospheric Model," *Proc. First Indo-German Conference on PDE, Scientific Computing and Optimization in Applications*, Trier, Germany, Sept. 8-10, 2004. UCRL-PROC-208350.

Mirin, A.A. and W.B. Sawyer, "Implementation of the FV Dycore in the Community Atmosphere Model," *Finite-Volume Dynamical Core Workshop*, Princeton, NJ, Nov. 1, 2004. UCRL-PRES-207460.

Kosovic, B., G. Sugiyama, W. Hanley, G. Johannesson, J. Nitao, S. Larsen, R. Serban, A. Mirin, G. Loosmore, J. Lundquist and K. Dyer, "Data-Driven Event Reconstruction for Atmospheric Releases," *Second Sandia Workshop on Large-scale PDE-Constrained Optimization: Towards Real-time and Online PDE-Constrained Optimization*, Santa Fe, NM, May 19-21, 2004. UCRL-POST-204204.

Sugiyama, G., K. Dyer, B. Hanley, G. Johannesson, B. Kosovic, S. Larsen, G. Loosmore, J. Lundquist, A. Mirin, J. Nitao and R. Serban, "Markov-Chain Monte-Carlo and Sequential Monte-Carlo Approaches to Dynamic Data-Driven Event Reconstruction for Atmospheric Releases," *Second Workshop on Monte-Carlo Methods*, Boston, MA, Aug. 27-28, 2004. UCRL-POST-206484.

Kosovic, B., G. Sugiyama, K. Dyer, W. Hanley, G. Johannesson, S. Larsen, G. Loosmore, J. Lundquist, J. Nitao, A. Mirin and R. Serban, "Dynamic Data-Driven Event Reconstruction for Atmospheric Releases," *Eighth Annual George Mason University Transport and Dispersion Modeling Conference*, Fairfax, VA, July 13-15, 2004. UCRL-PRES-205169.

Caldeira, K., B. Govindasamy, S. Thompson, A. Mirin, M. Wickett and C. Delire, "A Three-Dimensional Coupled Climate-Carbon Simulation of a Business-as-Usual Carbon Emissions Pathway to Year 2300," *American Geophysical Union Meeting*, San Francisco, CA., Dec. 13-17, 2004. UCRL-ABS-206473.

Govindasamy, B., S.L. Thompson, A. Mirin, M. Wickett and C. Delire, "Carbon Cycle Sensitivity to Climate Change: Results from a Comprehensive GCM-Based Climate and Carbon Cycle Model," *American Geophysical Union Meeting*, San Francisco, CA., Dec. 13-17, 2004. UCRL-ABS-206468.

Cohen, R.H., W.P. Dannevik, A.M. Dimits, D.E. Eliason, A.A. Mirin, Y. Zhou, D.H. Porter, and P.R. Woodward, "Three-Dimensional Simulation of Richtmyer-Meshkov Instability With a Two-Scale Initial Perturbation," *Phys. Fluids*, **14**, 2002, p. 3692. UCRL-JC-144836.

Mirin, A.A., R.H. Cohen, B.C. Curtis, W.P. Dannevik, A.M. Dimits, M.A. Duchaineau, D.E. Eliason, D.R. Schikore, S.E. Anderson, D.H. Porter, P.R. Woodward, L.J. Shieh and S.W. White, "Very High Resolution Simulation of Compressible Turbulence on the IBM-SP System, (Gordon Bell Award for Performance, 1999), Supercomputing 99 Conference, Portland, OR, Nov. 13-19, 1999. UCRL-JC-134237.

**WILFRED M. POST**  
**Environmental Science Division**  
**Oak Ridge National Laboratory**  
**P.O. Box 2008, Bldg. 1509**  
**Oak Ridge, TN 37831-6335**

**EDUCATION**

1978 Ph.D. Ecology, University of Tennessee, Knoxville  
1975 M.S. Botany, University of Wisconsin, Madison  
1971 B.S. Mathematics, University of Wisconsin, Madison

**PROFESSIONAL EXPERIENCE**

1997 - current Senior Scientist, Oak Ridge National Laboratory, Environmental Sciences Division  
1980 - 1997 Research Staff Member, Oak Ridge National Laboratory, Environmental Sciences Division  
1985 - present Adjunct Professor, University of Tennessee, Department of Ecology and Evolutionary Biology

**SELECTED AWARDS:**

Research Accomplishment Award, Technical Publication; Lockheed Martin Energy Research Corporation (1990); Technical Communication Award, Merit in Scholarly and Professional Articles, East Tennessee Chapter of the Society for Technical Communication (1990); Technical Communication Award, Distinguished in Scholarly and Professional Articles, East Tennessee Chapter of the Society for Technical Communication (1991); Energy System's Team Technical Achievement Award, Martin Marietta Energy Systems (1991). Highly cited researcher in ecology/environment (in top 250 researchers in subject category based on citations from 1981-1999), ISI HighlyCited.com (2002).

**RESEARCH:**

Wilfred Post has over 90 open literature publications in terrestrial ecosystem ecology. Particular emphasis is in the area of global terrestrial ecosystem carbon cycling and relationships of ecosystem dynamics to environmental, edaphic, and biological conditions. He is a recognized expert on soil carbon dynamics, nutrient relationships between soil and vegetation, and the impact of species composition on ecosystem processes. He has developed new approaches to representing the impact of land-use change, and climate change in terrestrial biogeochemistry models and also developed global data sets for the evaluation of global terrestrial biogeochemistry models. His current work now centers on developing data-assimilation methods to confront terrestrial ecosystem models with data from a variety of sources (atmospheric trace gas measurements, eddy-covariance networks, soil and biomass inventories) to estimate model parameters and initial conditions and to improve ecosystem models.

**5 MOST RELEVANT PUBLICATIONS (90+ total)**

Gu, L., W.M. Post, and A.W. King. 2003. Fast labile carbon turnover obscures sensitivity of heterotrophic respiration from soils to temperature: a model analysis. *Global Biogeochemical Cycles* 18:GB1022, doi:10.1029/2003GB002119.

Post W.M., R.C. Izaurralde, J.D. Jastrow, B.A. McCarl, J.E. Amonette, V.L. Bailey, P.M. Jardine, T.O. West, J. Zhou 2004. Carbon sequestration enhancement in U.S. soils. *BioScience* 54:895-908.

Jain, A.K., T.O. West, X. Yang, and W.M. Post. 2005. Assessing the Impact of Changes in Climate and CO<sub>2</sub> on Potential Carbon Sequestration in Agricultural Soils. *Geophysical Research Letters* 32, L19711, doi:10.1029/2005GL023922.

Post, W. M., and K. C. Kwon. 2000. Soil carbon sequestration and land-use change: processes and potential. *Global Change Biology* 6:317-328.

Post, W. M., A. W. King, and S. D. Wullschleger 1997. Historical variations in terrestrial biospheric carbon storage. *Global Biogeochemical Cycles* 11:99--109.

**Mark Taylor**  
**Exploratory Simulation Technologies**  
**MS 0318, Sandia National Lab., Albuquerque NM 87185**  
[mataylo@sandia.gov](mailto:mataylo@sandia.gov)

### Education

- 1992, Ph.D., Courant Institute of Mathematical Sciences, New York University, New York, NY. Awarded the Courant Institute 1993 Kurt O. Friedrichs Prize for an Outstanding Thesis.
- 1988, B.G.S., University of Michigan, Ann Arbor MI.

### Professional Appointments

- Since 02/04, Principal Member of Technical Staff, Exploratory Simulation Technologies, Sandia National Laboratories, Albuquerque, NM.
- 9/98-1/04, Technical Staff Member, Computer and Computational Sciences, Los Alamos National Laboratory, Los Alamos, NM.
- 09/92-8/98, Software Engineer III, Computational Sciences Section, National Center for Atmospheric Research, Boulder, CO.
- 9/89-8/92, NSF Graduate Fellow, Courant Institute of Mathematical Sciences, New York University, NY.

### Relevant previous work

Mark was one of the first to develop a cubed-sphere dynamical core for global atmospheric circulation modeling. He demonstrated the scalability and accuracy of this model by running a 1B grid point simulation of the polar vortex on a 10,000 processor system. Mark was also the lead developer of a Navier-Stokes code and performed a record setting 8B grid point decaying turbulence simulation. He has also done extensive research in numerical methods for geophysical applications, focusing on high order finite element methods.

### Selected Publications

- A. F. X. Giraldo and M.A. Taylor, *Triangular Diagonal Mass Matrix Spectral Elements based on Cubature Points for the Shallow Water Equations on the Sphere*, under review, *J. Eng. Mech.* (2006).
  - B. B. T. Nadiga, M. Taylor and J. Lorenz, *Ocean Modelling for Climate Studies: Eliminating Short Time-Scales in Long-Term, High-Resolution Studies of Ocean Circulation*, to appear, *Math. Comp. Modelling* (2006).
  - C. Dennis, Fournier, Spitz, St.-Cyr, Taylor, Thomas, Tufo, *High Resolution Mesh Convergence Properties and Parallel Efficiency of a Spectral Element Atmospheric Dynamical Core*, *Int. J. High Perf. Computing Appl.*, **19** (2005).
  - D. S. Kurien and M. A. Taylor, *Direct Numerical Simulation of Turbulence - Data Generation and Statistical Analysis*, *Los Alamos Science*, **29** (2005).
  - E. M. A. Taylor, B. A. Wingate and L. P. Bos, *A Cardinal function algorithm for computing multivariate quadrature points*, to appear, *SIAM J. Numer. Anal.*, 2005.
  - F. A. Fournier, M. A. Taylor and J. Tribbia, *The Spectral Element Atmosphere Model (SEAM): High-resolution parallel computation and localized resolution of regional dynamics*, *Monthly Weather Review*, **132** (2004).
  - G. D. Komatitsch, R. Martin, J. Tromp, M.A. Taylor and B.A. Wingate, *Wave propagation in 2-D elastic media using a spectral element method with triangles and quadrangles*, *J. Comp. Acoustics*, **9** (2001).
  - H. M. Taylor and B. Wingate, *A generalized diagonal mass matrix spectral element method for non-quadrilateral elements*, *Appl. Num. Math.* **33** (2000).
  - I. W. Spitz, M. Taylor and P. Swartztrauber, *Fast and high-order solutions to the spherical shallow water equations*, *Appl. Numer. Math.* **33** (2000).
- M. Taylor, R. Loft, J. Tribbia, *Performance of a spectral element atmospheric model (SEAM) on the HP Exemplar SPP2000*, NCAR Technical Note, NCAR/TN-439+EDD (1998).
  - M. Taylor, J. Tribbia and M. Iskandarani, *The spectral element method for the shallow water equations on the sphere*, *J. Comput. Phys.* **130** (1997).
  - D. Haidvogel, E. Curchitser, M. Iskandarani, R. Hughes and M. Taylor, *Global modeling of the ocean and atmosphere using the spectral element method*, *Atmosphere-Ocean Special*, **35** (1997)

**Mariana Vertenstein**  
**Software Engineer IV**  
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**National Center for Atmospheric Research**  
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**Education:**

Harvard University, Ph.D., Chemical Physics, 1987

Dissertation: "A Microscopic Theory of Membrane Transport"

Harvard University, M.A., Physics, 1983

Massachusetts Institute of Technology, M.S., Chemical Engineering, 1979

M.S. Thesis: "Characterization of Platinum Black by Physical Adsorption of Krypton"

Massachusetts Institute of Technology, B.S., Chemical Engineering, 1978

B.S. Thesis: "Physical Adsorption of Krypton on Platinum Black"

**Employment:**

2004-Present: Software Engineer IV (Head of CCSM Software Engineering Group), Climate and Global Dynamics Division, National Center for Atmospheric Research (NCAR), Boulder, CO

2003-2004: Software Engineer IV, Climate and Global Dynamics Division, NCAR, Boulder, CO

1989-2003: Software Engineer III, Climate and Global Dynamics Division, NCAR, Boulder, CO

1987-1989: Network Analyst, Bolt, Beranek and Newman Communications Corporation, Cambridge, MA

**Peer-Reviewed Publications** (principal authorship):

Vertenstein, M., and D. Ronis, 1984: A Microscopic Theory of Membrane Transport II: Darcy-Brinkman Flow." *J. Chem. Phys.*, **80**, 5754.

Vertenstein, M., and D. Ronis, 1986: A Microscopic Theory of Membrane Transport III: Transport in Multiple Barrier Systems." *J. Chem. Phys.*, **85**, 1628.

Vertenstein, M., and D. Ronis, 1987: A Theory of Electrolyte Solutions Near a Polarizable Surface." *J. Chem. Phys.*, **87**, 4132.

Vertenstein, M. and D. Ronis, 1987: On the Approximation of Diffusion Memory Functions by Time Correlation Functions in Inhomogenous Systems." *J. Chem. Phys.*, **87**, 5457.

**Peer-Reviewed Publications** (co-authorship):

Bonan, G.B., K.W. Oleson, M. Vertenstein, S. Levis, X. Zeng, Y. Dai, R. E. Dickinson, and Z.-L. Yang, 2002: The land surface climatology of the Community Land Model coupled to the NCAR Community Climate Model. *J. Clim.*, **15**, 3123-3149.

Bonan, G.B., S. Levis, S. Sitch, M. Vertenstein, and K.W. Oleson, 2003: A dynamic global vegetation model for use with climate models: Concepts and description of simulated vegetation dynamics. *Global Change Biol.*, **9**, 1543-1566.

Oleson, K.W., G.B. Bonan, S. Levis, and M. Vertenstein, 2003: Effects of land use change on U.S. climate: Impact of surface datasets and model biogeophysics. *Climate Dynamics*, **23**: 117-132.

Hoffman, F.M., M. Vertenstein, J. B.White III, and H. Kitabata, 2005: Vectorizing the Community Land Model. *The International Journal of High Performance Computing Applications*, **19**, Fall 2005.

Dickinson, R. E., K. Oleson, G. Bonan, F. Hoffman, P. Thornton, M. Vertenstein, Z.-L. Yang, and X. Zeng, 2006: The Community Land Model and its climate statistics as a component of the Community Climate System Model. *J. Clim.*, in press.



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### **Professional Preparation**

B.S., Physics 1958, Oregon State University  
M.S., Meteorology, 1960, Oregon State University  
Ph.D., Meteorology, 1964, Pennsylvania State University

### **Appointments**

1995-present: Senior Scientist; Section Head, Climate Change Research Section, Climate & Global Dynamics Division, National Center for Atmospheric Research (NCAR), Boulder, Colorado

1987-1995: Director, Climate & Global Dynamics Division; Senior Scientist; Leader, Climate Sensitivity and CO<sub>2</sub> Research Group, NCAR

### **Synergistic Activities**

Since 1990, Washington has served on the Secretary of Energy's Biological and Environmental Research Advisory Committee (BERAC). Since 1996, he has been the chair of the Subcommittee on Global Change for BERAC. He served on the Modernization Transition Committee and the National Centers for Environment Prediction Advisory Committee of the U. S. National Weather Service. From 1978 to 1984, he served on the President's National Advisory Committee on Oceans and Atmosphere. From 1998-2002, he served on to the National Oceanic and Atmospheric Agency Science Advisory Board. From 2000-2002 he was a member of DOE's Advanced Scientific Computing Advisory Committee.

Washington is a fellow of the American Meteorological Society (AMS) and the American Association for the Advancement of Science (AAAS), a Distinguished Alumnus and an Alumni Fellow of Pennsylvania State University and Oregon State University. From 1991 to 1995, he was a member of the AAAS Board of Directors, and he served as President of AMS in 1994.

Washington received the Le Verrier Medal of the Societe Meteorologique de France in 1995. The U.S. Department of Energy awarded him the Biological and Environmental Research Program Exceptional Service Award for Atmospheric Science in 1997, for the development and application of advanced coupled atmospheric-ocean general circulation models to study the impacts of human activities on future climate. Also in 1997, he was inducted into the National Academy of Sciences Portrait Collection of African Americans in Science, Engineering, and Medicine. In 1999, Washington received the National Weather Service Modernization Award. In January 2000 Washington was awarded the Dr. Charles Anderson Award from the American Meteorological Society for pioneering efforts as a mentor and passionate supporter of individuals, educational programs, and outreach initiatives designed to foster a diverse population of atmospheric scientists. Washington was appointed to the National Science Board in 1994 and reappointed to the Board in 2000. He was elected Chair in 2002 and re-elected Chair in 2004.

## Publications

- Meehl, G.A., W.M. Washington, J.M. Arblaster, T.W. Bettge, and W.G. Strand Jr., 2000: Anthropogenic forcing and decadal climate variability in sensitivity experiments of 20th and 21st century climate. *Journal of Climate*, **13**, 3728-3744.
- Washington, W.M. et al., 2000: Parallel Climate Model (PCM): Control and transient simulations. *Climate Dynamics*, **16/10-1**, 755-774.
- Meehl, G. A., W. M. Washington, T. M. L. Wigley, J. M. Arblaster, and A. Dai, 2003: Solar and greenhouse gas forcing and climate response in the 20th century. *Journal of Climate*, **16**, 426-444.
- Santer, B.D., T.M.L. Wigley, G.A. Meehl, M.F. Wehner, C. Mears, M. Schabel, F.J. Wentz, C.M. Ammann, J. Arblaster, T. Bettge, W.M. Washington, K.E. Taylor, J.S. Boyle, W. Brüggemann, and C. Doutriaux, 2003: Influence of satellite data uncertainties on the detection of externally-forced climate change. *Science*, **300**, 1280-1284.
- Meehl, G.A., W.M. Washington, C. Ammann, J.M. Arblaster, T. M.L. Wigley and C. Tebaldi, 2004: Combinations of natural and anthropogenic forcings and 20<sup>th</sup> century climate. *Journal of Climate*, **17**, 3721-3727
- Washington, W.M. and C.L. Parkinson, 2005: An Introduction to Three-Dimensional Climate Modeling, 2<sup>nd</sup> Edition. University Science Books, ISBN: 1-891389-35-1, 353 pp.
- Meehl G.A., W.M. Washington, W.D. Collins, J.M. Arblaster, A. Hu, L.E. Buja, W.G. Strand and H. Teng, 2005: How much more global warming and sea level rise? *Science*, **307**, 1769-1772.
- Washington, W.M., A. Dai, and G.A. Meehl, 2005: Climate Change Modeling: A Brief History of the Theory and Recent 21st Century Ensemble Simulations. In: *Frontiers in the Science of Climate Modeling*, J.T. Kiehl and V. Ramanathan (eds.), Cambridge University Press, in press.
- Barnett, T.P., D. Pierce, K. AchutaRao, P. Gleckler, B. Santer, J. Gregory and W. Washington, 2005: Penetration of a warming signal into the world's oceans: Human Impacts, *Science*, **309**, 284-287.
- Washington, W.M., 2005: Computer Modeling the 20<sup>th</sup> and 21<sup>st</sup> Century Climate, American Philosophical Society, in press.

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**Education**

Ph.D., 1983, University of Wisconsin-Madison (Nuclear Engineering)

M.S., 1980, University of Wisconsin-Madison (Nuclear Engineering)

B.S., 1978, University of Delaware, Graduated with High Honors (Physics)

**Professional Experience**

*2002-present:* Staff Scientist, Scientific Computing Group, Computational Research Division, Lawrence Berkeley National Laboratory, Berkeley, CA

*1998-2002:* Physicist, Program for Climate Modeling and Intercomparison, Lawrence Livermore National Laboratory, Livermore, CA

*1991-1998:* Physicist, Climate System Modeling group, A-division, Lawrence Livermore National Laboratory, Livermore, CA

*1985-1991:* Physicist, Code Development group, B-division, Lawrence Livermore National Laboratory, Livermore, CA

*1983-1984:* Post doctoral Research Associate, Nuclear Engineering Department, University of Wisconsin-Madison

**Recent Relevant Publications**

1. B. D. Santer, T. M. L. Wigley, G. A. Meehl, M. F. Wehner, C. Mears, M. Schabel, F. J. Wentz, C. Ammann, J. Arblaster, T. Bettge, W. M. Washington, K.E. Taylor, J. S. Boyle, W. Brüggemann, and C. Doutriaux, Influence of Satellite Data Uncertainties on the Detection of Externally Forced Climate Change, *Science* 300 (2003) 1280-1284
2. **B. D. Santer, M. F. Wehner, T. M. L. Wigley, R. Sausen, G. A. Meehl, C. Ammann, J. Arblaster, W. M. Washington, J.S. Boyle, W. Brüggemann, Contributions of Anthropogenic and Natural Forcing to Recent Tropopause Height Changes, *Science* 301 (2003) 479-483.**
3. Curt Covey, Krishna M. AcutaRao, Peter J. Gleckler, Thomas J. Phillips, Karl E. Taylor and Michael F. Wehner, Coupled ocean-atmosphere climate simulations compared with simulations using prescribed sea surface temperature: Effect of a “perfect ocean”. *Global and Planetary Change* 41 (2004) 1-14
4. N.P. Gillett, A.J. Weaver, F.W. Zwiers, and M.F. Wehner, Detection of volcanic influence on global precipitation, *Geophysical Review Letters* 31 (2004) L12217
5. N.P. Gillett, M.F. Wehner, S.F.B. Tett, Testing the linearity of the response to combined greenhouse gas and sulfate aerosol forcing, *Geophysical Review Letters* 31 (2004) L14201
6. B. D. Santer, T. M. L. Wigley, A. J. Simmons, P. Kahlberg, G. A. Kelly, S. Uppala, C. Ammann, J. S. Boyle, W. Brüggemann, C. Doutriaux, M. Fiorino, C. Mears, G. A. Meehl, R. Sausen, K.E. Taylor, W. M. Washington, M. F. Wehner and F. J. Wentz, Identification of anthropogenic climate change using a second generation analysis. *J. Geophysical Research* 109 (2004) D21104
7. M.F. Wehner, Predicted 21<sup>st</sup> century changes in seasonal extreme precipitation events in the Parallel Climate Model, *J. Climate* 17 (2004) 4281-4290
8. B.D. Santer, T.M.L. Wigley, C. Mears, F.J. Wentz, S.A. Klein, D.J. Seidel, K.E. Taylor, P.W. Thorne, M.F. Wehner, P.J. Gleckler, J.S. Boyle, W. Collins, K.W. Dixon, C. Doutriaux, M. Free, Q. Fu, J.E. Hansen, G.S. Jones, R. Ruedy, T.R. Karl, J.R. Lanzante, G.A. Meehl, V. Ramaswamy, G. Russell, and G.A. Schmidt, Amplification of Surface Temperature Trends and Variability in the Tropical Atmosphere. *Science*. 309 (2005) 1551-1556
9. Michael Wehner, “Changes in daily precipitation and surface air temperature extremes in the IPCC AR4 models.” *US CLIVAR Variations*, 3, (2005) pp 5-9

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**Climate Dynamics**  
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## **EDUCATION**

Ph.D.	1988	Computer Science	Stanford	University
M.S.	1983	Computer Science	Stanford	University
B.A.	1980	Mathematics / Computer Science	Indiana University	

## **PROFESSIONAL EXPERIENCE**

Computer Science and Mathematics Division, Oak Ridge National Laboratory (ORNL):

2003 – present            Senior Research and Development Staff

1987 – 2002             Research and Development Staff

## **SELECTED RECENT PUBLICATIONS**

1. L. Oliker, J. Carter, M. Wehner, A. Canning, S. Ethier, A. Mirin, G. Bala, D. Parks, P. Worley, S. Kitawaki and Y. Tsuda. *Leading Computational Methods on Scalar and Vector HEC Platforms*. In Proceedings of the ACM/IEEE Conference on High Performance Networking and Computing (SC05), Seattle, WA, November 12-18, 2005.
2. P. Worley and J. Drake. *Performance Portability in the Physical Parameterizations of the Community Atmospheric Model*. International Journal for High Performance Computer Applications, 19 (3), August 2005, pp. 187-202.
3. P. Worley, J. Candy, L. Carrington, K. Huck, T. Kaiser, G. Mahinthakumar, A. Maloney, S. Moore, D. Reed, P. Roth, H. Shan, S. Shende, A. Snively, S. Sreepathi, F. Wolf, and Y. Zhang. *Performance Analysis of GYRO: A Tool Evaluation*. In Proceedings of the 2005 SciDAC Conference, San Francisco, CA, June 26-30, 2005.
4. T. H. Dunigan, Jr., J. S. Vetter, and P. H. Worley, *Performance Evaluation of the SGI Altix 3700*, in Proceedings of the 2005 International Conference on Parallel Processing, Oslo, Norway, June 14-17, 2005.
5. P. Worley, S. Alam, T. Dunigan, Jr., M. Fahey and J. Vetter. *Comparative Analysis of Interprocess Communication on the X1, XD1, and XT3*. In Proceedings of the 47th Cray User Group Conference, Knoxville, TN, May 16-19, 2005.

## **SYNERGISTIC ACTIVITIES**

Worley's research interests include parallel algorithms for scientific computing and performance evaluation of parallel applications and computer systems. Worley currently leads Oak Ridge National Laboratory's participation in the Department of Energy (DOE) SciDAC project in performance evaluation (Performance Evaluation Research Center). He is also a lead performance engineer for the National Science Foundation and DOE Community Climate System Model (CCSM), the principal investigator for the Performance Evaluation and Analysis Consortium End Station at the National Center for Computational Sciences Leadership Computing Facility, and a co-chair of the Software Engineering Working Group for the CCSM.

Recent professional activities include: organizing committee for the SIAM (Society for Industrial and Applied Mathematics) Conference on Parallel Processing for Scientific Computing: 2004, 2005; Tutorials Committee, SC03 and SC04 (2003, 2004); ACM SIGMETRICS Electronic Bulletin Board moderator (1996-2004); Secretary of the SIAM Activity Group on Supercomputing: 2001-2002.

## 7 DESCRIPTION OF FACILITIES AND RESOURCES

This proposal makes heavy use of supercomputing resources at the Leadership Computing Facility (located in the National Center for Computational Science at Oak Ridge), the Climate System Lab (located at the National Center for Atmospheric Research in Boulder), the National Energy Science and Engineering Research Center (located at the Lawrence Berkeley National Lab in Berkeley), and the Advanced Computing Laboratory (located at the Los Alamos National Lab in Los Alamos). The primary allocation for the development team funded under this project has been granted as part of the Climate Science End Station using the Cray X1e and Cray XT3 in the LCF. In excess of 500,000 node hours have been allocated for development activities within the Climate End Station. The biogeochemistry inter-comparison work is also covered by a separate allocation within the Climate End Station. In addition, resources are being provided on the IBM Blue Gene/L computer at Argonne National Laboratory.

### 7.1 Oak Ridge National Laboratory

The Center for Computational Sciences (CCS) was established in 1992 and is a designated User Facility. The CCS has the following goals:

- Focus on grand challenge science and engineering applications
- Procure the largest scale systems (beyond vendors design point) and develop software to manage and make them useful
- Deliver leadership-class computing for science and engineering
  - By 2005: **50x** performance on major scientific simulations
  - By 2008: **1000x** performance
- Educate and train next generation computational scientists

The CCS houses the computing platforms and has a long history of taking delivery of emerging, yet promising architectures to drive computational sciences at the leading edge.

**Physical Facility.** The new Computational Sciences building, which is located on the secure campus of ORNL, has 40,000 square feet of raised floor computer room designed specifically for leadership-class computer systems. The facility currently can provide up to 12 megawatts of power and 3,600 tons of cooling with redundant capacity to allow concurrent operation and maintenance. More than 16,000 square feet of raised floor space is readily available to house the proposed systems. The proposed systems will require 600 square feet, leaving more than 15,000 square feet for further expansion of systems.

**Power** is supplied from the Tennessee Valley Authority (TVA). The electrical infrastructure was built to meet the reliability requirements of the uranium enrichment activities of the U.S. Government. The TVA feeder circuits average one unplanned interruption every 10.7 years, and the internal distribution network supplying the computer center has averaged one unplanned outage every 2.6 years over the last 46 years. The repair time for these outages has ranged from a few minutes up to three hours. For the past six consecutive years, TVA has served its customers with 99.999 percent reliability<sup>1</sup>. At this writing, TVA is installing a new state-of-the-art substation that will have two independent 161 kilovolt supply sources with a capacity of 150 MW at ORNL for expanding available power for the computers and other facilities on the campus. Construction of this \$16M substation began in July 2005 and will be completed in mid-2006. By June of 2008, a third 161 kilovolt supply source will be installed for additional redundancy and to boost capacity to 250 MW.

**Cooling** is provided by chilled water that can be connected through computer room air handling units for air-cooled systems, or directly connected to the computers for systems that require direct chilled water cooling. The cooling system provides a redundant chiller to allow the center to continue to operate in the event of a chiller failure or required maintenance. At this writing, the center has 3,600 tons of chiller capacity. ORNL is in the process of upgrading the chiller capacity to be able to accommodate up to 40 MW of power and to provide redundancy by linking the chiller system into the laboratory-wide chilled water system. The combination of power and cooling upgrades will allow the ORNL to house as many as three 10-12 MW petascale computer systems simultaneously.

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<sup>1</sup> <http://www.tva.gov/power/xmission.htm> / [http://www.search.com/reference/Tennessee\\_Valley\\_Authority](http://www.search.com/reference/Tennessee_Valley_Authority)

**Network Connectivity.** ORNL is connected to every major research network at rates of 10 gigabits per second or greater. Connectivity to these networks is provided via optical networking equipment owned and operated by ORNL that runs over leased fiber optic cable. This equipment has the capability of simultaneously carrying either 192 10-gigabit per second circuits or 96 40-gigabit per second circuits and connects the CCS computing facility to major networking hubs in Atlanta and Chicago. Currently, only 16 of the 10-gigabit circuits are committed to various purposes, allowing for virtually unlimited expansion of the networking capability. As part of this proposal, we will expand the current TeraGrid connection from 10 to 30 gigabits per second. Currently, the connections into ORNL include: TeraGrid, Internet2, ESnet, and Cheetah at 10 gigabits per second as well as UltraScienceNet and National Lambda Rail at 20 gigabits per second. ORNL operates the Cheetah research network for NSF and the UltraScience Net research network for DOE.

The CCS local-area network is a common physical infrastructure that supports separate logical networks, each with varying levels of security and performance. Each of these networks is protected from the outside world and from each other with access control lists and network intrusion detection. Line rate connectivity is provided between the networks and to the outside world via redundant paths and switching fabrics. A tiered security structure is designed into the network to mitigate many attacks and to contain others. The new Cray system will be connected in the TeraGrid enclave to the TeraGrid Force10 E600 router via a 10 Gbps link.

**Visualization and Collaboration.** ORNL has state-of-the-art visualization facilities that can be used on site or accessed remotely. ORNL's Exploratory Visualization Environment for REsearch in Science and Technology (EVEREST) is a 30' wide by 8' high PowerWall for data exploration and analysis. Twenty-seven projections are virtually seamlessly edge-matched for an aggregate resolution of more than 11,000 by 3,000 pixels. This projection environment is driven by a 64-node rendering and analysis cluster comprised of dual-processor Opteron workstations. This cluster is networked to the resources in the National Center for Computational Sciences (NCCS) and performs additional visualization-related functions including computation, pre-analysis, and pre-rendering. The rendering cluster has been demonstrated with a variety of COTS and open-source visualization tools including VisIt, CEI Insight, Paraview, OpenDX, AVS/Express, VMD, and VTK. Our rendering environment currently utilizes 64-bit SuSE Linux, Chromium, Distributed Multi-Head X (DMX), and recent graphics cards with pixel shader support. The facility itself has a 600 square-foot projection area, and a 1000 square-foot viewing area. The viewing area can accommodate a wide range of groups, from a couple researchers to a 25-member collaboration. The ORNL-developed PowerWall Toolkit is a GUI environment which enables groups to use the EVEREST PowerWall as a large desktop pixel space with static imagery, movies, and interactive 3D visualizations. Other visualization capabilities include an LCD array and an immersive display.

**Archives and Access.** A high-performance, scalable filesystem is vital to data-intensive applications. Archival storage is provided by the High Performance Storage System (HPSS) operated by ORNL. ORNL has an HPSS installation with a capacity of up to 5 petabytes of data and regularly supports data transfers of more than 10 TB per day. Both the bandwidth and capacity of HPSS can be increased as needed. The CCS will deliver a shared secondary file storage system to enable sharing of data among the computer systems, data analysis systems, visualization systems, and archival storage. A project is currently underway with Cray and other strategic partners to implement a single high-speed shared file system linking all of the computing systems within the CCS. The underlying technology of this file system will be based on the LUSTRE file system developed by Cluster File Systems Inc.

**Physical and Cyber Security.** ORNL has a comprehensive physical security strategy including fenced perimeters, patrolled facilities, and authorization checks for physical access. An integrated cyber security plan encompasses all aspects of computing. Cyber security plans are risk-based and separate systems of differing security requirements into enclaves of similar requirements allowing the appropriate level of protection for each system, while not hindering the science needs of the projects.

**Systems Engineering, Administration, and Operations.** ORNL has a professional, experienced operational and engineering staff comprised of groups in HPC Operations, Technology Integration, User Services, and Scientific Computing. The ORNL computer facility is staffed 24 hours a day, 365 days a year to provide for continuous operation of the center and for immediate problem resolution. On evenings and weekends, the operators provide first-line problem resolution for users with additional user support and system administrators on-call for more difficult problems. Primary CCS systems include the following:

- **Jaguar:** a 5,296 processor Cray XT3 system providing a peak performance of over 25 teraflops and over 10 TB of memory. Planned upgrades of Jaguar are to 100 TF in 2006 and to 400 TF in 2007.
- **Phoenix:** a Cray X1E, with 1,024 multistreaming vector processors (MSPs) and 2 TB of globally addressable memory. Each MSP has 2 MB of cache, and four MSPs form a node with 8 GB of shared memory. Memory bandwidth is very high, up to half the cache bandwidth. The interconnect functions as an extension of the memory system, offering each node direct access to memory on other nodes at high bandwidth and low latency. The peak performance of Phoenix is 18.5 teraflops.
- **OIC:** ORNL Institutional Cluster is a collection of eight SGI Xeon clusters providing 640 dual-processor nodes and almost 10 TF of peak performance.
- **Cheetah:** a 27-node IBM Power-4 system. Each Power-4 node of Cheetah has thirty-two 1.3-GHz Power4 processors. Twenty of the nodes have 32 GB of memory, five nodes have 64 GB of memory and two nodes have 128 GB of memory. The peak performance of Cheetah is 4.5 teraflops.
- **Ram:** a 256-processor SGI Altix with 2 TB of shared memory. Each processor is the Intel Itanium2 1.5 GHz processor. The full system runs a single Linux image and the large shared memory facilitates analysis of very large data sets. The peak performance of Ram is 1.5 teraflops.

The **Joint Institute for Computational Sciences (JICS)** facility represents a \$10M investment by the State of Tennessee and features a state-of-the-art distance learning center with 66 interactive seating; conference rooms, informal / open meeting space, executive offices for distinguished scientists and directors, and incubator suites for students and visiting staff. Users of the NCASE will have ready access to this facility.

## **7.2 Argonne National Laboratory Facilities and Resources**

Personnel associated with this proposal will have access to facilities at Argonne National Laboratory, and in particular to facilities associated with the Mathematics and Computer Science Division at Argonne.

Argonne National Laboratory has computing and networking facilities located in the Mathematics and Computer Science Division. These resources include major parallel computing clusters, visualization systems, advanced display environments, collaborative environments, and high-capacity network links.

As one of the nine participants in the NSF's Distributed Terascale Facility, Argonne operates the TeraGrid's visualization facility. The entire TeraGrid is a 13.6 TF grid of distributed clusters using Intel McKinley processors with over 6 TB of memory and greater than 600 TB of disk space. The full machine is distributed between NCSA, SDSC, Caltech, the Pittsburgh Computer Center, Purdue, Indiana University, the Texas Advanced Computing Center, and U Chicago/Argonne. The individual clusters are connected by a dedicated 40 Gb/s link that acts as the backbone for the machine. The Argonne component of the machine consists of 16 dual IA-64 nodes for computation, 96 dual Pentium IV nodes with G Force Ti 4600 graphics accelerators for visualization, and 20 TB of storage.

A second supercomputer at Argonne, which is available to researchers for production computing, is "Jazz". This Linux system, which has achieved a sustained teraflop, ranks among the 50 fastest computers in the world. Jazz has 350 compute nodes, each with a 2.4 GHz Pentium Xeon with 1.5GB of RAM. The cluster uses Myrinet 2000 and Ethernet for interconnect and has 20 TB of on-line storage in PVFS and GFS file systems.

In addition, Argonne has a cluster dedicated for computer science and open source development called "Chiba City". Chiba City has 512 Pentium-III 550MHz CPUs for computation, 32 Pentium-III 550 CPUs for visualization and 8 TB of disk. Chiba City is unique testbed that is principally used for system software development and testing.

Argonne's most recent addition to its supercomputing facilities is a one-rack IBM Blue Gene/Light. The system includes a 2048-processor compute node with a peak performance of 5.7 teraflops.

Another facility available to researchers is the recently constructed wireless sensor network research and deployment laboratory. The lab includes Mica2 motes with a wide range of sensors, including weather boards and GPS. The motes, StarGate gateway nodes, servers, and a digital image capture device allow researchers to develop and test deployments.

Argonne also is a participant in the I-WIRE project, which links to the TeraGrid and StarLight, as well as linking facilities at Argonne to various research institutions in Illinois.

Argonne has substantial visualization devices as well, each of which can be driven by the TeraGrid visualization cluster, by Chiba City, or by a number of smaller dedicated clusters. These devices include the ActiveMural (an 11 million pixel

large-format tiled display) and several smaller tiled displays such as the portable MicroMural, which has approximately 3 million pixels.

Furthermore, Argonne currently supports numerous Access Grid nodes, ranging from AG nodes in continual daily use to AG2 development nodes.



## **Statistical Approaches to Aerosol Dynamics for Climate Simulation**

**Program Area:** Scientific Application Partnership: Mathematics

**Principal Investigator:** Robert McGraw (BNL)

**Senior Personnel:** Wei Zhu (SUNY – Stony Brook)

**Scientific Application Partner:** A Scalable and Extensible Earth System Model for Climate Change Science (PI - John B. Drake, Oak Ridge National Laboratory)

**Participating Institutions:** Brookhaven National Laboratory (BNL) and State University of New York at Stony Brook

**Projected Funding Request:** FY07 - \$315K, FY08 - \$326K, FY09 - \$337K, Total \$979K for three years.

## **1. Abstract**

The quadrature method of moments (QMOM), developed in recent years in collaborations between BNL scientists and SUNY-SB mathematicians, provides a statistically-based alternative to modal and sectional methods for aerosol simulation. Key moments of the aerosol population, including number, mass, and mixed moments entering the covariance matrix of a principal components analysis, are tracked in place of the distribution itself. The new approach is highly efficient, yet provides the comprehensive representation of natural and anthropogenic aerosols, and of their mixing states and direct and indirect effects, that the CCSM will require. In addition to furthering its partnership with SUNY-SB, the proposed SAP will leverage findings from current BNL science programs related to aerosols (DOE ASP), aerosol-cloud interaction (DOE ARM), and climate simulation (NASA-GISS) to the maximum extent possible to meet CCPP objectives in collaboration with the inter-laboratory science team.

## **2. Background**

### **2.1 Objectives**

The goal of the DOE Climate Change Prediction Program (CCPP), including the SciDAC Climate Modeling and Simulation Science Application, is:

- *To determine the range of possible climate changes over the 21<sup>st</sup> century and beyond through simulations using a more accurate climate system model that includes the full range of human and natural climate feedbacks with increased realism and spatial resolution.*

This Science Application Partnership (SAP) will support that goal through its development of statistically-based approaches to aerosol simulation. These approaches tend to be highly efficient and will contribute to maximizing the length of simulations and number of ensembles that can be performed to facilitate the aggressive schedule of climate change simulations required for upcoming assessment products. This SAP has been called out in the inter-Laboratory science application proposal: “A Scalable and Extensible Earth System Model for Climate Change Science”, submitted under this SciDAC call (PI: John Drake of ORNL) and will contribute in an integral way to that proposed activity. Indeed this is the only SAP called out as part of that inter-Laboratory proposal to improve the representation of aerosols in the Community Climate System Model (CCSM).

The specific objectives of the proposed SAP can be summarized as follows:

- *To develop new statistical approaches for improving the representation of aerosols, aerosol microphysical processes, and aerosol-cloud interactions in the CCSM.*
- *To supply a new aerosol microphysical module based on these findings in time for CCSM5.*

### **2.2 Significance**

In contrast to greenhouse gases, radiative forcing by aerosols cannot be characterized simply by mass concentration as has been employed in many past and current evaluations (Schmidt et al., 2006). Rather, the direct effects of aerosol on atmospheric radiation strongly depend upon the sizes, shape, chemical composition, and mixing state of the particle distribution (Jacobson, 2001, 2002). Understanding the complex processes that shape this variability is a major scientific challenge (Asrar et al., 2001). Similarly, size-resolved simulations of aerosol microphysics, including number and mass concentrations are necessary to understanding and modeling the indirect effect of aerosols on clouds (Adams and Seinfeld, 2002). Anthropogenic aerosols are believed to have two effects on cloud

properties: (1) The increase in the number of cloud condensation nuclei results in a larger number of smaller droplets and brighter clouds (the Twomey effect) (Schwartz et al., 2002), (2) The smaller droplets tend to inhibit rainfall increasing cloud lifetime and average cloud cover (Rosenfeld, 2000). These indirect effects of aerosol on clouds have been characterized as contributing perhaps the largest of all uncertainties about global climate forcings (NRC, 2001). It is thus imperative for future assessments of aerosol forcing that the aerosol number, size distribution, chemical composition, and mixing state be represented in models in sufficient detail to make accurate estimates of cloud activation and optical properties of the aerosol if the uncertainty that presently attaches to estimates of this forcing is to be appreciably reduced. The aerosol mixing state, for example, plays a major role in determining particle optical properties, solubility and cloud activation efficiency, yet has not been adequately represented in traditional aerosol models. These aerosol properties are likewise of great significance to the interpretation of ground based and remote sensing measurements.

As described below, we in the aerosol microphysics community have made considerable progress in developing the advanced methods and highly efficient modular components necessary to represent both the direct and indirect effects of aerosols in atmospheric models. It is thus timely and imperative for improved assessment of climate effects that these new developments be incorporated in the next generation Earth system model. The development of highly efficient size and composition resolved aerosol modules based on the quadrature method of moments (QMOM) affords a timely opportunity to fill this need, and specifically to update the representation of aerosols and their direct and indirect effects in the CCSM.

### ***2.3 Relation to current state-of-the art***

Traditional approaches to aerosol modeling have mainly centered on the use of “modal” and “sectional” methods. Modal methods typically divide the aerosol into a small number of modes of prescribed shape and having uniform composition within each mode. The method is efficient but generally not very accurate. Sectional methods divide the aerosol into a number of size classes. High accuracy requires good size resolution in order to minimize numerical diffusion, with the result that a large number of class variables (scalars) needs to be carried in the model. A high-resolution sectional calculation is useful, even vital, as a validation tool for off-line testing of more approximate methods, but is an unlikely candidate for use in climate simulation. Thus it is clear that new and efficient approaches are needed for the aerosols.

The method of moments, especially as developed over recent years in collaborations between BNL scientists and SUNY-SB mathematicians (Yoon and McGraw, 2004a; 2004b),

provides a statistically-based alternative for aerosol simulation. The new approach is highly efficient and especially suited to simulations of the multicomponent aerosols that the CCSM will require. Key moments of the aerosol population, including number, mass, and the mixed moments entering the covariance matrix of a principal components analysis, are tracked in place of the distribution itself. This greatly reduces the number of aerosol scalars required by the model without compromising the accuracy with which the physical and optical properties of the aerosol are computed – properties computed directly from the moments. The quadrature method of moments (QMOM) has been advanced in recent years to the point where it is now widely regarded as an extremely accurate method and a viable alternative to bin-sectional and modal methods for describing the dynamics of particle populations in models. **The QMOM has a potential future with the CCSM: It is clearly more efficient than sectional and more accurate than modal methods.**

## 2.4 Preliminary Studies

This section presents an overview of some of the more significant advances achieved in the representation of aerosols by the method of moments. Parameterizations to describe how aerosols activate to form cloud droplets (these set requirements on the aerosol module), and new results for parameterization of the autoconversion process governing the transition from cloud droplets to precipitation are also summarized.

### 2.4.1 The quadrature method of moments

Gaussian quadrature provides a systematic method for approximate evaluation of integrals of the form given by Eq. 2.1:

$$I = \int_0^{\infty} \sigma(r) f(r) dr \approx \sum_{i=1}^N \sigma(r_i) w_i \quad (2.1)$$

where  $\sigma(r)$  is a known kernel function, in this case a function of the particle radius. For our purpose the weight function,  $f(r)$ , is the aerosol size distribution, and  $I$ , depending on the nature of the kernel is some integral property of the distribution.

Two key properties of quadrature underlie the power of the QMOM: (1) for  $N$  quadrature points  $\{r_i; w_i\}$  the approximate equality of Eq. 2.1 is exact for polynomial kernels of degree  $2N - 1$ , and (2) the quadrature abscissas and weights,  $\{r_i\}$  and  $\{w_i\}$ , respectively depend only on the moments of  $f(r)$ :

$$\mu_k = \int_0^{\infty} r^k f(r) dr = \sum_{i=1}^N (r_i)^k w_i \quad (2.2)$$

for  $k = 0, 1, 2, \dots, 2N - 1$ . Thus one does not require full knowledge of  $f(r)$  in order to evaluate integral properties of the aerosol as it suffices to know only the lower order moments. Efficient methods for obtaining quadrature abscissas and weights from moments have been developed for the univariate case, i.e. an aerosol distribution that, like  $f(r)$  above, is specified using only a single particle radius (or mass) coordinate [See for example McGraw, 1997 or the Numerical Recipes subroutine OTHOG (Press et al., )]. An important goal of the statistical approach is to develop methods for extending the assignment of quadrature points to multivariate particle distribution functions (pdfs) as described below in Sec. 3.

The physical and optical properties of an aerosol can be estimated from its moments using Eq. 2.1. Figure 1 illustrates a particularly difficult case where  $\sigma(r)$  is the Mie-scattering angular distribution kernel at a single wavelength and in a particular scattering direction for a spherical particle of radius  $r$  (McGraw et al., 1995). The behavior of  $\sigma(r)$  is shown at four scattering directions ranging from forward scattering ( $\theta = 0$ ) to backscattering at  $180^\circ$ . The total scattering due to the aerosol, at any specified angle, is an integral of type  $I$  (Eq. 2.1). Property 1 gives an indication of the accuracy to expect. Thus if the kernel were a fifth-degree polynomial (solid curves in Fig. 1) the obtained result would be exact for  $N=3$ . The figure shows that the true kernels are indeed reasonably well fit by polynomials except in the  $180^\circ$  backscattering case where strong oscillations in the kernel are not captured well by the fit. Comparison of both sides of the approximate equality of Eq. 2.1 for representative known particle size distributions shows the method leads to nonsystematic errors in the range  $\pm 5\%$ , except in the  $180^\circ$  backscattering case where errors reached over 40%. Moreover, these results were for a single wavelength – the most unfavorable case. Many practical applications average over multiple wavelengths, as in the solar spectrum, and the errors tend to cancel to obtain much more accurate results. With further averaging over a vertical column of grid cells and multiple aerosol types (the reported results are for a single homogeneous aerosol) the error is even further reduced. The utility of moment methods for properties estimation has been enhanced by the development of methods such as Randomized Minimization Search Technique (RMST) and Multiple Isomoment Distribution Aerosol Surrogate (MIDAS), which used the first six moments to compute aerosol optical properties to within 1-2% of those obtained from the full particle distribution function (PDF) (Yue et al., 1997; Wright, 2000). These methods can be used even for pathologically non-polynomial kernels, such as the step function kernels often used in models of cloud droplet activation (Wright et al., 2002), although here a better approach would be to develop parameterizations for aerosol-cloud interaction directly in terms of moments (Sec. 3).

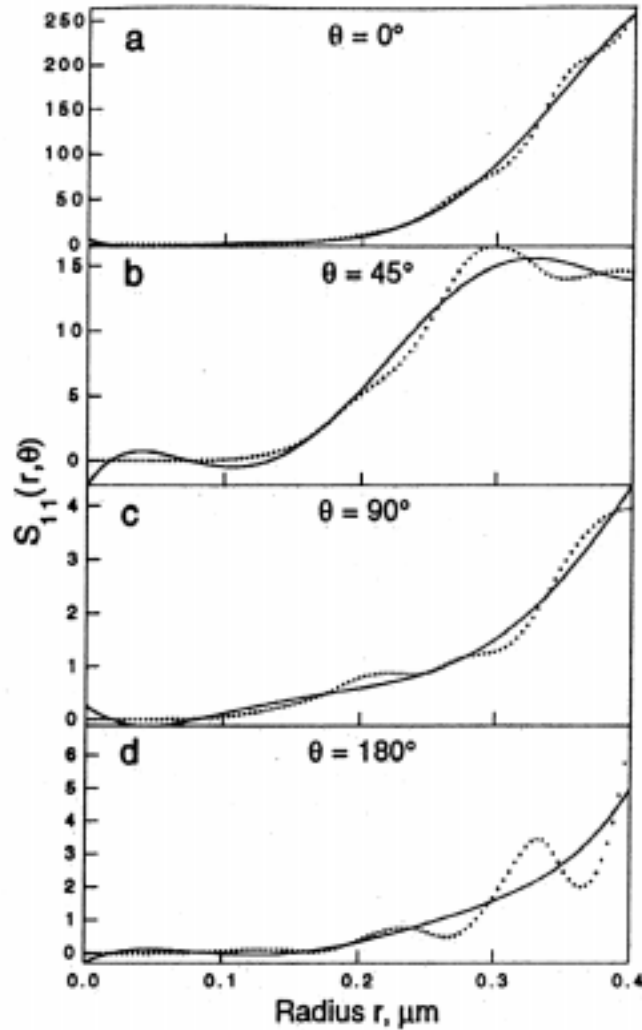


Figure 1. Mie scattering angular distributions (unnormalized). Dotted curves result from Mie scattering calculations at a wavelength of  $0.6328 \mu\text{m}$ . Solid curves are fifth-degree polynomial fits. To the extent that the Mie curves can be approximated by the corresponding polynomial forms the quadrature approximation of Eq. 2.1 is exact (from McGraw et al., 1995).

The quadrature approximation to integrals of type  $I$ , also leads to the moment closure necessary to simulate general aerosol evolution processes using only moments. We will illustrate this idea here for condensation growth. Results for other aerosol processes including coagulation, dry deposition, even cloud activation, follow in similar fashion. Let  $dr/dt = \phi(r)$  be an arbitrary particle growth rate. Then from Eq. 2.1 (McGraw and Wright, 2003):

$$\frac{d\mu_k}{dt} = k \int_0^\infty r^{k-1} \phi(r) f(r) dr \approx k \sum_{i=1}^N (r_i)^{k-1} \phi(r_i) w_i. \quad (2.3)$$

The abscissas and weights are the same as before – independent of kernel and dependent only on lower order moments. Equations 2.2 and 2.3 provide an example of closure for moment evolution equations that is the basis for the QMOM (McGraw, 1997).

These results have immediate consequences for simulation efficiency – i.e., one need not track the full aerosol distribution as just a few moment scalars are sufficient for obtaining aerosol physical and optical properties and closure of the moment dynamics. Moreover, approximations for estimating particle size distributions from moments have been developed and although the solutions are not unique the latest results are promising (Wright, 2000; Diemer and Olson, 2002).

#### 2.4.2 Recent applications

Recent years have seen development of the QMOM to the point where it is now widely regarded as an extremely accurate method and a viable alternative to bin-sectional and modal methods for describing the dynamics of particle populations (see for example Marchisio et al., 2003a, 2003b and Upadhyay and Ezekoye, 2003 for independent assessments of QMOM accuracy in chemical engineering applications). A recent monograph includes a fifteen page appendix describing the QMOM and new applications including closure of the moment equations for turbulence, and especially for simulating particle population dynamics in turbulent flows (Fox 2003). Along similar lines, the QMOM is now available as a user specified option in the popular computational fluid dynamics code FLUENT (Wan et al., 2004).

Its remarkable efficiency makes the QMOM ideal for use in atmospheric models. The method has been used for the representation of aerosols in chemical transport models (CTMs) on the sub-hemispheric (Wright et al., 2000) and regional scales (Yu et al., 2003). As described above, the QMOM tracks key moments of the aerosol population directly, without need for a priori assumptions regarding the form of the particle size distribution, while overcoming difficulties associated with closure of the moment evolution equations encountered in the ordinary MOM. An early QMOM aerosol dynamics module 6M (for 6 radial moments) includes a range of aerosol microphysical and chemical processes and allows for arbitrary growth laws for condensation and coagulation, nucleation of new particles, and precursor gas and liquid-phase chemistry (Wright et al., 2001a; Yu et al., 2003). Comparison with results obtained using a high-resolution discrete model of the particle dynamics, demonstrated that the accuracy of 6M is good relative to uncertainties associated with other processes represented in atmospheric CTMs (Wright et al., 2001a). For example differences in the mass/volume



moments and in the partitioning of chemical species such as sulfur (VI) between the gas and aerosol phases remained under 1% and differences in particle number rarely exceeded 15% (Wright et al., 2001).

### 2.4.3 Multivariate extension of moment methods

In addition to particle mass loading, the chemical and physical properties of aerosols are determined by particle number density, composition, and size distribution. In the atmosphere, particle number and composition control the indirect effects that aerosols have on climate through their influence on cloud activation, drizzle production, and cloud radiative properties. Another example points to the mixing state of black carbon aerosols as having a significant influence on radiative forcing (Jacobson, 2001). Unlike the limiting cases of externally or internally mixed aerosols, the modeling of general mixing requires a multivariate/multicoordinate representation that can accommodate multiple particle species and variable surface properties, as well as the distribution of particle size. Successful extensions of moment methods to particle distribution functions characterized by more than a single mass or radius coordinate have been achieved in collaborations with Yale University for bivariate applications (Wright et al., 2001b; Rosner et al., 2003) and with our SAP partners at SUNY-SB for the fully multivariate case (Yoon and McGraw, 2003a; 2003b).

Bivariate calculations were made for the Koch-Friedlander model of nonspherical particles undergoing simultaneous coagulation and sintering (Koch and Friedlander, 1990). This well-known model provides an interesting test case for simulation of non-spherical particles of mixed size and shape (Wright et al., 2001b). Particles are characterized by two coordinates: surface area,  $a$ , and volume,  $v$ . Figure 2 shows the bivariate pdf initially (Panel a) and at a later time (Panel b) on the 150x150 grid. Sectional approaches require an unmanageable number of size bins in higher dimensions (here 22500) and just obtaining the evolved bivariate distribution shown in Panel b required about 10 calendar days on a Sun Spark Enterprise computer. (The area and volume grids in Panels a and b are logarithmically spaced and there is substantial evolution of the distribution from a to b). Moments were computed from the sectional representation and compared with the moments computed by the (bivariate) QMOM. Panels c and d of Fig. 2 show evolution of the bivariate mixed moments defined as:

$$M_{kl} = \langle v^k a^l \rangle = \int_0^\infty \int_0^\infty v^k a^l n(v, a) dv da \quad (2.4)$$

where  $n(v, a)$  is the bivariate number distribution function. QMOM calculation times ranged from several seconds (using 9 bivariate moments/ 3 quadrature points) to several minutes (using 36 bivariate moments/ 12 quadrature points) on a PC (Pentium II processor), the longer calculation requiring a nonlinear search routine to invert 36 moments to obtain the 12 quadrature

points. Maximum error, relative to the sectional benchmark calculation, ranged from 1% (using 36 bivariate moments/ 12 quadrature points) to 20% (using 9 bivariate moments/ 3 quadrature points), which is quite good considering the small number of quadrature points and orders of magnitude range spanned by the moments themselves (Fig. 2). This orders-of-magnitude savings in computation time illustrates the dramatic efficiency of moment methods. It is for these kinds of problems, where the aerosol population needs to be represented by more than one coordinate, that the full advantages of the method of moments becomes evident.

The great computational efficiency of the QMOM makes this method an ideal approach for extension to fully multivariate aerosol dynamics simulations. The most significant obstacle had been the lack of a systematic and efficient means for assigning quadrature points in higher coordinate dimensions - and this has now been overcome through an extension of the QMOM using the statistical method of principal components analysis (PCA) (Yoon and McGraw, 2004a, 2004b). The idea for using PCA originated with Prof. Zhu, and AMS student Choongseok (Paul) Yoon undertook the development of this idea as part of his doctoral research project while working at BNL. In this interesting application of statistics, which might be called “dynamic PCA” the covariance matrix evolves in time as the aerosol distribution evolves. The resulting PCA-QMOM has been tested at the box model level via comparisons with results from the high-resolution bivariate ( $v,a$ ) sectional model, discussed above, and compared with analytic test cases for coagulation and condensation in higher coordinate dimensions where a sectional calculation of the multivariate pdf, or indeed even visualizing this higher dimensional distribution function, is impractical (Yoon and McGraw, 2004b). Illustrative calculations from the PCA-QMOM are shown in Fig. 3 for one of the analytic test cases using three aerosol coordinates (species masses  $m_1$ ,  $m_2$ , and  $m_3$ ). These results are discussed further under Approach, where a proposed module designed to implement the QMOM is described. It is interesting that for all known test cases where an analytic solution for the aerosol dynamics exists, the QMOM is also exact.

In our view, the inherent complexity of aerosol processes, coupled with the need to strike a balance between model complexity and computational efficiency, will make the use of moment-based methods or some other similar statistical approach, obligatory and widespread in the future - especially for multivariate particle populations where representation of the full multidimensional pdf is not an option.

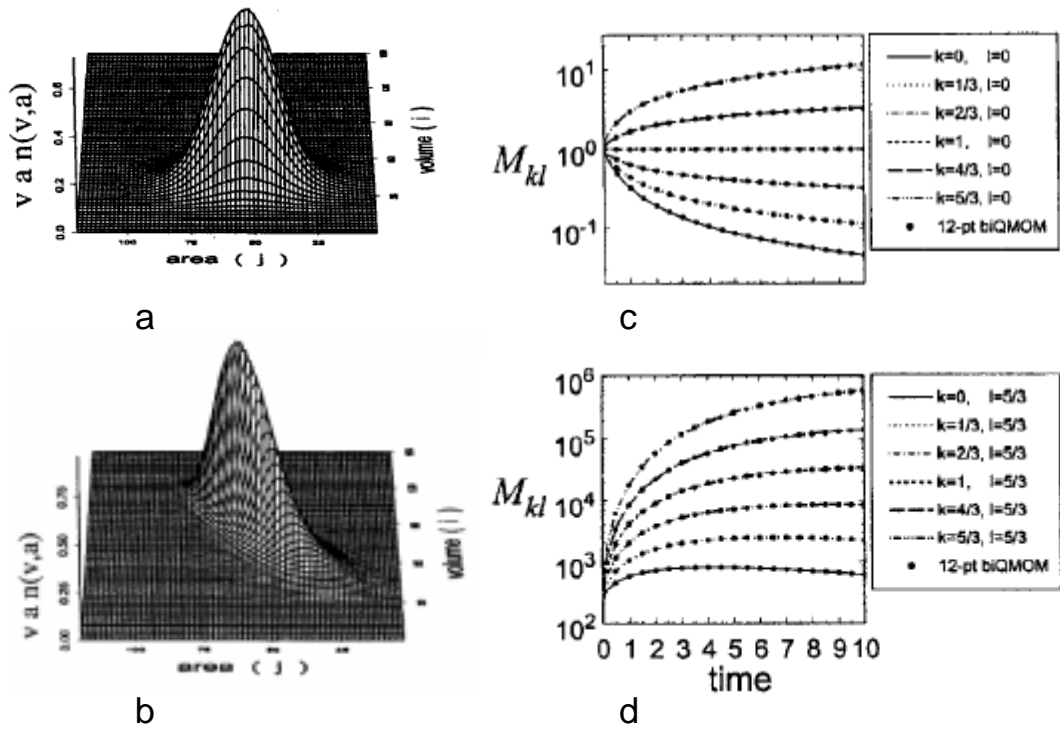


Figure 2: Evolution of a bivariate pdf under simultaneous coagulation and sintering. Panels a and b: 2D discrete model with 150x150 size sections; a. initial distribution ( $t=0$ ), b. evolved distribution at  $t=10$  with  $t$  in reduce coagulation time units. Panels c and d compare moments obtained from discrete model integration (points) with the moments evolved directly using the bivariate QMOM (curves). Results for 12 bivariate mixed moments (from Wright et al. 2001b).

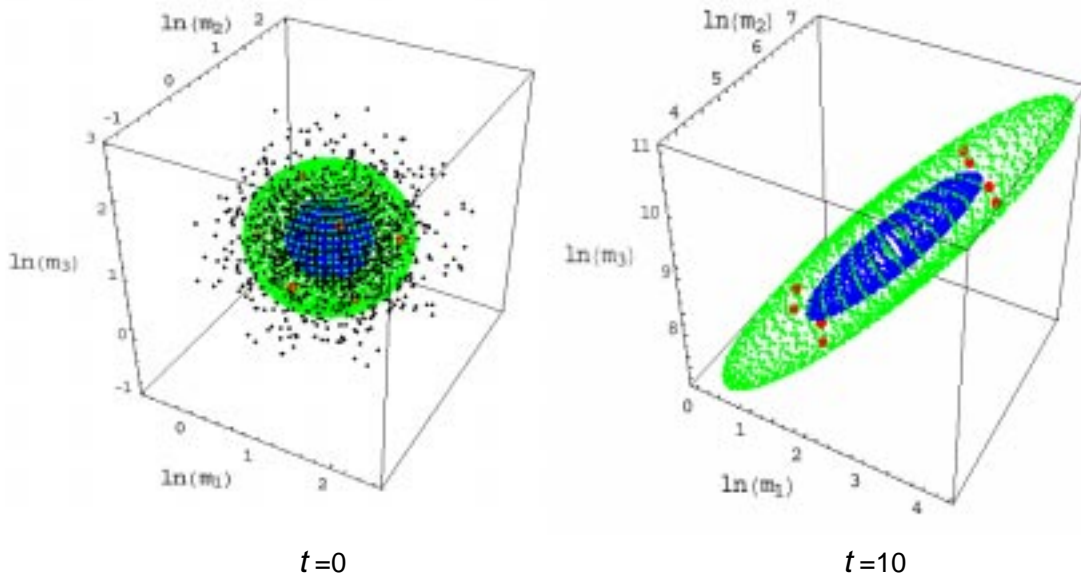


Figure 3: Evolution of a three component generally-mixed aerosol. Figure shows evolution of the  $\sigma$  (blue) and  $2\sigma$  (green) probability surfaces under coagulation and condensation (from Yoon and McGraw, 2003b).

#### 2.4.4 Parameterization of aerosol-cloud interactions

Clouds cover on average about 60% of the Earth's surface and play crucial roles in regulating the Earth's energy balance and water cycle; yet they remain the major source of uncertainty in climate models. Aerosols have major influences on clouds and through clouds on climate. First, aerosols are responsible for cloud formation, which requires the activation of aerosol particles to form cloud droplets through heterogeneous nucleation (the first indirect aerosol effect). Aerosol particles, depending on their number concentration and wetting properties, determine the cloud droplet number concentration,  $N_D$ , which in turn has a major effect on the subsequent autoconversion process whereby large cloud droplets collect smaller ones and become embryonic raindrops (second indirect aerosol effect). Meteorological conditions including temperature and concentration of water vapor also play an important role in determining number concentration through their influence on the fraction of aerosol particles that activate to become cloud droplets. Meteorological conditions also determine cloud liquid water content,  $L$ , and the cloud turbulence conditions that also play major roles in autoconversion.

Parameterizations for cloud activation vary considerably as to the level of aerosol microphysical detail that they include. The GISS GCM currently employs a mass-only aerosol representation based on multiple regression relationships used to predict cloud droplet number over land (mass concentrations of sulfate and organic matter) and over oceans (mass concentrations of sulfate, organic matter, and sea salt) (Menon et al., 2002). Other parameterizations require a higher level of size/composition detail than available in mass-only aerosol models. Examples here include parameterizations based on single or multiple lognormal, or sectional size representations of the aerosol population (Abdul-Razzak and Ghan, 2002), and recent extension of the Abdul-Razzak parameterization to include effects from particle composition and surface properties (Rissman et al., 2004). Clearly, the requirements of any aerosol-cloud parameterization to be used set a lower limit on the level of microphysical detail that the climate aerosol module must include. Recent parameterizations also include the important role played by droplet dispersion on radiative forcing (Liu and Daum, 2002). The method of moments is sufficiently flexible that it can include a variety of such parameterizations for the first indirect effect.

Parameterization of the second aerosol indirect effect has proven especially difficult (Liu and Daum, 2004). Lacking theoretical foundation, there is large discrepancy (several orders of magnitude) among existing parameterizations for the autoconversion rate. In several recent papers (McGraw and Liu, 2003; 2004; 2006) the kinetic potential (KP) of nucleation theory has been adapted to provide a new theoretical foundation for understanding drizzle formation and the second aerosol indirect effect; namely, the tendency for aerosols to

increase cloud droplet number concentrations and for increased droplet number concentrations to suppress rain (Rosenfeld, 2000). The KP drizzle theory provides an explanation for a long-standing puzzle concerning the precipitation process in warm clouds (McGraw and Liu, 2004): droplets of significant fall velocity size would seem to take longer to form than the lifetime of a typical rain cloud. Drizzle in the KP description is identified as a barrier crossing process that transforms cloud droplets to drizzle size with a rate dependent on turbulent diffusion, droplet collection efficiency, and cloud droplet size (through  $N_D$  and  $L$ ). The barrier regulates the rate at which cloud droplets can enter the collection regime such that those few that do enter experience less competition and can grow much more quickly to significant fall velocity size. A parameterization for the transient drizzle rate is presented in McGraw and Liu (2004).

Important to current parameterizations based on this model, the barrier maximum yields a critical droplet size, here approximately 20-30 micron in radius, having balanced condensation, collection, and evaporation rates. This newly identified critical radius provides a microphysical basis for improving Kessler-type empirical parameterizations of autoconversion rate (Liu et al., 2004; 2005; 2006), and has already been included in one parameterization employed recently in a climate model (Rotstayn and Liu, 2005).

### 3. Technical Approach

The technical approach is designed with two purposes in mind. First, under Task 1, we propose to develop the mathematical foundation and methods needed to expand the power, efficiency, and flexibility of new statistical approaches to aerosol simulation. Second, under Task 3, we propose to incorporate these findings into a new aerosol module designed to be compatible with the CCSM modeling framework and available for use in time for CCSM5. Parameterizations for aerosol microphysical properties and aerosol-cloud interactions are under rapid development, and becoming better rooted in physics, due in large part to DOE support through its ASP and ARM programs. Task 2 will leverage findings from several BNL programs in this area to make the newest and best parameterizations available to the climate modeling community, generally, and for use in the new aerosol module proposed under Task 3.

#### 3.1 Task structure

##### 3.1.1 Task 1: *Developing new capabilities for aerosol simulation using advanced statistical methods and improvements to the QMOM (Years 1-3)*

**Multivariate statistics:** A central concern of all aerosol microphysical models is how to capture the relevant aspects of particle size and composition while striking a balance between model complexity and the efficiency required for use in climate models. Thus the question emerges: What is the smallest set of variables needed to reliably represent aerosol properties in models? One cannot, and fortunately need not, answer this question for each individual particle; the answers need to be provided for the bulk of the material that contributes to the climate influence of aerosols. With these considerations in mind, we have directed much effort over the past several years to the development of statistically-based moment approaches suitable, simultaneously, for classification, model simplification (i.e. reduction in the number of aerosol internal coordinates) and rendering of the aerosol dynamics (Yoon and McGraw, 2004a; 2004b). These activities will continue with focus on the needs of the CCSM under this Task.

The results shown in Fig. 3 illustrate an early application of the statistical approach to simulation of a generally-mixed three-component aerosol evolving under simultaneous coagulation and condensation (Yoon and McGraw, 2004b). For this test an initial distribution, lognormal in each coordinate, was chosen and statistically sampled to generate the multitude of points in compositional coordinate space shown in the figure for  $t = 0$ . Here  $m_i$  is the mass of species  $i$  in the particle. To implement the PCA-QMOM we begin with the initial distribution, or its moments, and obtain the variances and co-variances that enter the covariance matrix,  $\Sigma$ . For a 3-component system this is a 3x3 symmetric matrix constructed using moments through second order. These are listed below in Eq. 3.1. Assignment of quadrature points (red points in the figure) is immediate once the eigenvalues (or principal values) of  $\Sigma$  have been determined.

The moments themselves are updated using the quadrature points, as in the usual QMOM. These are then used to update  $\Sigma$ , and so on, yielding a closed system of equations for evolving the moments (Yoon and McGraw, 2004b). One advantage of the method is that it requires no a priori assumptions about the form of the size distribution to track moments. Nevertheless one is free to use distributions such as lognormal distributions consistent with the tracked moments to help visualize the pdf, or to estimate physical and optical properties of the aerosol using parameterizations where distributions are required (e.g. the cloud activation parameterization of Abdul-Razzak and Ghan (2002)), or, as described in connection with Task 3, to exploit certain similarities between the QMOM and modal methods.

To gain perspective on computational burden expected from the advection of aerosol moments in a global model, consider the 10 mixed mass moments tracked during evolution of the three component generally-mixed aerosol shown in Fig. 3. These are

$$\{N, \langle m_1 \rangle, \langle m_2 \rangle, \langle m_3 \rangle, \langle m_1^2 \rangle, \langle m_2^2 \rangle, \langle m_3^2 \rangle, \langle m_1 m_2 \rangle, \langle m_1 m_3 \rangle, \langle m_2 m_3 \rangle\}. \quad (3.1)$$

$N$  is particle number concentration,  $m_i$  is species mass, and averages are defined as in Eq. 2.4.. (The last six members of this set are the second order moments that appear in the covariance matrix.) An analogous set of 10 *spatial* moments for the distribution of an advected tracer within each 3D grid cell is carried in the Prather second-order moment advection scheme. Thus we expect similar computational burden for moment advection as in the Prather scheme. Of course this estimate does not include the computational burden required to update the mass moments within each grid box, which is where the aerosol microphysical processes come into play, but this step is known from much experience to be very fast in the computationally efficient QMOM (c.f. the fast computer times cited in connection with the  $v$ - $a$  box model calculations of Sec. 2.4.3). In application of PCA to the bivariate  $v$ - $a$  model only 6 moments are required, namely, any subset of moments from Eq. 3.1 that includes only two coordinates. The calculations are even faster in this case than with the 9 moment scheme described in Sec. 2.4.3 and the accuracy is about the same.

Even with this success there remains much room for improvement. Figures 2 and 3 show evolution of a single aerosol pdf. Generally, as with the multi-modal method more than one pdf is required to represent the aerosol. The main difference is that in the usual modal approximation the pdf is univariate, whereas with the PCA-QMOM it is multivariate. In either case it is important to optimize this partitioning. This is primarily a classification issue whose resolution is perhaps best achieved through the statistical analysis of measurements of aerosol composition and mixing state (described below).

Another important issue relates to certain necessary convexity conditions that any valid moments set must satisfy (Rosner et al., 2003). [Necessary and sufficient conditions for a valid moment set can be framed in terms of certain Hankel-Hadamard determinates constructed from the moments which must be positive definite (Shohat and Tamarkin, 1963)]. Generally the evolution of moments preserves validity of a moment set, however in climate models where nonlinear advection algorithms are used, correlations between moments can be broken when moments are advected as independent scalars, leading to invalid sets. One way to avoid moment failures is to implement the so-called Direct QMOM or DQMOM (Marchisio et al., 2003a; 2003b, Fox, 2003) wherein quadrature points are evolved directly during the advection step with two scalars, number and mass, assigned to each point. Other approaches are currently under development and will be considered along with the DQMOM under this Task and as part of module development (Task 3).

***Composition and mixing state:*** Most atmospheric models assume that the aerosol is either externally or internally mixed. Each of these extreme cases can be represented using a single-coordinate pdf. Multi-modal and multi-sectional methods sample the composition space of general mixtures to some degree, but multivariate methods are required to treat the general mixing case to describe, for example, the pdfs shown in Figs. 2 and 3. Field measurements indeed support a full spectrum of mixed particle states. Aerosol mixing state determines particle optical properties (e.g. black carbon coated with sulfate), solubility, and cloud activation efficiency. Thus it is important to have a good description of general mixed aerosols for use in climate models. The proposed research seeks to develop systematic criteria for characterization of mixing and apply these criteria to develop a compact representation of mixing state in terms of multivariate mixed moments and optimized quadrature point assignments.

As an aerosol evolves its mixing state tends to change from external to internal mixing. Insights into this evolution can be gained through inspection of the covariance matrix,  $\Sigma$ . Figure 3 shows the 1- $\sigma$  and 2- $\sigma$  probability surfaces; obtained from the eigenvalues and eigenvectors of  $\Sigma$ , or equivalently from the quadrature points, assuming the pdf is a trivariate lognormal distribution. The initial stages of dimensional reduction are observed as the aerosol approaches internal mixing: all particles of the same mass have nearly the same composition. This is seen in the elongation of the probability surfaces with time; revealing the emergence of a single dominant coordinate (here a function of total particle mass) that is characteristic of the approach to internal mixing under coagulation. (Initially all 3 coordinates were of equal importance). The identification of dimensional reduction is a well known application of PCA, seen here to carry over to aerosol simulations based on the PCA-QMOM. Closely related to mixing state analysis is the notion of classification that needs also to be addressed under this Task. Several approaches are next described.



***Classification and optimization of aerosol representation:*** Our AMS partners at SUNY-SB have extensive experience in the mining and classification of large data sets (Zhu et al., 2002; Zhu et al., 2003; Wang et al., 2006). Similar algorithms are currently being applied to the analysis and classification of aerosol mass spectroscopic data in a project being developed by BNL/AMS student (Bin Xu). This Summer we plan to utilize funding from DOE ASP to apply these methods to the data sets now being generated by several Aerodyne Aerosol Mass Spectrometers as part of the large Mexico City campaign currently in progress (March 2006). Classification and regression tree methods have been incorporated into “SpectrumMiner”, which uses what we call the interactive dendrogram (Imrich et al., 2002) for visualization. SpectrumMiner has been applied in preliminary studies to the classification of ambient aerosols using single-particle mass spectroscopic data collected during field campaigns in Houston and Korea (Imrich et al., 2002). Hierarchy nodes are placed on concentric circles whose radii are determined by the dissimilarity of the node’s sub tree. Individual particles appear as leaf nodes along the circumference of the outer circle. Successfully larger nodes (higher-level and with more particles) appear towards the center and it is these inner branches and nodes that represent the bulk of the material that is contributing to the climate influence of aerosols. Our hypothesis is that similar classification methods can productively guide aerosol model development.

Linkages between modeling and measurement will be pursued during Year 2 and we will determine whether similar classification and regression algorithms can be used to optimize how the aerosol is represented in climate models. Specific goals will include, for example, optimization of modal (class) partitioning and quadrature-point assignment, and determining which multivariate compositional moments are best to track during the course of a climate simulation. A good example of how to proceed can be found in recent studies by Jimenez and co-workers (e.g. Zhang et al., 2005). These authors employ multivariate and factor analysis to investigate the major organic aerosol components identified in an Aerodyne Mass Spectrometer data set acquired at the EPA Pittsburgh Supersite during September 2002. Using mathematical deconvolution techniques, and a priori understanding of the organic data, two mass spectral marker peaks (at  $m/z$ 's 44 and 57) were selected as the first guess principal components (most likely peaks associated with  $\text{CO}_2^+$  and  $\text{C}_4\text{H}_9^+$ , respectively). The reconstructed organic concentrations of hydrocarbon-like and oxygenated organic aerosols (HOA and OOA) explained 99% of the variance in the measured time series of spectra. From the standpoint of modeling guidance, the study suggest that strong consideration be given to the representation of HOA (similar to diesel exhaust, and freshly emitted traffic aerosols in urban areas), and OOA (similar to aged highly processed and oxidized organic aerosols sampled in rural areas) in atmospheric models. It is clear from this example that the measurement and modeling communities can each benefit from a cross-fertilization of ideas driven by a common need for advanced statistical methodologies similar to those we propose. Field-deployable mass-spectroscopic techniques now furnish the composition of multicomponent aerosols in real time,

and in some cases on a particle-by-particle basis. The analysis of such measurements has spurred the development of sophisticated software tools for multivariate data visualization, analysis, and compression. The need for microphysically-based simulations that can be compared with these new kinds of measurements has, in turn, motivated our ideas to develop multivariate, statistically-based aerosol dynamic models – with the added benefit that these same methods are efficient enough for practical climate simulation.

### *3.1.2 Task 2: Parameterizations for climate models (Years 1-3)*

Parameterizations are required in many components of climate modeling including aerosol dynamics and direct and indirect feedbacks. Here we describe several new parameterizations under development at BNL with support from current DOE ASP and DOE ARM science programs. These include parameterizations for new particle formation, water uptake with changes in relative humidity, sea salt aerosol production flux, and for aerosol-cloud interactions and indirect effects, including drizzle formation. Findings from these activities will be leveraged as part of Task 2 especially for use in the CCSM.

The essential output variables of the aerosol dynamics module designed under Task 1 and implement under Task 3 will be in the form of quadrature points and/or moments. These variables will be advected as scalars and passed to, for example, the aerosol optical properties and aerosol-cloud interaction parameterization modules as meteorological conditions warrant. From this multivariate information, the modules will be designed to generate various zero to two dimensional projections such as total aerosol species mass, multiple lognormal distributions (or modes) for univariate size representation along various composition coordinates, and multivariate lognormal distributions for representing more general mixing states. These are the formats required for input to the currently available cloud activation parameterizations described in Sec. 2.4.4 (see Menon et al., 2002; Abdul-Razzak and Ghan, 2002; and recent extensions of Abdul-Razzak and Ghan to include composition effects on surface tension and wetting by Rissman et al., 2004). New parameterizations that relate both the relative spectral dispersion (standard deviation of the cloud droplet distribution divided by the mean) and droplet concentration to pre-cloud aerosol properties, updraft, and turbulence parameters, will also be considered for used in the CCSM as these are developed.

Subgrid cloud processes and the indirect effects of aerosols on clouds need to be parameterized in GCMs, and parameterizations of the subgrid process have been often developed empirically and have tunable parameters. The empirical parameterizations, and especially the tunable parameters associated with them, often do not have solid theoretical bases. To improve this situation, a concerted effort has been made by BNL under its DOE ARM program to derive parameterizations from first principles. A typical example is the development

of new parameterizations for the autoconversion process (the first step for cloud droplets growing into small raindrops). Application of the new autoconversion parameterization to a GCM has produced promising results without arbitrarily tuned parameters (Rotstayn and Liu 2005). BNL will propose leveraging the best of these parameterizations for use in the CCSM in a form that makes best utilization of the moment sequences already tracked in the QMOM. Emphasis will be on aerosol-cloud interactions, especially on parameterizations of cloud turbulence, and aerosol indirect effects on droplet dispersion, cloud optical properties, and cloud lifetime.

BNL is currently developing parameterizations for atmospheric new particle formation under a DOE ASP program and will leverage these results for use in the CCSM. The new parameterization, also developed using multivariate statistical methods, will include nucleation as well as the subsequent competition between growth and coagulation loss that governs the formation of particles of climate-significant size (McGraw, 2005). BNL has also introduced a parameterization for emissions of sea salt aerosol. The new parameterization includes source terms for both particle number and particle size, with dependence on meteorological conditions, and is well suited for use in climate models (Lewis and Schwartz, 2004). BNL will also incorporate a new parameterization for the water uptake and related aerosol optical properties (Lewis, 2006). Activities under Task 2 will include leveraging these findings from DOE ASP and DOE ARM programs to insure that the resulting parameterizations are compatible with the CCSM.

### *3.1.3 Task 3: QMOM aerosol module development (Years 1-3)*

For its proposed implementation in time for CCSM5, the QMOM will be introduced gradually, beginning with 1-pt quadrature (number and mass moments) to benefit from PNL's concurrent implementation of the modal method. The 1-pt QMOM has been tested recently and found to give accuracy comparable to the modal method (Upadhyay and Ezekoye, 2003). Multiple quadrature point methods for fully multivariate pdfs will be introduced first for the mixed mode. In this mode (MXX in Fig. 4) aerosols tend to end up with aging, so this is perhaps the most important mode, albeit the one that is the most neglected in the traditional modal and sectional approaches to aerosol dynamics. The MXX mode should provide an excellent testing ground both for studying the general mixing states of atmospheric aerosols and for development of the new statistical methods envisaged for Task 1.

	PRIMARY MODES	SECONDARY MODES	TERTIARY+ MODES
<b>Mechanism I</b> 14 modes 45 variables	AKK, ACC, DDD, SSA, SSC, OCC, BC1	DSS, BC2, BC3, DBC, BOC, BCS	MXX
<b>Mechanism II</b> 14 modes 45 variables	AKK, ACC, DDD, SSA, SSC, OCC, BC1	DSS, BC2, OCS, DBC, BOC, BCS	MXX
<b>Mechanism III</b> 11 modes 35 variables	AKK, ACC, DDD, SSA, SSC, OCC, BC1	DSS, BC2, BOC	MXX
<b>Mechanism IV</b> 8 modes 28 variables	ACC, DDD, SSS, OCC, BC1	DSS, BC2,	MXX

Figure 4. Modal structures developed for the NASA-GISS climate model. Primary modes: AKK = Aitken, ACC = inorganic accumulation, DDD = insoluble mineral dust, SSA = accumulation mode sea salt, SSS = total sea salt, OCC = organic carbon, BC1 = insoluble black carbon. Secondary modes are derived from the primary modes through condensation and coagulation processes. MXX = mixed mode. The user specifies which mechanism to use. (From Wright et al., 2006).

Module development will benefit from similarities between 1-pt quadrature and the modal methods (Upadhyay, R. R., and Ezekoye, O. A, 2003). Input/Output structures will be designed to be similar to those of the modal method and we envisage working with and sharing information, methods, and parameterizations with PNL investigators as findings develop - in full support of PNL's proposed implementation of the modal method as described in the inter-Laboratory proposal. BNL will also leverage findings from its current NASA program which requires building a QMOM module for the GISS GCM. The first version of the BNL module, called MATRIX (for Multiconfiguration Aerosol Tracker of mIXing state), was delivered to NASA in Feb. 06 and is currently being implemented in the GCM. An illustration of the flexibility of the multiconfiguration framework of MATRIX is shown in Fig. 4. Note that the modal structures here are somewhat subjective – as is the usual case (e.g Jacobson, 2001; 2002). For example, DDD represents insoluble mineral dust with less than 5% sulfate coating. On further addition of sulfate, particles are transferred to the DSS soluble mineral dust mode. Such criteria are obviously somewhat arbitrary. The proposed classification methods introduced under Task 1 should provide a firmer statistical foundation to such assignments.

### **3.2 Tasks by individual**

**Robert L. McGraw**, Principal Investigator (BNL). Responsible for project leadership and technical direction.

**Wei Zhu**, co-Principal Investigator (SUNY-SB). Responsible for many of the activities described under Task 1 and for student direction. Will lead the design of the mathematical and statistical framework for those activities described under Task 1.

**Douglas Wright**, co-Investigator (BNL). Contribute to the activities of Task 1 and to module development for Task 3

**Yangang Liu**, co-Investigator (BNL). Development of parameterizations for aerosol-cloud interaction and indirect effects under Task 2.

**Ernie Lewis**, co-Investigator (BNL). Development of parameterizations for aerosol water uptake (hygroscopicity) and sea salt aerosol emissions under Task 2.

### **3.3 Milestones**

Year 1: Continue development of multivariate extensions of the QMOM. Selection of optimal moment sets for multicomponent aerosols. Development of new statistical approaches for the systematic classification of aerosol mixing states. Initiate construction of QMOM module and incorporation of microphysical parameterizations.

Year 2: Apply Visual Statistical Analyzer (ViStA) framework and similar methods, developed for classification of field aerosol measurements, to optimize modal (class) structures for aerosol simulation. Apply Bayesian statistical methods to their characterization of evolving aerosol populations. Complete benchmark validations of the QMOM aerosol module using high-resolution sectional and analytic methods.

Year 3: Completion of QMOM module validation studies. Prepare for integration into the CCSM.

## **4. Consortium Arrangements**

The proposed statistical approaches to aerosol simulation are inherently more interesting from a mathematical perspective than either the sectional or modal methods, and require a

correspondingly greater level of mathematical sophistication for their development. To effectively perform the proposed work we are building on an already successful collaboration between the BNL Atmospheric Sciences Division and the Applied Mathematics and Statistics (AMS) Department at SUNY-SB.

#### **4.1 Why this team?**

There is a strong history of productive collaboration between our groups. In recent years BNL has taken on several AMS students who have completed, or are in the late stages of completing, their doctoral research in applied mathematics while at BNL. Especially relevant to the proposed SAP is the work of Paul Yoon, an AMS student whose research was jointly supervised by Professor Zhu and Dr. McGraw. That effort has resulted in a major advancement of the multivariate QMOM for simulating the general mixing states of multicomponent aerosols. Key progress was achieved through influx of new ideas from the field of principal components analysis (PCA) (Yoon and McGraw, 2004a; 2004b). We view this as only the first breakthrough step in the application of advanced statistical methods to the science of aerosol simulation. Other statistical models such as Bayesian models, etc. will be studied as part of the proposed SAP. More recently a second AMS student (Mr. Bin Xu) has been working in the BNL Atmospheric Sciences Division on visual statistical analysis and data mining methods and software. We envisage that similar statistical methods, developed initially to facilitate the analysis of atmospheric field measurements, will serve both to guide the science of aerosol simulation, for example by identifying the aerosol classes and mixing states most important to track during simulation, and help motivate new collaborations between the measurement and modeling communities.

#### **4.2 Project management**

The proposed SAP will be a partnership between BNL and SUNY-SB with BNL leading the science application work, in support of CCSM, and SUNY-SB leading the applied mathematics research. We envisage taking on perhaps two additional graduate students as part of the proposed effort. These students, as yet unidentified, would carry out their research both at SUNY-SB and BNL, and under the joint direction of Professor Zhu and BNL staff – the protocol we have used in the past. Ideally we hope to support one student from math (M) and one from computer science (CS) so as to develop a complementary set of skills for addressing the first and second of the SAP objectives, respectively, listed in Section 2.1. Students benefit from the close proximity of our two institutions, and from the combination of computational and scientific resources and staff expertise.

**Statistical Approaches to Aerosol Dynamics for Climate Simulation**

ORGANIZATION Brookhaven National Laboratory				Budget Page No: <u>1</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Dr. Robert McGraw, Principal Investigator				Requested Duration: <u>12</u> (Months) Year 1	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Man-Mo.		Funds Requested by Applicant
			CAL	ACAD	SUMR
1. McGraw, R			2	0	0
2. Wright, D			2		
3. Liu, Y			2		
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. ( 3 ) TOTAL SENIOR PERSONNEL (1-6)			7	0	0
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( 1 ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)			1		\$7,739
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)					\$70,518
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					\$28,912
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$99,431
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					\$0
E. TRAVEL			1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)		\$0
			2. FOREIGN		
TOTAL TRAVEL					\$0
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					\$0
2. TUITION & FEES					\$0
3. TRAINEE TRAVEL					\$0
4. OTHER (fully explain on justification page)					\$0
TOTAL PARTICIPANTS ( 0 ) TOTAL COST					\$0
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					\$0
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					\$0
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES - ITD Support/Services @ 3.75% of Total Salaries + Fringe Benefits					\$3,580
5. SUBCONTRACTS					\$0
6. OTHER - SHOP SERVICES					\$0
TOTAL OTHER DIRECT COSTS					\$3,580
H. TOTAL DIRECT COSTS (A THROUGH G)					\$103,010
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
39.45% General & Administrative (G&A) on Item (H) Total Direct Costs Less Item (D.) Equipment Plus					
7.0% Material Burden on Item (E) Travel, Item (G.1.) Mat'l's & Supplies, Item (G.5.) Subcontracts & Item (D.) Equipment Plus					
31.2% G&A Common Support on Item (G.4.) Computer Services Plus 20% Organizational Burden,					
11.5% Space Charge, .35% Waste Management Fee & 2.46% Electric Power on Items A+B+C;					
TOTAL INDIRECT COSTS					\$86,990
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$190,000
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					\$0
L. TOTAL COST OF PROJECT (J+K)					\$190,000

DOE F 4620.1

(04-93)

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U.S. Department of Energy

Budget Page

(See reverse for Instructions)

OMB Control No.

1910-1400

OMB Burden Disclosure

Statement on Reverse

Statistical Approaches to Aerosol Dynamics for Climate Simulation

ORGANIZATION Brookhaven National Laboratory				Budget Page No: <u>2</u>		
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Dr. Robert McGraw, Principal Investigator				Requested Duration: <u>12</u> (Months) Year 2		
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Man-Mo.		Funds Requested by Applicant	
			CAL	ACAD	SUMR	Funds Granted by DOE
1.	McGraw, R		2	0	0	
2.	Wright, D		2			
3.	Liu, Y		2			
4.						
5.						
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7.	( 3 ) TOTAL SENIOR PERSONNEL (1-6)		7	0	0	\$62,779
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)						
1.	( ) POST DOCTORAL ASSOCIATES					
2.	( 1 ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)		1			\$7,739
3.	( ) GRADUATE STUDENTS					
4.	( ) UNDERGRADUATE STUDENTS					
5.	( ) SECRETARIAL - CLERICAL					
6.	( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)						\$70,518
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)						\$30,307
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)						\$104,225
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)						
TOTAL PERMANENT EQUIPMENT						\$0
E. TRAVEL						
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)						\$0
2. FOREIGN						
TOTAL TRAVEL						\$0
F. TRAINEE/PARTICIPANT COSTS						
1. STIPENDS (Itemize levels, types + totals on budget justification page)						\$0
2. TUITION & FEES						\$0
3. TRAINEE TRAVEL						\$0
4. OTHER (fully explain on justification page)						\$0
TOTAL PARTICIPANTS ( 0 ) TOTAL COST						\$0
G. OTHER DIRECT COSTS						
1. MATERIALS AND SUPPLIES						\$0
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION						\$0
3. CONSULTANT SERVICES						
4. COMPUTER (ADPE) SERVICES - ITD Support/Services @ 3.75% of Total Salaries + Fringe Benefits						\$3,752
5. SUBCONTRACTS						\$0
6. OTHER - SHOP SERVICES						\$0
TOTAL OTHER DIRECT COSTS						\$3,752
H. TOTAL DIRECT COSTS (A THROUGH G)						\$107,977
I. INDIRECT COSTS (SPECIFY RATE AND BASE)						
39.45% General & Administrative (G&A) on Item (H) Total Direct Costs Less Item (D.) Equipment Plus						
7.0% Material Burden on Item (E) Travel, Item (G.1.) Mat'ls & Supplies, Item (G.5.) Subcontracts & Item (D.) Equipment Plus						
31.2% G&A Common Support on Item (G.4.) Computer Services Plus 20% Organizational Burden,						
11.5% Space Charge, .35% Waste Management Fee & 2.46% Electric Power on Items A+B+C;						
TOTAL INDIRECT COSTS						\$91,392
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)						\$199,369
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES						\$0
L. TOTAL COST OF PROJECT (J+K)						\$199,369



*Statistical Approaches to Aerosol Dynamics for Climate Simulation*

ORGANIZATION Brookhaven National Laboratory				Budget Page No: <u>3</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR McGraw, R				Requested Duration: <u>12</u> (Months) Year 3	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Man-Mo.		Funds Requested by Applicant
			CAL	ACAD	SUMR
1. McGraw, R			2	0	0
2. Wright, D			2		
3. Liu, Y			2		
4.			1		
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. ( 3 ) TOTAL SENIOR PERSONNEL (1-6)			8	0	0
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( 1 ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)			1		
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)					\$70,518
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					\$31,519
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$102,036
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					\$0
E. TRAVEL			1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)		\$0
			2. FOREIGN		
TOTAL TRAVEL					\$0
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					\$0
2. TUITION & FEES					\$0
3. TRAINEE TRAVEL					\$0
4. OTHER (fully explain on justification page)					\$0
TOTAL PARTICIPANTS ( 0 ) TOTAL COST					\$0
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					\$0
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					\$0
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES - ITD Support/Services @ 3.75% of Total Salaries + Fringe Benefits					\$3,902
5. SUBCONTRACTS					\$0
6. OTHER - SHOP SERVICES					\$0
TOTAL OTHER DIRECT COSTS					\$3,902
H. TOTAL DIRECT COSTS (A THROUGH G)					\$105,938
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
39.45% General & Administrative (G&A) on Item (H) Total Direct Costs Less Item (D.) Equipment Plus					
7.0% Material Burden on Item (E) Travel, Item (G.1.) Mat'ls & Supplies, Item (G.5.) Subcontracts & Item (D.) Equipment Plus					
31.2% G&A Common Support on Item (G.4.) Computer Services Plus 20% Organizational Burden,					
11.5% Space Charge, .35% Waste Management Fee & 2.46% Electric Power on Items A+B+C;					
TOTAL INDIRECT COSTS					\$95,266
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$201,204
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					\$0
L. TOTAL COST OF PROJECT (J+K)					\$201,204

**Statistical Approaches to Aerosol Dynamics for Climate Simulation**

ORGANIZATION Brookhaven National Laboratory				Budget Page No: <u>4 - Summary</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR McGraw, R				Requested Duration: <u>36</u> (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)				DOE Funded	
				Man-Mo.	
				Funds Requested	
				Funds Granted	
				by Applicant	
				by DOE	
1.	McGraw, R	7	0	0	
2.	Wright, D	7			
3.	Liu, Y	7			
4.					
5.					
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)				
7.	( 3 ) TOTAL SENIOR PERSONNEL (1-6)	23	0	0	\$197,139
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1.	( ) POST DOCTORAL ASSOCIATES	4			\$24,173
2.	( 1 ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER				
TOTAL SALARIES AND WAGES (A+B)				\$221,313	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				\$90,738	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				\$312,049	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT				\$0	
E. TRAVEL				\$0	
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				\$0	
2. FOREIGN					
TOTAL TRAVEL				\$0	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)				\$0	
2. TUITION & FEES				\$0	
3. TRAINEE TRAVEL				\$0	
4. OTHER (fully explain on justification page)				\$0	
TOTAL PARTICIPANTS ( 0 ) TOTAL COST				\$0	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				\$0	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				\$0	
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES - ITD Support/Services @ 3.75% of Total Salaries + Fringe Benefits				\$11,234	
5. SUBCONTRACTS				\$0	
6. OTHER - SHOP SERVICES				\$0	
TOTAL OTHER DIRECT COSTS				\$11,234	
H. TOTAL DIRECT COSTS (A THROUGH G)				\$323,283	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
39.45% General & Administrative (G&A) on Item (H) Total Direct Costs Less Item (D.) Equipment Plus					
7.0% Material Burden on Item (E) Travel, Item (G.1.) Mat'ls & Supplies, Item (G.5.) Subcontracts & Item (D.) Equipment Plus					
31.2% G&A Common Support on Item (G.4.) Computer Services Plus 20% Organizational Burden,					
11.5% Space Charge, .35% Waste Management Fee & 2.46% Electric Power on Items A+B+C;					
TOTAL INDIRECT COSTS				\$273,647	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				\$596,931	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES				\$0	
L. TOTAL COST OF PROJECT (J+K)				\$596,931	

DOE F 4620.1  
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**BUDGET JUSTIFICATION**

**SECTION**

**A. Senior Personnel** **\$ 97,750**

The personnel costs, as budgeted, include three summer months per year for the Principal Investigator. Faculty monthly summer salaries are budgeted at 1/9 of academic year salary.

SUNY Research Foundation fringe benefit rate is calculated at 15.5% each year.

All salaries in years two through three include a three percent COLA increase per year.

**B. Other Personnel** **\$ 135,655**

Support for two graduate students during the calendar year at a rate of \$19,920 per year per student.

SUNY Research Foundation fringe benefit rates are calculated as follows:

	Year 1	Year 2	Year 3
Graduate Students	12.0%	13.5%	15.0%

Salaries and wages are competitive with those of other public and private research universities of similar research standing to Stony Brook.

**F. Other Direct Costs** **\$ 20,736**

Graduate Student Tuition costs are included for the two graduate students at six credits per year calculated at the current New York State resident rate of \$3,456.

**G. Total Direct Costs** **\$ 254,141**

**H. Indirect Costs** **\$ 128,372**

Indirect costs are calculated on all direct costs, except tuition, at a rate of 55.0%.

**I. Total Cost of Project** **\$ 382,513**

# Cover Page

Scientific Discovery through Advanced Computing  
LAB 06-04

## Local Refinement Methods for Atmospheric Modeling Scientific Application Partnership

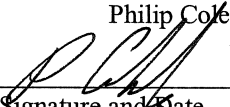
For the period July 1, 2006 – June 30, 2009

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Philip Colella  
  
2/28/06  
PI Signature and Date

Horst Simon  
  
2/27/06  
Official Signature and Date

Co-Investigator(s): **LBNL**: Daniel Martin; **LLNL**: Caroline Bono; **University of Michigan**: Christiane Jablonowski

Requested Funding:      Year 1: \$496,588  
                                    Year 2: \$509,557  
                                    Year 3: \$520,077  
Total Funding Requested: \$1,526,222

Use of Human Subjects: No  
Use of Vertebrate Animals: No





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## 1 Abstract

We will develop a block-structured local refinement simulation capability for global-scale atmospheric modeling, as a Science Applications Partnership under the joint sponsorship of the SciDAC2 Scalable and Extensible Earth System Model for Climate Change Science Project and the Applied Partial Differential Equations Center for Enabling Technology (APDEC). The goal of this project, to be carried out over a three-year period, is to develop a prototype of an atmospheric dynamical core that would be suitable for use in a production climate simulation code such as the Community Climate System Model (CCSM). Our approach will be based on finite-volume discretizations of a non-hydrostatic model for atmospheric fluid dynamics and transport on mapped multiblock (cubed-sphere) grids that are surface-fitted in the vertical direction. Technical issues to be addressed are the behavior of moisture models at refinement boundaries, high-order spatial accuracy, vertical refinement, and the efficacy of dynamic grid adaptation.

## 2 Summary

The desirability of having multiresolution methods is becoming increasingly clear to the climate modeling community. Examples of settings that require localized regions with increased grid resolution include tropical convection, the effects of localized orographic features, and the need to perform detailed studies of regional effects of climate change. Structured local refinement provides a general and flexible approach for providing such a multiscale capability. In this project, we propose developing a block-structured local refinement simulation capability for global-scale atmospheric modeling, as a Science Applications Partnership under the joint sponsorship of the SciDAC2 Scalable and Extensible Earth System Model for Climate Change project (hereafter referred to as the "SciDAC Climate project") and the Applied Partial Differential Equations Center for Enabling Technology (APDEC). The goal of this project, to be carried out over a three-year period, is to develop simulation codes based on local refinement for solving the fluid dynamics and transport equations - the so-called dynamical core - of the atmospheric modeling component of a climate model. At the end of the three years, we expect to have a prototype of a dynamical core that would be suitable for use in a production climate simulation code such as the Community Climate System Model (CCSM). Special emphasis will be placed on parallel computing aspects such as the scalability of the adaptive grid approach and the efficiency of the load-balancing and domain decomposition strategy.

Our approach will be based on finite-volume discretizations of a non-hydrostatic model for atmospheric fluid dynamics and transport. The underlying discretization of space will be surface-fitted in the vertical direction, and mapped-multiblock (cubed-sphere) in the horizontal directions, with block-structured local refinement applied to the rectangular grids in abstract coordinate space. Besides static grid adaptations, we will in particular support dynamic adaptive mesh refinement, with the local grid density changing as a function of space, time, and data. While static zonal refinement has been used in weather prediction applications, such a dynamic strategy has not previously been available in production climate codes.

The implementation of these simulation codes will be built using a C++ framework for AMR calculations developed by APDEC. The present project will be leveraged by software developed under APDEC 2, with close coordination of the planning for both projects.

## 3 Background and Significance

The goal of this research is to develop a novel nonhydrostatic atmospheric general circulation model on a cubed-sphere grid that utilizes innovative numerical and computational techniques allowing for local mesh refinements with ultra-high resolutions in regions of interest. The proposed project has the potential to make

a major scientific contribution to climate modeling. This is especially true with respect to the many multi-scale challenges that future climate system models face. Examples of multi-scale interactions in need of high local resolutions include phenomena like tropical cyclones, convective regions or steep mountainous terrain. The enhanced local mesh resolutions will enable us to capture the small-scale physical processes and to reliably simulate their consequent interactions with the large scale flow.

### 3.1 Review: Nonuniform Resolutions and Adaptive Meshes in Atmospheric Modeling

The use of increased horizontal grid resolutions over areas of interest has been discussed for regional atmospheric modeling over the past three decades (see also the overview in Fox-Rabinovitz et al. (1997)). In particular, both nested grids and stretched grids have been suggested in the literature. Static nested grids are widely used for local weather predictions and regional climate models to downscale a global large-scale simulation. Examples include NCAR's limited-area "Weather and Research Forecasting Model" WRF (Skamarock et al. 2005) and the Canadian Regional Climate Model CRCM (Caya and Laprise 1999). Here, a fixed-size refined grid is permanently embedded in a coarse-resolution General Circulation Model (GCM), which initializes the fine grid and periodically updates the lateral boundary conditions of the nested area. Most often, different sets of equations, physics approximations and numerical schemes are used in the two domains. Therefore, special care must be taken to avoid numerical and physical inconsistencies across the fine-coarse grid boundaries. In addition, nested grids might also be placed within the same model to allow for further refinement steps (Skamarock et al. 2005). Such an approach can also be viewed as a statically adaptive mesh application which considerably improves the consistency along the mesh interfaces. Even multiply-nested movable grids are feasible as demonstrated by Wang (2001) with a primitive-equation model. In this simulation, the grid movement is guided by the position of an idealized cyclone, with the total number of grid points remaining constant during the nested-grid model run.

In general, nested-grid configurations make it possible to combine realistic large-scale simulations with meso-scale forecasts for selected domains. Two coupling strategies need to be distinguished. These are the one-way (Davies 1976) and two-way (Zhang et al. 1986) interaction of the two model areas. The former is the simplest, and predominantly used, nested-grid technique where the fine grid information does not affect the solution in the coarse region. The latter includes a feedback mechanism that updates the coarse grid data with fine grid information wherever the two grids coincide. Typically, ratios between 2-5 are chosen for the resolution jump (Denis et al. 2002).

Stretched grids, on the other hand, vary their resolution rather modestly. Typical stretching factors between neighboring grid points lie in the range of 2-10% (Fox-Rabinovitz et al. 1997, 2006). Stretched spherical grids are most commonly used for global-scale forecast models (Côté et al. 1998; Fox-Rabinovitz et al. 2001; McGregor 2004) that focus their resolution in a single predefined area, and coarsen the grid in distant domains. A clear advantage of the smoothly varying resolution is the minimization of the lateral boundary reflections, which can produce spurious noise at abruptly changing nested-grid interfaces. Stretched grids are therefore an alternative way of downscaling the large-scale circulation to the meso-scale regime while guaranteeing a consistent two-way interaction across the continuous multi-scale mesh. The stretching can be either implemented as a global coordinate transformation as suggested by Schmidt (1977) or in a user-customized fashion. Examples of the conformal Schmidt transformation on a cubed-sphere grid are shown by McGregor (1996, 2005). Here, it is important to note that the total number of grid points stays constant during the simulation as mentioned before for the nested-grid setups. This limits the ability of the model to readily adapt the resolution in multiple regions. Nevertheless, some flexibility is added when movable stretched grids are employed. These can be viewed as global, time-dependent remapping techniques. Recently, such a method was applied to a 3D anelastic nonhydrostatic dynamical core by Prusa and Smolarkiewicz (2003) who used a priori information to steer the global mesh redistribution over time.

In contrast, the goal of dynamic grid adaptations addressed in this proposal is not to move the grid

globally, but rather to refine the mesh at run time to resolve any important physical process that needs additional grid resolution, and to coarsen the grid if the additional resolution is no longer needed. The same algorithmic and software tools are needed to support both static and dynamic refinement, and we will use the term adaptive mesh refinement (AMR) to denote both methods. Dynamically adaptive grids have long been used in astrophysical, aeronautical and other computational fluid dynamics problems (Berger and Olinger 1984; Berger and Colella 1989). However, in atmospheric science they were first applied in the late 80s when Skamarock et al. (1989) and Skamarock and Klemp (1993) published their adaptive grid techniques for 3D regional models in Cartesian coordinates. More recently, Bacon et al. (2000) and Boybeyi et al. (2001) introduced the adaptive non-hydrostatic limited-area weather and dispersion model OMEGA which addresses atmospheric transport and diffusion questions. This model is based on unstructured, triangular grids on the sphere with rotated Cartesian coordinates that can be dynamically and statically adapted to features of interest. Meanwhile, OMEGA has been used as a regional hurricane forecasting system in spherical geometry (Gopalakrishnan et al. 2002; Bacon et al. 2003).

Furthermore, a variety of statically and dynamically adaptive advection models as well as shallow-water codes have been proposed in the literature. An overview of adaptive advection techniques is provided in Jablonowski et al. (2006b) who also applied a block-structured AMR method to the NCAR/NASA Lin-Rood finite volume advection algorithm (Lin and Rood 1996). This approach utilized the spherical block-structured adaptive mesh library by Oehmke (2004). To date, statically adaptive shallow-water models on the sphere were developed by Ruge et al. (1995), Fournier et al. (2004), Barros and Garcia (2004) and Giraldo and Warburton (2005). Dynamically adaptive shallow-water models in the Cartesian geometry were designed by Behrens (1998), Giraldo (2000) and Borthwick et al. (2001). Note that Behrens (1998) and Giraldo (2000) based their approaches on unstructured adaptive mesh triangulations whereas Borthwick et al. (2001) utilized adaptive quadtree grids. Most recently, dynamically adaptive 2D shallow-water codes and a 3D hydrostatic dynamical core in spherical geometry have been introduced. In particular, Jablonowski (2004); Jablonowski et al. (2004, 2006a) discussed a block-structured spherical AMR technique for the NCAR/NASA 3D finite volume primitive-equation model and its corresponding shallow-water version, and Lauter (2004) and Behrens et al. (2005) presented an adaptive 2D shallow-water code with unstructured triangulated meshes.

### 3.2 Challenges and Open Questions

Grid refinement techniques in atmospheric modeling are a relatively new and powerful tool and offer an interesting future alternative to today's standard uniform grid approaches. If adaptive grids are capable of actually resolving selected features of interest as they appear, such as convection in tropical regions, then the corresponding parameterizations can locally be dropped and replaced by the underlying physics principles. This poses new and interesting questions concerning the small-scale large-scale flow interactions. Every scale of atmospheric motion affects every other scale due to the nonlinearity in the equations. Thus the trend of increased spatial resolution for short-term weather predictions and even long-term climate predictions (Duffy et al. 2003) is on-going and today mostly determined by the availability of sufficient computing resources. As a result, resolving the so-called mesoscale phenomena with typical length scales of tens or hundreds of kilometers has been one of the key aspects to improving forecasts in past decades. As pointed out by Boville (1991), improvements can be found in nearly all aspects of the climatic state at finer resolutions. However, Boyle (1993) and Williamson et al. (1995) also noted that improving the horizontal resolution alone does not necessarily lead to a more accurate climate prediction. The nonlinear dynamics-physics interactions demand a careful assessment of the physics parameterizations with respect to the underlying computational mesh. Our team is aware of this challenge.

The discussion about suitable horizontal resolutions raises an important research problem for atmospheric AMR applications. What are the features of interest for an adaptive climate simulation and will the

adaptive model be capable of detecting them early on the relatively coarse initial grid? In meteorological flows that are, from a global climate perspective, dominated by large-scale wave perturbations, detectable features of interest on a coarse grid may be characterized by the atmospheric wave activity with corresponding vorticity patterns, pressure gradients, temperature fronts or tracer distributions.

Adaptive models, even if statically adaptive with only few refinement levels, are expected to play another key role with respect to today's orography treatment in General Circulation Models, especially for climate studies. Static adaptations in mountainous terrain with reinitialized orography profiles can improve the rather crude representation of topographic features on the computational grid. This will lead to a more realistic topographic forcing of waves on all atmospheric scales. As an alternative, static refinement options for climate studies could also include broad bands in the midlatitudes or tropics in order to capture the baroclinic wave activities or dominant tropical convective regions at higher resolutions.

Dynamically and statically adaptive grids offer an attractive framework for future high resolution climate studies that can focus on certain geographical regions or atmospheric events. So far, dynamically adaptive general circulation models on the sphere are not standard in the atmospheric science community. Whether adaptive atmospheric models for climate research will be successfully utilized in the future crucially depends on two major issues. First, it must be shown that adaptive atmospheric modeling is not just feasible, but also accurate with respect to the resulting flow patterns and furthermore, is capable of detecting the features or regions of interest reliably. Second, adaptive model simulations must also be computationally less expensive than comparable uniform high resolution runs. As a consequence and with respect to the fact that climate modeling is a grand-challenge application, any adaptive climate model and its numerics need to perform and scale well on current and future distributed-memory and hybrid parallel computer architectures.

Adaptive modeling is a truly interdisciplinary scientific computing effort. Not only does it raise exciting atmospheric science questions, but also interesting computer science and applied mathematics aspects. Our team, consisting of atmospheric and computational scientists as well as applied mathematicians, is well-prepared to meet this challenge by integrating computational science with a climate-research driven application.

## **4 Preliminary Studies**

### **4.1 Hydrostatic Finite Volume Dynamical Core with AMR**

Climate and weather systems are true multi-scale phenomena that are characterized by widely varying spatial and temporal scales. Solving such a problem more efficiently and accurately requires variable resolution that tracks small-scale features embedded in a large-scale flow. Recently, adaptive grid techniques have been applied to a revised version of the NCAR/NASA current dynamical core for climate and weather research (Lin and Rood 1997; Lin 2004). This hydrostatic global dynamics package in flux form is built upon the conservative Lin and Rood (1996) transport algorithm, which utilizes the oscillation-free Piecewise Parabolic Method (PPM, Colella and Woodward (1984)). The adaptive model design (Jablonowski 2004; Jablonowski et al. 2006b) is based on two fundamental building blocks: a block-structured data layout and a spherical adaptive grid library for parallel processors (Oehmke and Stout 2001; Oehmke 2004). Two model configurations are available: the full 3D hydrostatic dynamical core on the sphere and the corresponding 2D shallow-water configuration that is extracted out of the 3D version. This shallow-water setup serves as an ideal testbed for the horizontal discretizations and the 2D adaptive mesh strategies. The model can be flexibly run with static and dynamic grid adaptations. Static adaptations are used to vary the resolution in pre-defined regions of interest. This includes static refinements near mountain ranges or static coarsenings in the longitudinal direction for the implementation of a so-called reduced grid in polar regions. Dynamic adaptations are based on flow characteristics and guided by refinement criteria that detect user-defined features

of interest during a simulation. In particular, flow-based refinement criteria, such as vorticity or gradient indicators, are implemented. Refinements and coarsenings occur according to pre-defined threshold values.

An example of the block-structured latitude-longitude grid on the sphere is given in Figs. 1(a) and (b). In Fig. 1(b) a single region of interest, an idealized mountain as indicated by the contour lines, is refined at a maximum refinement level of 3. This corresponds to the finest grid resolution of  $0.625^\circ \times 0.625^\circ$ . Each block is self-similar and contains an identical number of grid cells per block. Neighboring blocks only differ by one refinement level (factor of 2) which guarantees accurate inflow and outflow conditions at fine-coarse grid boundaries.

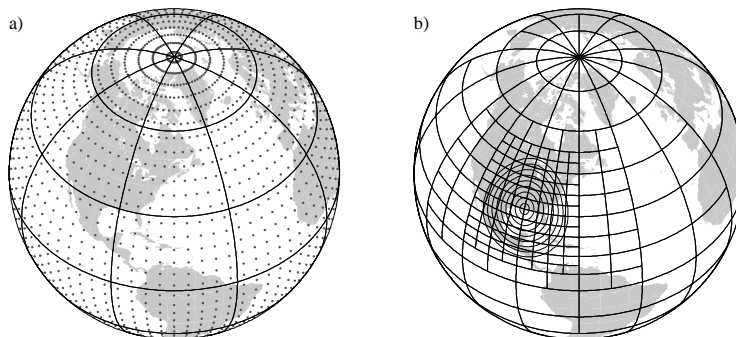


Figure 1: (a) Block-structured latitude-longitude grid with  $6 \times 9$  grid points per block, (b) adapted blocks with 3 refinement levels.

Statically and dynamically adaptive grids have been successfully tested in 2D shallow-water simulations and 3D hydrostatic dynamical core assessments on the sphere. Figure 2(a) shows a 2D shallow-water simulation of a mountain-induced wave at day 15 (test case 5 in Williamson et al. (1992)). The geopotential height field is dominated by a lee wave that propagates into the Southern Hemisphere. Here, a combination of statically and dynamically refined grids is applied. Besides the statically refined orography field, the evolution of the flow field is tracked by a vorticity-based adaptation criterion. It reliably detects the wave train over the course of the simulation. No distortions or noise are visible at fine-coarse grid boundaries.

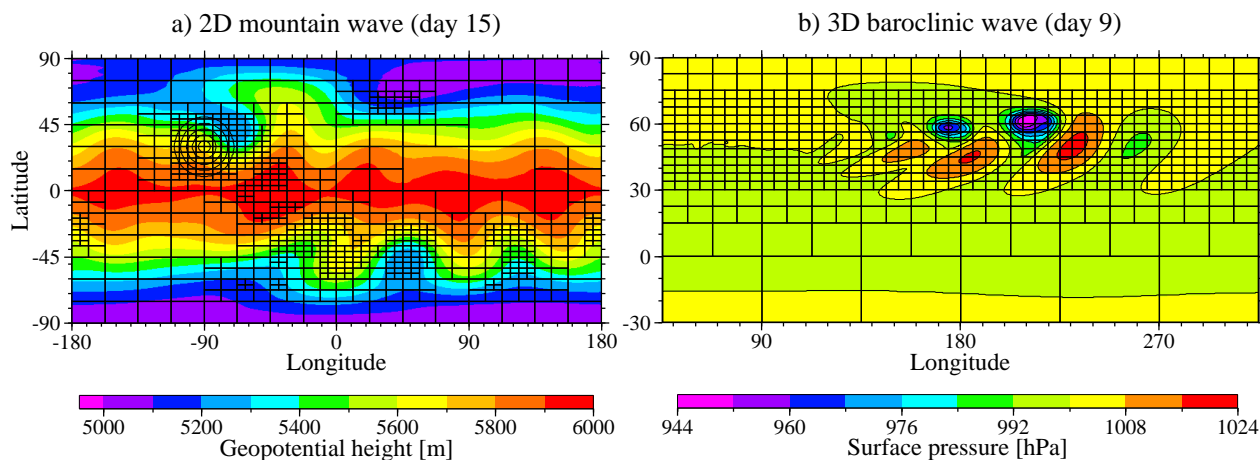


Figure 2: (a) Geopotential height field (day 15) of a 2D shallow-water test case describing the flow over an idealized mountain. The dynamic adaptations with 3 refinement levels are invoked whenever the relative vorticity exceeds the threshold  $|\zeta| \geq 2 \times 10^{-5} s^{-1}$ . (b) 3D baroclinic wave test case with 3 static refinement levels, surface pressure at day 9. The adapted blocks with  $6 \times 9$  grid points per block are overlaid. The finest resolution in both examples is  $0.625^\circ \times 0.625^\circ$ .

In addition, the adaptive 3D hydrostatic dynamical core has been tested with a newly developed idealized test case (Jablonowski and Williamson 2006b,a). This test describes the evolution of a baroclinic wave that is triggered by a small perturbation overlaying the steady state balanced initial conditions. Explosive cyclogenesis can be observed after model day 8. Figure 2(b) illustrates the surface pressure field at day 9 shortly before wave breaking events set in. In this simulation, the static adaptations with 3 refinement levels

( $0.625^\circ \times 0.625^\circ$ ) improve the resolution of the storm track in the Northern Hemisphere. The increased resolution leads to an accurate prediction of the developing system without the need of a fine resolution in the whole model domain. The surface pressure field varies smoothly across grid boundaries and matches the corresponding uniform-grid reference solution very closely (Jablonowski et al. 2006a).

## 4.2 Gravity Waves

Gravity waves develop in climate and weather systems. They propagate at relatively high speeds (about  $300\text{ m/s}$ ), and special care must be taken in an AMR framework to avoid spurious reflections at the coarse/fine boundaries and problems near the poles (Jablonowski (2004)). It is therefore important to have a good understanding of gravity wave dynamics and set the stage for an AMR framework through a formulation with well-posed boundary-value problems.

In Gatti-Bono and Colella (2006), we looked at gravitationally-stratified atmospheric flows at low Mach and Froude numbers and proposed a new algorithm to solve the compressible Euler equations that fulfills the following three requirements:

- the asymptotic limits are recovered numerically;
- the acoustic dynamics, the dynamics due to stiff gravity waves, and the advective dynamics, can be separated out and each treated with a suitable explicit or implicit method;
- the formulation admits well-posed general boundary-value problems, an essential property for the development of block-structured local refinement methods, which, for example, does not hold for hydrostatic models (Oliger and Sundstrom (1978)).

The algorithm is based on an extension of the allspeed projection algorithm developed by Colella and Pao (1999) to the case of an anelastic Hodge decomposition of the velocity field into solenoidal and potential components, along with a corresponding splitting of the pressure field. This splitting is further modified to correctly represent the dynamics of gravity waves for thin layers. This allows us to use an implicit method for treating the acoustic modes, combined with a semi-implicit method for the anelastic dynamics. We combine this method with appropriate spatial discretizations, including an embedded boundary treatment of orography. The resulting method has as a time step limitation the CFL condition for the fast gravity waves. Since the compressible flow equations have a well-posed boundary-value formulation, the overall method is well-posed. In addition, the individual PDEs that are solved in the various substeps have well-posed boundary-value formulations, thus making it a suitable starting point for an extension to locally refined meshes. Furthermore, since the splitting is of the full equations, there is a natural embedding of the thin-layer asymptotics into a more complete fundamental system of equations in multiscale calculations, in which the resolved horizontal scales become locally comparable to the vertical scales.

In a second study (Gatti-Bono and Colella (2005)), we combined the splitting of Gatti-Bono and Colella (2006) with ideas from normal mode analysis to deal with the time scale introduced by gravity waves, which is much shorter than the advective time scale and therefore reduces the time step significantly. The numerical method aims to allow for time steps of the order of the advective time step without sacrificing the accuracy of the slower gravity modes. The components associated with the fast dynamics are computed using vertical normal eigenmodes and corresponding one-dimensional horizontal wave equations obtained from an asymptotic analysis (Gatti-Bono and Colella (2006)). These stable estimates of the fast dynamics replace the unstable components that were calculated with a time step larger than the CFL condition for the fastest gravity wave. Several methods can be used to compute the stable estimates for the fast gravity waves modes depending on the physics of the application at hand. In Gatti-Bono and Colella (2005), we presented an implicit method where the fastest modes were damped. The strength of the method is that it allows for the damping of selected modes, therefore making it possible to damp only the fastest gravity



waves without impacting the dynamics of the slower modes that are physically important. If the fast modes need to be resolved accurately, an explicit method with subcycling in time can be used. This method can be used with a wide variety of numerical methods for compressible equations since it only requires that the acoustic dynamics be treated implicitly.

### 4.3 APDEC Framework

One of the principal characteristics of the algorithms described above is that they are difficult to implement: they are more complicated than traditional finite difference methods, and often the data structures involved are not easily represented in the traditional procedural programming environments used in scientific computing. To manage this algorithmic complexity, we use a collection of libraries written in a mixture of Fortran and C++ that implement a domain-specific set of abstractions for the combination of algorithms described above. In this approach, the high-level data abstractions are implemented in C++, while the bulk of the floating point work is performed on rectangular arrays by Fortran routines.

The design approach used here is based on two ideas. The first is that the mathematical structure of the algorithm domain specified above maps naturally into a combination of data structures and operations on those data structures, which can be embodied in C++ classes. The second is that the mathematical structure of the algorithms can be factored into a hierarchy of abstractions, leading to an analogous factorization of the framework into reusable components, whose natural organization is as a hierarchy of layers.

- **Layer 1:** Classes for representing data and computations on unions of rectangles, including a mechanism for managing the distribution of rectangular patches across processors, and an interface to Fortran for obtaining acceptable uniprocessor performance. This is meant to support an underlying coarse-grained model of SPMD parallelism based on domain decomposition.
- **Layer 2:** Classes for representing inter-level interactions, such as averaging and interpolation, interpolation of coarse-fine boundary conditions, and managing conservation at coarse-fine boundaries.
- **Layer 3:** Interface classes that implement control structures, such as Berger-Oliger timestepping or various iterative methods for solving linear systems, without knowing the details of the data, using a combination of inheritance and class templates. Core solver components for elliptic and hyperbolic PDEs are developed based on these classes.
- **Layer 4:** Implementations of specific applications or classes of applications using these tools, such as a Berger-Oliger algorithm for hyperbolic conservation laws or for incompressible flow, and AMR multigrid for Poisson's equation.
- **Utility Layer:** Support for problem setup, I/O, and visualization that leverages existing de-facto standards, such as I/O, which is built on top of HDF5.

The resulting framework leads naturally to parallel implementations, with the low-level communications hidden from the user by the Layer 1 and Layer 2 APIs, and the SPMD semantics of loops over patches requiring full reentrancy of patch-level modules.

We have developed the basic infrastructure corresponding to Layers 1 and 2 in the APDEC architecture required to support AMR calculations both for problems without complex geometries and for embedded boundary methods. This includes parallel data structures for data defined on nested hierarchies of unions of rectangles; high-level interfaces for exchanging ghost cells between rectangular patches at the same level; averaging and interpolation between different levels of refinement; tools for the computation of coarse / fine boundary conditions and for maintaining conservation at refinement boundaries for finite-volume discretizations. We have a variety of tools for grid generation and load balancing, including efficient implementation

of Berger-Rigoutsos and fixed-size patch grid generators, and of localized knapsack and space-filling curve algorithms for load balancing.

We have also developed interface classes including ones for Berger-Oliger time stepping, and for the iterative methods such as point relaxation, BiCGStab, multigrid, and AMR-multigrid. We have implemented a variety of solvers based on these interfaces, including parallel solvers for second-order accurate finite-volume discretizations of self-adjoint elliptic problems on unions of rectangles, and on nested-grid hierarchies. We have developed unsplit higher-order Godunov methods, with both PLM and PPM spatial discretizations, for first-order hyperbolic systems in both conservative and quasilinear form, with user-supplied physics-dependent operations provided through an interface class.

## 5 Research and Design Methods

### 5.1 Algorithmic and Design Choices

#### 5.1.1 The Dry Nonhydrostatic Shallow-Atmosphere Equations

We propose utilizing the fully compressible nonhydrostatic equations with a shallow-atmosphere approximation. Such an approximation is justified for models with model tops below 100 km which is the primary region of interest for climate applications. The nonhydrostatic equations are chosen to allow for local mesh refinements down to a scale of a few kilometers. In particular, the nonhydrostatic approach guarantees consistent well-posed boundary conditions at internal mesh interfaces. The equations of motion for the velocity components  $\vec{v} = (u, v, w)$  in spherical longitude-latitude  $(\lambda, \varphi)$  coordinates with a vertical  $z$  coordinate (height above ground) are given by

$$\begin{aligned} \frac{du}{dt} - \frac{uv \tan \varphi}{a} - f v + \frac{1}{\rho a \cos \varphi} \frac{\partial p}{\partial \lambda} &= F_u \\ \frac{dv}{dt} + \frac{u^2 \tan \varphi}{a} + f u + \frac{1}{\rho a} \frac{\partial p}{\partial \varphi} &= F_v \\ \frac{dw}{dt} + \frac{1}{\rho} \frac{\partial p}{\partial z} + g &= F_w \end{aligned}$$

with  $t$  being time and

$$\frac{d}{dt}(\cdot) = \frac{\partial}{\partial t}(\cdot) + \frac{u}{a \cos \varphi} \frac{\partial}{\partial \lambda}(\cdot) + \frac{v}{a} \frac{\partial}{\partial \varphi}(\cdot) + w \frac{\partial}{\partial z}(\cdot).$$

Here,  $a$  denotes the Earth's radius,  $g$  indicates the (constant) gravitational acceleration,  $\rho$  stands for the density of dry air,  $p$  symbolizes the pressure and  $f = 2\Omega \sin \varphi$  is the Coriolis parameter with  $\Omega$  the angular rotation rate of the earth.  $(F_u, F_v, F_w)$  represent frictional forces. In addition, the mass continuity equation for dry air in conservation form is expressed by

$$\frac{\partial \rho}{\partial t} + \frac{1}{a \cos \varphi} \left[ \frac{\partial(\rho u)}{\partial \lambda} + \frac{\partial(\rho v \cos \varphi)}{\partial \varphi} \right] + \frac{\partial(\rho w)}{\partial z} = 0$$

The thermodynamic equation and ideal gas law for dry air are given by

$$\begin{aligned} \frac{dp}{dt} &= \frac{c_p}{c_v} R_d T \left( \frac{d\rho}{dt} + \frac{\rho Q}{c_p T} \right) \\ p &= \rho R_d T \end{aligned}$$

where  $T$  is the temperature,  $R_d$  stands for the dry specific gas constant,  $Q$  represents the time rate of heating/cooling per unit mass and  $c_p$  and  $c_v$  denote the specific heat at constant pressure and at constant volume, respectively.

In the design phase of the project we will discuss a variety of forms of this equation set, e.g. the vector-invariant and flux forms, while taking map scale factors for the cubed-sphere geometry into account. In addition, the vertical coordinate  $z$  will be transformed to a terrain-following coordinate system (see also discussion in the following section). Initially, we will implement and evaluate the dry dynamical core and its corresponding single-level shallow-water version. At a later stage, moisture will be added to the system which leads to slight changes in the equation set. These are for example outlined in Skamarock et al. (2005).

### 5.1.2 The Grid: “Cubed-Sphere” Approach

The main concern when describing a spherical geometry is the possibility of getting a potential singularity at the poles as is the case with spherical polar coordinates or lat-long grids. We will use a “cubed-sphere” mapping (Ronchi et al. (1996)). It is a mapped grid method in which the six faces of a unit cube are projected onto the spherical physical domain and determine six identical regions on the sphere. Four regions line the equator and two regions are centered around the poles. On each of these regions, a local spherical coordinate system is defined. For the four patches along the equator, this corresponds to the usual spherical coordinates and for the patches centered at the geographical pole, the coordinate system passes through the geographical equator. In the vertical direction, the bottom of the grid is mapped to follow the orography. Some of the coordinate systems traditionally used include the Gal-Chen and Sommerville terrain-following coordinate system (Gal-Chen and Sommerville (1975)) and the terrain-following hydrostatic pressure coordinate system (Laprise (1992)), and we will support all of them since they are all the same mathematical object.

We can choose the dependent velocity variables to be the spherical variables with respect to each local spherical coordinate system. The introduction of six separate coordinate systems has the major advantage of preventing any singularity, but generates internal boundaries and the method used for coupling these different coordinate systems is crucial for the accuracy and stability of the solutions of the PDEs at hand. We will treat the internal boundaries very much like normal boundaries and use interpolation to compute the operator stencils for the different patches as shown in Figure 3. This is very similar to the ideas used for overset grids methods. Two of the main advantages are that the interpolation is well-defined even at the corners where three regions intersect, and that the interpolation can be done to any order preventing any loss of smoothness or accuracy at the block boundaries.

### 5.1.3 Numerical Method

We will use a finite-volume method to discretize the equations. The image of a cubic control volume in the mapping space becomes a control volume in physical space. The integral of a conserved quantity over a volume becomes a finite volume variable. The integrals of fluxes over faces define the numerical fluxes from which finite volume discretizations are defined. At the boundaries between the blocks, the fluxes are multivalued because they can be computed from either side of the boundary since each block face has its own set of ghost cells. For hyperbolic problem, we choose the upwind value and for elliptic problems, we use an average of the two flux values.

The fully compressible non-hydrostatic equations for a shallow atmosphere contain a background advection and a hierarchy of stiff waves: horizontal and vertical acoustic waves and horizontal gravity waves. We will explore several design options for handling the stiff waves. Because the acoustic waves impose a sharp restriction on the time stepping but do not have a significant effect on the dynamics of the atmosphere, we will at least treat the vertical acoustic waves implicitly. We will also consider treating all the acoustic waves

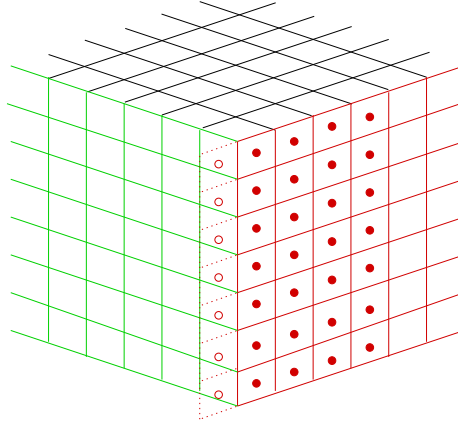


Figure 3: Intersection of 3 grids in the plane, analogous to the three-grid intersections that would appear in a cubed-sphere mapping. The red dashed lines correspond to ghost cells. The red dots represent a cell-centered quantity on the red grid and the open circles represent the quantity interpolated to the ghost cell.

implicitly through an anelastic allspeed method (Gatti-Bono and Colella (2006)). Each of these approaches have well-posed boundary conditions provided that the CFL condition is not violated. In Gatti-Bono and Colella (2006), backward-Euler is used in time, and the velocity is split into a cell-centered solenoidal part and a face-centered potential part containing the acoustic motions, through a projection method. The pressure is decomposed as well to separate the effects of the acoustic waves and the gravity waves. The acoustic pressure is solved implicitly with an elliptic solver that uses multigrid on anisotropic grids and is scalable in parallel. The small mesh spacing in the vertical direction requires a special smoother and this can be done either with semi-coarsening or line relaxation.

Advection will be treated either with unsplit PPM (Colella and Woodward (1984); Miller and Colella (2002)), or with a method of lines which combines fourth-order Runge-Kutta in time and PPM in space. The transported quantities (*e.g* mass) often have a positivity requirement which can be addressed through the use of limiters. The van Leer limiters generate a loss of accuracy at the extrema and bring the order down to first order. We want to achieve higher orders of accuracy, so we will use a combination of the flux-corrected transport limiters (Zalesak (1979)) and of the redistribution method presented in Hilditch and Colella (1997) that permits the combination of conservation and positivity for the advected quantities, together with higher-order accuracy at extrema.

#### 5.1.4 Adaptive Mesh Refinement

Our approach to multiresolution discretizations is based on a finite-volume version of the block-structured adaptive mesh refinement (AMR) algorithms of Berger and Olinger (1984) and Berger and Colella (1989). In this approach, the regions to be refined are organized into rectangular patches of several hundred to several thousand grid cells per patch. Thus, one is able to use the finite-volume rectangular grid methods described above as underlying discretization methods. Furthermore, the overhead in managing the irregular data is amortized over a relatively large amount of floating point work on regular arrays. For time-dependent problems, refinement is performed in time as well as in space. Each level of spatial refinement uses its own stable time step, with the time steps at a level constrained to be integer multiples of the time steps at all finer levels.

For the “cubed-sphere”, the refinement is done in the mapping space (Bell et al. (1989)) and leads to coarse/fine patches in physical space with each region having its own AMR hierarchy. The refinement

patches are therefore not allowed to cross the block boundaries. A refinement ratio of 4 will be used. The use of a smooth mapping within each block will eliminate spurious artifacts due to mesh interpolation (Dudek and Colella (1998)). The implicit solvers use geometric multigrid methods that work well in an AMR setting. For atmospheric flows, there are two options when refining: refining in the horizontal direction only or refining in the horizontal and vertical directions. We are planning to start with a refinement in the horizontal direction only, as it is most commonly done, and, during the course of the project, we will evaluate whether vertical refinement is needed.

We can foresee two major challenges when introducing refinement. The treatment of gravity waves must ensure that the problem is well-posed so as not to get spurious reflections at the coarse/fine boundary. Another problem that has been encountered when doing AMR is that of large errors in the moisture dynamics at refinement boundaries. These errors are thought to be driven by numerical artifacts in the horizontal divergence (Tribbia (2006)), which we will attempt to eliminate using techniques to preserve freestream conditions in AMR for incompressible flows (Martin and Colella (2000)).

## 5.2 Critical Design Issues

### 5.2.1 Accuracy

One of the main questions is the level of spatial accuracy required for long-time integration of climate models, particularly in connection with advective transport over long distances. Our baseline PPM discretization is fourth-order in space when viewed as a nodal point scheme. However, when viewed as a finite volume method, it is only second-order accurate, because the replacement of averages over cells and faces by their corresponding values at the centroids of those locations is only correct to second order in the mesh spacing. This becomes particularly apparent in connection with AMR, where the averaging of fluxes at grid-refinement boundaries is only as accurate as the quadrature used to compute the integrals of fluxes over the faces. For that reason, the two methods that we proposed in the previous section are only second-order accurate. Our approach to designing a fourth-order accurate finite-volume solver on AMR grids will be based on the ideas in Barad and Colella (2005), in which fourth-order accurate quadrature methods are used to convert between point values and average values. The APDEC center will be developing infrastructure for such solvers, which will provide the basis for our efforts in this area.

### 5.2.2 Stiff Gravity Waves

Because the fast gravity waves, *i.e.* the waves faster than the background advection, are stiff, they can restrict the time step through the CFL condition. In Gatti-Bono and Colella (2005, 2006), we presented a splitting method that separates the acoustic dynamics from the buoyant dynamics. The fastest gravity waves in the limit of a thin layer atmosphere propagate in the horizontal direction, and a vertical mode analysis yields a collection of two-dimensional wave equations for each normal mode corresponding to a mode of gravity wave propagation (Temperton and Williamson (1977, 1981); Williamson and Temperton (1981); Tribbia (1984); Temperton (1988)). All but a few of the two-dimensional waves have high wave speeds, with the remainder being resolved by the advective time step. By separating out that small number of stiff modes, and solving the corresponding wave equations in two dimensions using subcycling or an implicit method, we can use a time step for the remainder of the dynamics that is constrained only by the CFL condition for advection, leading to a more accurate and efficient method.

### 5.2.3 Inclusion of Moisture

The treatment of moisture processes is a challenging aspect in climate models. This is not only due to the relatively coarse resolutions of GCMs that are generally much coarser than the scales of most clouds but also

due to unique numerical problems when approximating cloud and precipitation phenomena. The numerical challenges are partly related to the wide range of moisture variables and values that can extend over several orders of magnitude.

We will include two water substances, water vapor and liquid water, in our modeling approach while paying special attention to their treatment at internal fine-coarse grid boundaries. This will ensure the consistency of the moisture processes across multiple scales. The ratio of the density of water vapor  $\rho_v$  to the density of dry air  $\rho$  is defined as the mixing ratio  $q_v = \rho_v/\rho$ . Analogous to the mass continuity equation, the changes in the amount of water vapor must be balanced by the moisture sources and sinks. In particular, the water vapor budget is described by the conservation law

$$\frac{\partial(\rho q_v)}{\partial t} + \frac{1}{a \cos \varphi} \left[ \frac{\partial(\rho q_v u)}{\partial \lambda} + \frac{\partial(\rho q_v v \cos \varphi)}{\partial \varphi} \right] + \frac{\partial(\rho q_v w)}{\partial z} = M + \rho E$$

where  $M$  is the time rate of change of water vapor per unit volume due to condensation (or freezing if ice particles are included) and  $E$  symbolizes the time rate of change of water vapor per unit mass due to evaporation from the surface and subgrid-scale diffusion in the atmosphere. A similar equation holds for the mixing ratio  $q_l$  of liquid water substances which comprises both cloud and precipitating rain droplets. The conservation law is given by

$$\frac{\partial(\rho q_l)}{\partial t} + \frac{1}{a \cos \varphi} \left[ \frac{\partial(\rho q_l u)}{\partial \lambda} + \frac{\partial(\rho q_l v \cos \varphi)}{\partial \varphi} \right] + \frac{\partial(\rho q_l w)}{\partial z} = -M - \rho E$$

where  $M$  and  $E$  represent the sources and sinks of liquid water, respectively. It is important to note that latent and sensible heat is exchanged if condensation and evaporation processes occur. These energy conversions will get incorporated into the nonadiabatic term  $Q$  of the thermodynamic equation discussed earlier in section 5.1.1.

We will address several moisture and simplified cloud processes during the course of the project. These include large scale condensation experiments and the inclusion of a convection scheme following Emanuel and Zivkovic-Rothman (1999).

#### 5.2.4 Dynamics & Physics Interplay

In atmospheric modeling, sub-grid scale processes that remain unresolved by chosen uniform grid resolutions are parameterized to take their average effect on the resolvable features into account. Generally, these parameterizations are grid-dependent although the scale of the grid box is not explicitly accounted for in physical packages. However, since the parameterizations are calculated for individual grid boxes, the scale of the forcing decreases with increasing horizontal mesh resolution. This raises questions concerning the convergence of model results. In particular, it is important to note that an increase in resolution does not necessarily lead to improved model predictions due to complex, nonlinear interactions between the dynamics and physics packages (Williamson 1999). For example, an increase in resolution might increase the sensitivity to errors in the modeled physical processes that can decrease the overall forecast quality. Therefore, grid-scale dependent parameterizations must be carefully examined when demanding that they function reliably over a wide range of grid scales.

This is in particular true for nested or adaptive mesh applications. For example, Skamarock and Klemp (1993) observed that the truncation error estimates in adaptive grid simulations with parameterized physics do not exhibit the expected rate of decrease when refining the mesh. Even error increases were apparent that cannot be found in dynamical core simulations without parameterized physics. As a consequence, a fundamental concern in adaptive mesh applications is the validity and consistency of grid-scale dependent physical parameterizations that are used over a wide range of refinement levels.

In addition, the influence of the lower boundary conditions in adaptive mesh applications is of equal importance. Atmospheric models rely on worldwide data sets for surface elevation, land/water coverage, soil types, land use, deep soil temperatures, deep soil moisture and sea surface temperatures at varying grid resolutions. These are used to derive important secondary parameters such as the surface roughness and albedo. Therefore, in adaptive mesh applications, the treatment of the refined lower boundary conditions needs to be carefully addressed in order to improve the overall accuracy.

We suggest following an incremental approach that focuses on the most dominant open research questions. In particular, we will assess selected physics parameterization packages like NCAR's radiation scheme in the Community Atmosphere Model CAM3 as well as simplified moisture modules to evaluate their behavior at fine-coarse grid boundaries. Here, special attention will be paid to avoiding spurious rainfall patterns at internal boundaries. In addition, we will assess adaptive orography fields with both idealized and real orography data sets.

### 5.2.5 Vertical and Horizontal Refinement

Setting the right criteria for grid refinements and coarsenings is very important due to the computational cost associated with adaptations. The ideal criteria are those that require minimum computational efforts to evaluate and still indicate the refinement and coarsening regions reliably. In general, two basic adaptation principles need to be distinguished, namely, the "physical" flow-based adaptation indicators and the local truncation error estimators. The latter are built upon a purely numerical approach since they limit the global solution or local discretization error of the numerical scheme. This technique was for example used by Berger and Olinger (1984) and further assessed by Skamarock (1989) and Skamarock and Klemp (1993). Here, Richardson-type truncation error estimators were applied that are based on the difference of the numerical solution on fine and coarse overlapping meshes. In practice though, flow-based adaptation criteria are predominantly used in adaptive grid applications. They typically rely on measures of a solution gradient or curvature that are compared to user-defined and problem dependent thresholds. In addition, assessments of the vorticity, potential vorticity, divergence or instability indicators like the Richardson number are feasible options for atmospheric AMR applications.

The key question is what the regions or features of interest in a short-term or long-term model run are. This question will be addressed during the course of the project. In particular, we will evaluate a variety of flow-based refinement and coarsening strategies and furthermore assess static refinement regions in mountainous terrain. The chosen criterion must be well-suited to the atmospheric research problem. Here, numerous decisions need to be made. Among them are the choice of the vertical level at which a refinement criterion is evaluated as well as the selection of one or more primary model variables. Alternatively, post-processing quantities, like the mean sea level pressure or potential vorticity gradients on isentropes (as in Hubbard and Nikiforakis (2003)), could be assessed that, as a consequence, would require extra computations during the adaptation cycle. It is important to point out that the length of an ideal adaptation cycle is also problem-dependent. It relies on the time scales of the features of interest; for example quickly changing cloud systems require very short assessment periods on the order of minutes. On the other hand, the evolution of a low pressure center can be sufficiently captured on a time scale of hours. In any case, it must be guaranteed that the tracked feature cannot be transported out of the refined area during the selected time interval. This creates a fine balance between accuracy and computational overhead.

Primarily, our research will be focused on horizontal refinement regions that are able to scale the global domain down to the nonhydrostatic regime (on the order of a few kilometers). This raises important questions with respect to the vertical resolution. As pointed out by Lindzen and Fox-Rabinovitz (1989) and Fox-Rabinovitz and Lindzen (1993) inconsistencies between the horizontal and vertical resolutions could arise. Therefore, assessing the feasibility of vertical refinement regions is indicated.

### 5.3 Software Development

This project depends on the use of the APDEC framework for AMR methods. APDEC will be responsible for developing the Layer 1 - Layer 3 components of the mapped multiblock infrastructure (see section 4.3), which the present team will use as a basis for developing the atmospheric model. We will also conform to the software development standards of the APDEC team. In particular, we will use the following staged development of new capabilities in the project.

(i) A design document is created and updated regularly. This document contains a mathematical description of the algorithm and / or programming abstractions, and a description of the application programming interface (API), in terms of function prototypes or C++ class headers. The document will also describe in detail the test programs that will be implemented and outline what criteria are met by passing the tests.

(ii) After step (i) is complete, the API prototypes are coded, followed by the test programs, followed by the API implementation. At this point debugging commences until all tests pass. Additional tests may be added throughout this process. Completion of this phase of the development process is documented with a written report, as well as the submission of the completed software and tests for review. Also, at this time, reference manual entries for the software must be generated from annotated header files using doxygen.

(iii) After step (ii) is complete, the software is released for validation.

At the end of each step, a review will be performed by both APDEC and the SciDAC Climate Project, before the work in the next step is begun.

### 5.4 Evaluation Methods

During all stages of the modeling project we will assess our progress and performance with adequate test cases. Our evaluation methods are split into two parts: the 2D shallow-water assessments and the 3D dynamical core tests. This split reflects our incremental approach to the modeling effort and ensures the quality of each milestone. We propose testing our finite-volume discretization on the cubed-sphere grid with the following selected test cases. Each test covers unique scientific and numerical modeling aspects. The order of the test cases indicates the increase in complexity for each step.

**Evaluation of the horizontal discretization: 2D shallow-water tests.** The shallow-water equations describe the nonlinear flow of an incompressible fluid. They represent the 2D atmospheric flow conditions in a single hydrostatic atmospheric layer and are therefore considered an idealized test-bed for all 3D atmospheric model developments. In particular, the shallow-water system addresses the majority of the modeling challenges that are associated with the temporal and horizontal discretization techniques in spherical geometry. These include the choice of the horizontal grid, the treatment of high-speed gravity waves, numerical dispersion and the stability of the numerical scheme. Within the climate modeling community, any novel numerical methodology will not be widely accepted unless it successfully passes the standard test suite for the spherical shallow-water equations as suggested by Williamson et al. (1992).

- **Tests of the advection algorithm.** Atmospheric motions on all scales are dominated by the advection process. The numerical solution to the advection problem is therefore fundamentally important for the overall accuracy of the flow solver. Besides the classical smooth cosine bell advection test we will also test the advection component with the solid-body rotation of a slotted cylinder that exhibits very sharp edges (Zalesak 1979). Furthermore, we will apply a challenging cyclogenesis test problem with a deformational flow (Nair and Machenhauer 2002; Nair et al. 2005) that describes the wrap-up of a vortex with increasingly stronger gradients over time. This test case mimics the observed evolution of cold and warm frontal zones. All advection tests are also idealized candidates for local mesh refinements.



- **Global steady-state nonlinear geostrophic flow.** This fundamental test case for the full nonlinear shallow-water system assesses the models ability to maintain a steady-state solution over time. It is the simplest measure of the adequacy of the numerical approach.
- **Forced nonlinear system with a translating flow.** The test evaluates the performance of the numerical scheme on the unsteady forced shallow-water equations. The flow field comprises a translating low pressure center in the Northern Hemisphere that is superimposed on a westerly jet stream. This setup resembles the observed properties of atmospheric flows in the middle troposphere (at about 5km above ground). The low pressure center is furthermore an ideal feature for local mesh refinements that, for example, resolve the predefined storm track at higher resolutions.
- **Zonal flow over an isolated mountain.** The test describes a zonal flow over an idealized mountain that generates a downstream wave train, shedding vortices in its wake. The initially smooth flow field develops sharp gradients and distinct vorticity patterns that provide an excellent opportunity to test the adaptive grid functionality. Both static mesh refinements near the mountain and dynamic flow-driven adaptation criteria will be assessed.
- **Rossby-Haurwitz wave.** Rossby-Haurwitz waves are the exact solutions to the nonlinear barotropic vorticity equation. In a shallow-water model, these solutions move from west to east without change of shape before numerical dispersion and truncation errors distort the regular wave pattern. In general, the flow resembles the horizontal structure of large-scale atmospheric weather systems. It exhibits very strong gradients and high wind speed regimes that allow an assessment of the diffusion, dispersion and stability properties of the horizontal and temporal discretization.

**Evaluation of the 3D nonhydrostatic dynamical core.** We propose testing the 3D nonhydrostatic dynamical core with a hierarchy of well-known and newly-developed test cases. These include tests of the dynamical core with and without the Earth's rotation as well as model runs in a quasi-climate mode. This approach not only allows us to test physical phenomena in isolation but also provides insight into the long-term model behavior and stability of the numerical method.

### Test cases for the non-rotating sphere

- **3D Advection tests with and without underlying orography fields.** We propose extending the 2D advection experiments by Schär et al. (2002) and Nair and Machenhauer (2002) to three dimensions in spherical geometry. The Schär et al. (2002) test case evaluates the advection of a tracer in the presence of idealized mountain ranges and therefore assesses the influence of an orography-following vertical coordinate system on the advection process. The deformational flow problem by Nair and Machenhauer (2002) describes the roll-up of one or two vortices in the global model domain and resembles the cyclogenesis processes in the atmosphere. These tests will be essential to testing the pure 3D advection algorithm.
- **Acoustic waves.** Acoustic waves can be triggered when perturbing a homogeneous pressure field in an isothermal atmosphere (see also Tomita and Sato (2004)). This test will assess the ability of the nonhydrostatic model to handle and damp out acoustic wave fields. In particular, it will test our implicit numerical treatment of the acoustic modes.
- **Gravity waves.** Similarly, gravity waves are triggered when perturbing the potential temperature distribution instead of the pressure field. Here, tests with a constant Brunt-Väisälä frequency will be performed that can be considered a 3D extension of the 2D Skamarock and Klemp (1994) gravity wave test problem. The test will be used to evaluate our treatment of high-speed gravity waves.
- **Mountain-induced gravity waves.** Gravity waves are also triggered by orographic features. We suggest performing a sequence of 3D mountain wave test cases as proposed by Qian et al. (1998). This requires the formulation of an idealized mountain profile like the bell-shaped witch-of-Agnesi curve and the inclusion of a sponge layer at upper levels. Different flow fields as well as mountain shapes and heights will be assessed.

The chosen parameters determine whether the model is in a hydrostatic or nonhydrostatic flow regime. In addition, linear (small-amplitude) and nonlinear (finite-amplitude) mountain waves will be investigated as determined by the inverse Froude number. This test is an ideal candidate for hydrostatic and non-hydrostatic adaptive-mesh simulations that focus their resolutions on the mountainous terrain.

### Test cases for the rotating sphere

- **Equatorially trapped Kelvin and mixed Rossby-gravity waves.** Following Gill (1980), Hoskins and Jin (1991) and Jin and Hoskins (1995) equatorial Kelvin and mixed Rossby-gravity waves can be triggered by a prescribed equatorial heat source. The heating pattern leads to a pair of westward traveling cyclones (the Rossby wave response) and eastward traveling wave packets (the Kelvin wave response). The latter have typical wavenumbers of 1 or 2 and long 11-15-day periods. This test assesses the global large-scale model response to localized thermal forcing mechanisms.
- **Rossby wave train triggered by idealized orography.** The 3D Rossby wave test can be considered a 3D extension of the 2D shallow-water flow over an idealized mountain (test case 5 in Williamson et al. (1992)). As shown in Qian et al. (1998), Smolarkiewicz et al. (2001) and Tomita and Sato (2004), the Rossby waves are induced by an idealized orography field. As in the irrotational mountain wave test case, different scenarios will be assessed. These include the hydrostatic and nonhydrostatic flow regimes for linear and nonlinear mountain waves. The use of local mesh refinements will be addressed.
- **Baroclinic waves in midlatitudes with and without moisture processes.** This test will be based on the deterministic Jablonowski and Williamson (2006b,a) baroclinic wave test case with added moisture fields, large-scale condensation and a convection scheme (e.g. the Emanuel and Zivkovic-Rothman (1999) convection algorithm). Adaptive mesh refinements can be applied along the storm track in the Northern Hemisphere where intense low and high pressure systems evolve over time. Here, precipitation is expected to develop along the sharp frontal zones. Such a test will be a step towards a full GCM with adaptive mesh functionality.

### Model evaluations in climate mode

- **Held-Suarez test with and without moisture.** In order to assess the statistical long-term behavior of the model we suggest running the dry Held and Suarez (1994) dynamical core benchmark. The test requires 1200-day model integrations with simple, pre-defined forcing functions that entirely replace the complex physics parameterization package. Most recently, a moist variant of the test has also been suggested by Galewsky et al. (2005). Here, a waterlike tracer is emitted at the surface and lost due to large-scale condensation processes. Both the dry and moist variants of the test are adequate representatives of idealized climate runs that in particular allow an assessment of local mesh refinement strategies for long-term model simulations. In addition, adaptive Held-Suarez tests with idealized and real orography fields are feasible.
- **Aqua-planet simulations.** An even more complex but still idealized test case for long-term climate model assessments has been proposed by Neale and Hoskins (2001). In these so-called aqua-planet simulations, the full physics parameterization package is retained but the lower boundary condition is drastically simplified. In particular, the complex land-surface model is replaced with a flat ocean surface using prescribed sea surface temperatures. We will assess variants of the aqua-planet experiment as soon as physics parameterization modules are added to our nonhydrostatic dynamical core. These will for example include NCAR's CAM3 radiation module and simple moisture processes.

## 6 Milestones

The project will be composed of two phases of 18 months each. In the first phase, we will develop a baseline version of the AMR mapped multiblock algorithm, using second-order accurate discretizations, semi-implicit treatment of acoustic waves, and horizontal refinement. At the end of the first phase, we evaluate the performance of that algorithm, and in consultation with the SciDAC Climate project determine which of the possible algorithmic improvements (e.g. fourth-order discretizations, vertical refinement, semi-implicit treatment of gravity waves) are needed, and plan the second phase of the project accordingly.

### 6.1 Phase I

**3 Months.** At the beginning of the project, we will meet with the investigators from the main climate program and define the requirements for our project including:

- **Scientific design document.** (lead: Jablonowski) This document will lay out the fluid equations and the physics modules for simplified moisture processes and radiation. In addition, we will address the interface for the orography database and the validation suite.
- **Algorithm design document.** (lead: Bono and Martin) This document will present our strategy for mapped multiblock and address top-level solver design issues. In particular we will discuss the different options for semi-implicit methods. We will present the discretization including possible fourth-order finite volume on mapped grids and time stepping. We will also discuss vertical refinement.
- **Software design document.** (lead: Bono and Martin) This document will address the software components of the low-level layers, such as multiblock and parallel communication in layer 1 or interpolation and flux accumulations in layer 2, and support for anisotropic refinements. We will define the tests that we will perform for verification and validation. We will present the plan for interoperability with the various frameworks for production climate codes, including CCSM, the Model Coupling Toolkit (MCT), and the Earth System Modeling Framework (ESMF).

#### 12 Months

- **Validation of the 2D shallow-water model.** (lead: Jablonowski) The shallow-water model provides an idealized testbed for the forthcoming 3D model developments. At this stage, we will thoroughly evaluate and review the numerical method and its implementation using a shallow-water test suite. AMR aspects will be discussed.
- **Verification of the prototype dry 3D dynamical core without rotation.** (lead: Bono and Martin) We will assemble the different solvers provided by APDEC into a prototype code for a dry atmosphere with no rotation. We will have implemented horizontal refinement capabilities and we will give the user two options to treat the acoustic waves by having a switch between using an allspeed method and treating the acoustic waves implicitly in the vertical direction only. The advection will be treated explicitly.

#### 18 Months

- **Implementation of baseline moisture processes.** (lead: Jablonowski) We start including moisture in our model which requires slight changes in the equation set. At this stage, we will assess the potential problems with moisture processes at fine-coarse grid boundaries that have traditionally been observed in AMR and nested grid applications. Our strategy will focus on avoiding spurious noise and rainfall at grid interfaces.
- **Validation of the dry 3D dynamical code without rotation.** (lead: Jablonowski)
- **Verification of the 3D implementation including rotational effects.** (lead: Bono and Martin)
- **Baseline testing of idealized (prescribed) adaptive orography fields.** (lead: Bono and Martin)
- **Baseline performance measurements.** (lead: Bono and Martin)

## 6.2 Decisions at the 18-Month Mark

At the 18-month mark, we expect to meet with the main climate project and evaluate the current milestones as well as discuss the additions of capabilities for the remainder of our project. We will first evaluate what needs to be implemented to have a well-behaved formulation that includes moisture. We will determine what improvements are required and plan how to carry them out. Possibilities include improving the numerical code by using higher-order schemes, treating the stiff gravity waves implicitly or by subcycling in time, or refining in the vertical direction.

## 6.3 Phase II

### 24 Months

- **Initial implementation of the improvements defined at the 18-month mark.** (lead: Bono and Martin)
- **Coupling to real orographic databases.** (lead: Bono and Martin) We will address the initialization issues with real orography fields in AMR applications. The standard high-resolution orography databases used in NCAR's mesoscale model WRF will be utilized.
- **Validation of the 3D dynamical core with rotation and simplified moisture processes.** (lead: Jablonowski) At this stage we will apply comprehensive idealized test cases that reveal the short-term model behavior. Both dry and moist model runs will be performed which not only assess small-scale and large-scale model responses but also the numerical treatment of internal boundaries in the AMR setup.
- **Creation of an interface with production climate codes.** (lead: Bono and Martin) We will evaluate the physics-dynamics coupling interface in NCAR's Community Atmosphere Model CAM3 and devise strategies for a coupled nonhydrostatic run. The target application will be an aqua-planet simulation.

### 30 Months

- **Model validations in climate mode.** (lead: Jablonowski) We will assess the long-term model behavior with and without moisture processes and orography fields in idealized climate experiments. These will include variants of the Held-Suarez benchmark and aqua-planet simulations which allow us to simplify the land surface boundary conditions. At this stage, we will also assess suitable refinement criteria for short-term and long-term model runs.
- **Enhanced physics modules.** (lead: Jablonowski) We will enhance our modeling capabilities by improving or adding selected physics modules. In particular, we will further tune the representation of moisture processes and include NCAR's CAM3 radiation scheme in our modeling system.
- **Improved performance and scalability measurements.** (lead: Bono and Martin)

### 36 Months

- **Comprehensive model validation with AMR functionality.** (lead: Jablonowski) We will assess the whole test suite and evaluate the adaptive mesh functionality of our modeling approach. The tests will assess static and dynamic refinement areas that focus on regions or features of interest. Regions of interest include the tropical belt due to its active convective regimes and steep mountainous terrain. We will also seek opportunities to track idealized tropical cyclones in aqua-planet simulations.
- **Test of the coupling interface to NCAR's CAM3 physics parameterizations.** (lead: Bono and Martin)
- **Prepare code for release.** (lead: Bono and Martin) This includes preparation of comprehensive documentation, users guides, and test software.

## 7 Management Plan

The work proposed here will be carried out at two DOE laboratories (LBNL and LLNL) and one university (University of Michigan). LBNL will be the coordinating institution, and Dr. Phillip Colella the coordinating PI (Colella is also the coordinating PI for APDEC). The applied mathematics component of the effort will comprise Dr. Caroline Bono of LLNL (0.5 FTE), Dr. Phillip Colella of LBNL (0.05 FTE) and Dr. Daniel Martin of LBNL (.55 FTE). The climate science component of the effort will be led by Prof. Christiane Jablonowski of the Atmospheric Sciences Department of the University of Michigan (\$150K / year). These investigators have been involved in various activities that uniquely prepare them for this undertaking. Jablonowski developed an AMR dynamical core based on the hydrostatic equations as part of her 2004 Ph.D. dissertation, which has given her a broad understanding of both the numerical and modeling issues surrounding the use of local refinement in atmospheric modeling. Bono has carried out numerical algorithm development projects using the APDEC framework, including a combined numerical and asymptotic analysis of the dynamics of non-hydrostatic models of gravitationally stratified fluids. The latter work yields a substantially improved understanding of the well-posedness of the general initial / boundary value problems for such models that is an important component of the design of local-refinement methods. Martin is one of the developers of the APDEC framework, with specific expertise in the design and implementation of local refinement methods for semi-implicit discretizations of fluid and transport equations. He was also the lead developer of the NASA CT project on AMR, with primary responsibility for meeting the project's extensive formal software process requirements. The coordinating PI Colella will provide leadership and an extensive experience in designing numerical methods for applied science problems.

The design of the algorithms and software will be a joint undertaking by the entire team. Bono and Martin will be the lead implementers. Jablonowski will be the lead on algorithm evaluation, model design, and verification and validation, as well as participating as appropriate in the day-to-day algorithm development. This project will be subject to the supervision of the SciDAC Climate project which will develop software interfaces and evaluation methods for the new dynamical core. Members of the project will participate in the SciDAC Climate project meetings and report progress through the SciDAC Climate project liason (Mark Taylor, SNL-NM) at regular intervals.

### 7.1 Evaluation Criteria

We give here a brief discussion of the extent to which the present proposal is responsive to the evaluation criteria in the Call for Proposals, as listed in the section entitled, "Merit Review".

#### 1. Scientific and Technical Merit of the Project

**a. Potential for Impact.** The possible impact on the successful development of AMR for climate modeling includes the ability to resolve important phenomena that are currently (and for the foreseeable future, in some cases) inaccessible using uniform grid methods. Examples are discussed in section 3.2.

**b. Demonstrated Capabilities of the Researchers.** The capabilities of the team are discussed at the beginning of this section.

**c. Connection to Previous Efforts.** See 1b. We will continue to consult extensively with the members of the SciDAC Climate project and other members of the climate modeling community as we move forward on this project.

**d. Likelihood of Broad Impact.** Since the target system for modeling is the non-hydrostatic equations, success of this project would be immediately applicable to mesoscale and microscale atmospheric simulations. The underlying multiblock mapped grid technologies are also being used in several other applications supported by APDEC.

**e. Software integration and long-term support.** We have as explicit milestones documentation, test cases, and the integration of the capabilities developed here into the CCSM codes. We will also benefit from the

plan for long-term support of the APDEC framework on which our implementation is based.

**f. Extent of broad community interaction.** The SciDAC Climate project is based on a broad consensus regarding the needs of the climate modeling community. By continuing consultation with the participants in that project, we can obtain the input required for us to be responsive to that community.

## **2. Appropriateness of Proposed Method and Approach**

**a. Quality of the Plan to Couple to Applications.** We have several mechanisms for meeting this requirement, including reviews of the project by APDEC and the SciDAC Climate project, determination and documentation of requirements, and regular consultation and reports to Mark Taylor, the liaison to this project from the SciDAC Climate project.

**b. Quality of Work Schedule and Deliverables.** The milestones in section 6, combined with the software development process described in section 5.3, provide well-defined goals and explicit metrics of progress, as well as a process for auditing that progress.

**c. Quality of Proposed Approach to Intellectual Property.** We will release the software developed by this project under a "Free BSD" license. Further details regarding our intellectual property approach are discussed in the appendix.

**d. Quality of plan for collaboration.** The fact that this project is staffed as a small integrated team (1.1 FTE at the national labs + a single-investigator team at Michigan) will enable the close coordination of the activities of the team members. The two DOE lab investigators Bono and Martin are located at the Northern California DOE laboratories LBNL and LLNL, and are also members of a single team within the APDEC center. They will meet face-to-face on a weekly basis. Particular effort will be taken to coordinate the efforts of the University of Michigan team and the DOE lab team, through regular conference calls and bimonthly face-to-face meetings in California or Michigan.

**e. Quality of plan for communication with other CETs.** APDEC has collaboration agreements with proposed centers in the areas of visualization and data analysis, performance engineering, scientific data management, and solvers, and will be responsible for providing technology for those centers to this project SAP.

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**U.S. Department of Energy**  
**Budget Page**  
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ORGANIZATION <b>Summary Total (Lawrence Berkeley National Laboratory and Academic Institution)</b>				Budget Page No: <u>1</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Phillip Colela, PhD.</b>				Requested Duration: <u>12</u> (Months) Year 1	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested
			CAL	ACAD	SUMR
					by Applicant
					by DOE
1.	Phillip Colella, Scientific Staff		0.05		\$8,214
2.	Dan Martin, Scientific Staff		0.55		\$54,720
3.	Christiane Jablonowski, Scientific Staff		0.25		\$27,616
4.	Caroline Bono, Scientific Staff		0.50		\$52,866
5.					
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE) TSM 110-119				
7.	( 4 ) TOTAL SENIOR PERSONNEL (1-6)		1.35		\$143,416
B. ( ) OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1.	( 1 ) POST DOCTORAL ASSOCIATES		0.75		\$35,100
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER				
TOTAL SALARIES AND WAGES (A+B)					\$178,516
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$178,516
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL			1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)		\$20,431
			2. FOREIGN		
TOTAL TRAVEL					\$20,431
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					\$10,928
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					\$2,900
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					\$1,581
5. SUBCONTRACTS					
6. OTHER					\$3,345
TOTAL OTHER DIRECT COSTS					\$18,754
H. TOTAL DIRECT COSTS (A THROUGH G)					\$217,701
I. INDIRECT COSTS					
TOTAL INDIRECT COSTS					\$278,887
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$496,588
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					\$496,588

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**U.S. Department of Energy**  
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 1910-1400  
 OMB Burden Disclosure  
 Statement on Reverse

ORGANIZATION Summary Total (Lawrence Berkeley National Laboratory and Academic Institution)				Budget Page No: <u>2</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Phillip Colela, PhD.				Requested Duration: <u>12</u> (Months) Year 2	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested
			CAL	ACAD	SUMR
					by Applicant
					by DOE
1.	Phillip Colella, Scientific Staff		0.05		\$8,461
2.	Dan Martin, Scientific Staff		0.55		\$56,361
3.	Christiane Jablonowski, Scientific Staff		0.25		\$27,226
4.	Caroline Bono, Scientific Staff		0.50		\$54,643
5.					
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE) TSM 110-119				
7.	( 4 ) TOTAL SENIOR PERSONNEL (1-6)		1.35		\$146,691
B. ( ) OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1.	( 1 ) POST DOCTORAL ASSOCIATES		0.75		\$36,504
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER				
TOTAL SALARIES AND WAGES (A+B)					\$183,195
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$183,195
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL			1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)		\$20,922
			2. FOREIGN		
TOTAL TRAVEL					\$20,922
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					\$10,296
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					\$2,996
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					\$1,589
5. SUBCONTRACTS					
6. OTHER					\$3,433
TOTAL OTHER DIRECT COSTS					\$18,313
H. TOTAL DIRECT COSTS (A THROUGH G)					\$222,430
I. INDIRECT COSTS					
TOTAL INDIRECT COSTS					\$287,127
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$509,557
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					\$509,557

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**U.S. Department of Energy**  
**Budget Page**  
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Statement on Reverse

ORGANIZATION <b>Summary Total (Lawrence Berkeley National Laboratory and Academic Institution)</b>				Budget Page No: <u>3</u>		
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Phillip Colela, PhD.</b>				Requested Duration: <u>12</u> (Months) Year 3		
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)		DOE Funded Person-mos.		Funds Requested	Funds Granted	
		CAL	ACAD	SUMR	by Applicant	by DOE
1.	Phillip Colella, Scientific Staff	0.05			\$8,715	
2.	Dan Martin, Scientific Staff	0.55			\$58,052	
3.	Christiane Jablonowski, Scientific Staff	0.20			\$25,438	
4.	Caroline Bono, Scientific Staff	0.50			\$56,282	
5.						
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE) TSM 110-119					
7.	( 4 ) TOTAL SENIOR PERSONNEL (1-6)	1.30			\$148,487	
B. ( ) OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)						
1.	( 1 ) POST DOCTORAL ASSOCIATES	0.75			\$37,964	
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3.	( ) GRADUATE STUDENTS					
4.	( ) UNDERGRADUATE STUDENTS					
5.	( ) SECRETARIAL - CLERICAL					
6.	( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)					\$186,451	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)						
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$186,451	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)						
TOTAL PERMANENT EQUIPMENT						
E. TRAVEL		1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)			\$21,429	
		2. FOREIGN				
TOTAL TRAVEL					\$21,429	
F. TRAINEE/PARTICIPANT COSTS						
1. STIPENDS (Itemize levels, types + totals on budget justification page)						
2. TUITION & FEES						
3. TRAINEE TRAVEL						
4. OTHER (fully explain on justification page)						
TOTAL PARTICIPANTS ( ) TOTAL COST						
G. OTHER DIRECT COSTS						
1. MATERIALS AND SUPPLIES					\$9,674	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					\$3,096	
3. CONSULTANT SERVICES						
4. COMPUTER (ADPE) SERVICES					\$1,590	
5. SUBCONTRACTS						
6. OTHER					\$3,435	
TOTAL OTHER DIRECT COSTS					\$17,795	
H. TOTAL DIRECT COSTS (A THROUGH G)					\$225,674	
I. INDIRECT COSTS						
TOTAL INDIRECT COSTS					\$294,403	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$520,077	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES						
L. TOTAL COST OF PROJECT (J+K)					\$520,077	

**U.S. Department of Energy**  
**Budget Page**  
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ORGANIZATION <b>Summary Total (Lawrence Berkeley National Laboratory and Academic Institution)</b>				Budget Page No: <u>4</u>		
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Phillip Colela, PhD.</b>				Requested Duration: <u>36</u> (Months) Summary - All Years		
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)		DOE Funded Person-mos.		Funds Requested	Funds Granted	
		CAL	ACAD	SUMR	by Applicant	by DOE
1.	Phillip Colella, Scientific Staff	0.15			\$25,390	
2.	Dan Martin, Scientific Staff	1.65			\$169,133	
3.	Christiane Jablonowski, Scientific Staff	0.70			\$80,280	
4.	Caroline Bono, Scientific Staff	1.50			\$163,791	
5.						
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE) TSM 110-119					
7.	( 2 ) TOTAL SENIOR PERSONNEL (1-6)	4.00			\$438,593	
B. ( ) OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)						
1.	( 1 ) POST DOCTORAL ASSOCIATES	2.25			\$109,568	
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3.	( ) GRADUATE STUDENTS					
4.	( ) UNDERGRADUATE STUDENTS					
5.	( ) SECRETARIAL - CLERICAL					
6.	( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)					\$548,161	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)						
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$548,161	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)						
TOTAL PERMANENT EQUIPMENT						
E. TRAVEL		1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)			\$62,781	
		2. FOREIGN				
TOTAL TRAVEL					\$62,781	
F. TRAINEE/PARTICIPANT COSTS						
1. STIPENDS (Itemize levels, types + totals on budget justification page)						
2. TUITION & FEES						
3. TRAINEE TRAVEL						
4. OTHER (fully explain on justification page)						
TOTAL PARTICIPANTS ( ) TOTAL COST						
G. OTHER DIRECT COSTS						
1. MATERIALS AND SUPPLIES					\$30,898	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					\$8,993	
3. CONSULTANT SERVICES						
4. COMPUTER (ADPE) SERVICES					\$4,760	
5. SUBCONTRACTS						
6. OTHER					\$10,212	
TOTAL OTHER DIRECT COSTS					\$54,863	
H. TOTAL DIRECT COSTS (A THROUGH G)					\$665,805	
I. INDIRECT COSTS						
TOTAL INDIRECT COSTS					\$860,417	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$1,526,222	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES						
L. TOTAL COST OF PROJECT (J+K)					\$1,526,222	

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ORGANIZATION Lawrence Berkeley National Laboratory				Budget Page No: <u>1</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Phillip Colela, PhD.				Requested Duration: <u>12</u> (Months) Year 1	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)				DOE Funded	
				Person-mos.	
				Funds Requested	
				Funds Granted	
				by Applicant	
				by DOE	
1.	Phillip Colella, Scientific Staff	0.05		\$8,214	
2.	Dan Martin, Scientific Staff	0.55		\$54,720	
3.					
4.					
5.					
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE) TSM 110-119				
7.	( 2 ) TOTAL SENIOR PERSONNEL (1-6)	0.60		\$62,934	
B. ( ) OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1.	( ) POST DOCTORAL ASSOCIATES				
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER				
TOTAL SALARIES AND WAGES (A+B)				\$62,934	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				\$62,934	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL				\$6,326	
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL				\$6,326	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				\$2,500	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES				\$831	
5. SUBCONTRACTS					
6. OTHER				\$1,098	
TOTAL OTHER DIRECT COSTS				\$4,429	
H. TOTAL DIRECT COSTS (A THROUGH G)				\$73,689	
I. INDIRECT COSTS					
Org Burden 17.6% -Base 91,856 Tvl Rate 14% - Base 6,326					
Proc. Burden 8.4% Base 2,500 LDRD Rate 9.1% - Base 115,446					
Gen Rate 46.3% -Base 109,085 Payroll Rate (Var). - Base 62,934					
TOTAL INDIRECT COSTS				\$106,312	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				\$180,001	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				\$180,001	



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U.S. Department of Energy

Budget Page

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OMB Control No.

1910-1400

OMB Burden Disclosure Statement on Reverse

ORGANIZATION Lawrence Berkeley National Laboratory				Budget Page No: <u>2</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Phillip Colela, PhD.				Requested Duration: <u>12</u> (Months) Year 2	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested
			CAL	ACAD	SUMR
					by Applicant
					by DOE
1.	Phillip Colella, Scientific Staff		0.05		\$8,461
2.	Dan Martin, Scientific Staff		0.55		\$56,361
3.					
4.					
5.					
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE) TSM 110-119				
7.	( 2 ) TOTAL SENIOR PERSONNEL (1-6)		0.60		\$64,822
B. ( ) OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1.	( ) POST DOCTORAL ASSOCIATES				
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER				
TOTAL SALARIES AND WAGES (A+B)					\$64,822
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$64,822
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL			1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)		\$6,453
			2. FOREIGN		
TOTAL TRAVEL					\$6,453
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					\$2,178
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					\$839
5. SUBCONTRACTS					
6. OTHER					\$1,186
TOTAL OTHER DIRECT COSTS					\$4,202
H. TOTAL DIRECT COSTS (A THROUGH G)					\$75,477
I. INDIRECT COSTS			Org Burden 17.6% -Base	94,859	Tvl Rate 14% - Base 6,453
			Proc. Burden 8.4% Base	2,178	LDRD Rate 9.1% - Base 119,152
TOTAL INDIRECT COSTS			Gen Rate 46.3% -Base	112,666	Payroll Rate (Var). - Base 64,822
TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$185,402
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					\$185,402

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**U.S. Department of Energy**  
**Budget Page**  
(See reverse for Instructions)

OMB Control No.  
1910-1400  
OMB Burden Disclosure  
Statement on Reverse

ORGANIZATION <b>Lawrence Berkeley National Laboratory</b>				Budget Page No: <u>3</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Phillip Colela, PhD.</b>				Requested Duration: <u>12</u> (Months) Year 3	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)				DOE Funded	
				Person-mos.	
				CAL	ACAD
				SUMR	
				Funds Requested	
				by Applicant	
				Funds Granted	
				by DOE	
1.	Phillip Colella, Scientific Staff			0.05	
2.	Dan Martin, Scientific Staff			0.55	
3.					
4.					
5.					
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE) TSM 110-119				
7.	( 2 ) TOTAL SENIOR PERSONNEL (1-6)			0.60	
B. ( ) OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1.	( ) POST DOCTORAL ASSOCIATES				
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER				
TOTAL SALARIES AND WAGES (A+B)					\$66,767
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$66,767
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL					\$6,582
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL					\$6,582
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					\$1,605
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					\$840
5. SUBCONTRACTS					
6. OTHER					\$1,188
TOTAL OTHER DIRECT COSTS					\$3,633
H. TOTAL DIRECT COSTS (A THROUGH G)					\$76,981
I. INDIRECT COSTS					
	Org Burden 17.6% -Base	98,183	Tvl Rate 14% - Base	6,582	
	Proc. Burden 8.4% Base	1,605	LDRD Rate 9.1% - Base	123,124	
	Gen Rate 46.3% -Base	116,511	Payroll Rate (Var). - Base	66,767	
TOTAL INDIRECT COSTS					\$113,984
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$190,965
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					\$190,965

**U.S. Department of Energy**  
**Budget Page**  
(See reverse for Instructions)

ORGANIZATION <b>Lawrence Berkeley National Laboratory</b>				Budget Page No: <u>4</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Phillip Colela, PhD.</b>				Requested Duration: <u>36</u> (Months) Summary - All Years	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)				DOE Funded Person-mos.	
				CAL	ACAD
				SUMR	Funds Requested by Applicant
					Funds Granted by DOE
1.	Phillip Colella, Scientific Staff		0.15		\$25,390
2.	Dan Martin, Scientific Staff		1.65		\$169,133
3.					
4.					
5.					
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE) TSM 110-119				
7.	( 2 ) TOTAL SENIOR PERSONNEL (1-6)		1.80		\$194,522
B. ( ) OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1.	( 1 ) POST DOCTORAL ASSOCIATES				
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER				
TOTAL SALARIES AND WAGES (A+B)					\$194,522
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$194,522
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL					\$19,360
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL					\$19,360
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					\$6,283
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					\$2,510
5. SUBCONTRACTS					
6. OTHER					\$3,471
TOTAL OTHER DIRECT COSTS					\$12,264
H. TOTAL DIRECT COSTS (A THROUGH G)					\$226,146
I. INDIRECT COSTS					
	Org Burden 17.6% -Base	493,665	Tvl Rate 14% - Base	46,136	
	Proc. Burden 8.4% Base	10,812	LDRD Rate 9.1% - Base	627,969	
TOTAL INDIRECT COSTS				Gen Rate 46.3% -Base	582,007
			Payroll Rate (Var). - Base	334,124	
TOTAL INDIRECT COSTS					\$330,221
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$556,367
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					\$556,367

## Lawrence Berkeley National Laboratory Budget Explanation

Cost estimates have been presented in this proposal to be comparable to other research institution's proposals. At Lawrence Berkeley National Laboratory (LBNL), actual costs will be collected and reported in accordance with the Department of Energy (DOE) guidelines. Total cost presented in this proposal and actual cost totals will be equivalent.

This SAP is an integrated team, with all of the members participating in all aspects of the project. However, each member of the team will have designated responsibilities regarding the Milestones given in section 6 of the proposal.

Professor Christiane Jablonowski (University of Michigan, \$150K / year), working with her students and postdoc, will be the lead on algorithm evaluation, model design, and verification and validation.

Dr. Caroline Bono (.5 FTE, LLNL) and Dr. Daniel Martin (.55 FTE, LBNL) will make up the code development team, and will have joint responsibility for meeting the milestones in those areas.

Each milestone in section 6 is assigned either to Jablonowski or to Bono / Martin.

Dr. Phillip Colella (.05 FTE, LBNL) is the coordinating PI for this project. He will be responsible for overall management and coordination with the APDEC CET, as well as providing technical expertise in AMR algorithm software design.

Dr. Mark Taylor (SNL-NM), while not funded by this SAP, is the designated point of contact in the SciDAC Climate Project for this SAP. He will coordinate the activities of this team with the larger climate activities.

### **DIRECT COSTS**

#### Senior Personnel – Item A.1-6

The salary figure listed for Senior Personnel is an estimate based on the current actual salary for an employee in her/his division plus 3.0% per fiscal year for inflation.

#### Fringe Benefits – Item C

Fringe Benefits for LBNL employees are estimated to be the following percent calculated on labor costs:

Career Employees – (FY06) 24.0%; (FY07) 24.9%; (FY08) 25.0%; (FY09) 25.9%; (FY10) 26.7%

Visiting Postdoctoral Fellows – (FY06) 11.3%; (FY07) 11.6%; (FY08) 11.4%; (FY09) 11.8%; (FY10) 12.2%

GSRAs – (FY06) 37.4%; (FY07) 37.4%; (FY08) 37.4%; (FY09) 37.4%; (FY10) 37.4%

Students/Other – (FY06) 3.1%; (FY07) 3.1%; (FY08) 2.4%; (FY09) 2.4%; (FY10) 2.4

#### Travel – Items E.1 and E.2

The senior staff members plan to attend domestic and/or foreign technical conferences/workshops in the areas of research covered by this proposal. Total cost includes plane fare, housing, meals and other allowable costs under government per diem rules.

Other Direct Costs – Item G.6

The estimated cost of telephone, computer usage, etc., calculated on person-months directly associated with the project.

**INDIRECT COSTS – Item I**

Organizational Burden

Use of organizational burden pools in LBNL Computing Sciences (CS) Division is the approved method for collection and distribution of indirect costs associated with personnel. These pools are established to collect costs associated with personnel engaged in a single operation or several closely related operations. The objective is to establish uniformity and compatibility in recording, distributing, and reporting organizational burden. The types of costs which can be charged to these pools are labor and labor-related costs of secretaries, division administration and general materials/service costs such as environmental, safety, and health, finance and budget provided for the general benefit of a division. The estimated LBNL CS Organizational Burden rate is 17.6% and is calculated on all CS research salaries.

Other LBNL on-site indirect estimated costs are as follows:

Procurement Burden – 8.4% calculated on all procurements and electricity

Travel – 14% calculated on all travel

General & Administrative General Rate – 46.3% calculated on all costs



# Face Page

**TITLE OF PROPOSED RESEARCH:**

Local Refinement Methods for Atmospheric Modeling (stand alone SAP for climate)

**1. CATALOG OF FEDERAL DOMESTIC ASSISTANCE #**

81.049

**2. CONGRESSIONAL DISTRICT:**

Applicant Organization's District: 10th

Project Site's District: 10th

**3A. I.R.S. ENTITY IDENTIFICATION OR SSN:**

95-6031193

**3B. DUNS Number:**

**4. AREA OF RESEARCH OR ANNOUNCEMENT TITLE#:**

SciDAC 2 Lab 06 04

**5. HAS THIS RESEARCH PROPOSAL BEEN SUBMITTED TO ANY OTHER FEDERAL AGENCY?**

YES  NO

PLEASE LIST \_\_\_\_\_

**6. DOE/OER PROGRAM STAFF CONTACT (if known):**

Anil Deane, 301-903-1465

**7. TYPE OF APPLICATION:**

New  Renewal  
 Continuation  Revision  
 Supplement

**8. ORGANIZATION TYPE:**

Local Govt.  State Govt.  
 Non-Profit  Hospital  
 Indian Tribal Govt.  Individual  
 Other  Inst. of Higher Educ.  
 For-Profit  Small Business  Disadvan. Business  
 Women-Owned  8(a)

**9. CURRENT DOE AWARD # (IF APPLICABLE):**

**10. WILL THIS RESEARCH INVOLVE:**

**10A. Human Subjects**  No  If yes  
Exemption No. \_\_\_\_\_ or  
IRB Approval Date \_\_\_\_\_  
Assurance of Compliance No: \_\_\_\_\_  
**10B. Vertebrate Animals**  No  If yes  
IACUC Approval Date \_\_\_\_\_ or  
Animal Welfare Assurance No: \_\_\_\_\_

**11. AMOUNT REQUESTED FROM DOE FOR ENTIRE PROJECT PERIOD \$** 522,092.00

**12. DURATION OF ENTIRE PROJECT PERIOD:**

07/01/06 to 06/30/09  
MM/DD/YY MM/DD/YY

**13. REQUESTED AWARD START DATE**

07/01/06  
MM/DD/YY

**14. IS APPLICANT DELINQUENT ON ANY FEDERAL DEBT?**

Yes (attach an explanation)  No

**15. PRINCIPAL INVESTIGATOR/PROGRAM DIRECTOR**

NAME Caroline Bono

TITLE Principal Investigator

ADDRESS 7000 East Avenue, L-560

Livermore, CA 94550

PHONE NUMBER (925) 424-2084

**SIGNATURE OF PRINCIPAL INVESTIGATOR/ PROGRAM DIRECTOR**

(please type in full name if electronically submitted)

Date 02/27/06

PI/PD ASSURANCE: I agree to accept responsibility for the scientific conduct of the project and to provide the required progress reports if an award is made as a result of this submission. Willful provision of false information is a criminal offense. (U.S. Code, Title 18, Section 1001).

**16. ORGANIZATION'S NAME** Regents of the University of California

ADDRESS Lawrence Livermore National Laboratory

7000 East Avenue

Livermore, CA 94550

**CERTIFYING REPRESENTATIVE'S**

NAME Steven F. Ashby

TITLE Computation, Deputy Associate Director

PHONE NUMBER (925) 422-1985

**SIGNATURE OF ORGANIZATION'S CERTIFYING REPRESENTATIVE**

(please type in full name if electronically submitted)

Date 2-27-06

CERTIFICATION and ACCEPTANCE: I certify that the statements herein are true and complete to the best of my knowledge, and accept the obligation to comply with DOE terms and conditions if an award is made as the result of this submission. A willfully false certification is a criminal offense. (U.S. Code, Title 18, Section 1001).

**NOTICE FOR HANDLING PROPOSALS**

This submission is to be used only for DOE evaluation purposes and this notice shall be affixed to any reproduction or abstract thereof. All Government and non-Government personnel handling this submission shall exercise extreme care to ensure that the information contained herein is not duplicated, used, or disclosed in whole or in part for any purpose other than evaluation without written permission except that if an award is made based on this submission, the terms of the award shall control disclosure and use. This notice does not limit the Government's right to use information contained in the submission if it is obtainable from another source without restriction. This is a Government notice, and shall not itself be construed to impose any liability upon the Government or Government personnel for any disclosure or use of data contained in this submission.

**PRIVACY ACT STATEMENT**

If applicable, you are requested, in accordance with 5 U.S.C., Sec. 562A, to voluntarily provide your Social Security Number (SSN). However, you will not be denied any right, benefit, or privilege provided by law because of a refusal to disclose your SSN. We request your SSN to aid in accurate identification, referral and review of applications for research/training support for efficient management of Office of Science grant/contract programs.

**U.S. Department of Energy  
Budget Page**  
(See reverse for Instructions)

Year 1

ORGANIZATION <b>Lawrence Livermore National Laboratory</b>				Budget Page No: <u>    1    </u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Caroline Bono</b>				Requested Duration: <u>    12    </u> (Months) Year 1	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested
			CAL	ACAD	SUMR
					by Applicant
					by DOE
1.	Caroline Bono		6.00		\$52,866
2.					
3.					
4.					
5.					
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE) TSM 110-119				
7.	( ) TOTAL SENIOR PERSONNEL (1-6)		6.00		\$52,866
B. ( ) OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1.	( ) POST DOCTORAL ASSOCIATES				
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER				
TOTAL SALARIES AND WAGES (A+B)					\$52,866
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					\$22,468
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$75,334
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL					\$5,000
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL					\$5,000
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					\$4,250
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					\$500
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					\$750
5. SUBCONTRACTS					
6. OTHER					\$2,247
TOTAL OTHER DIRECT COSTS					\$7,747
H. TOTAL DIRECT COSTS (A THROUGH G)					\$88,081
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS					\$80,741
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$168,822
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					\$168,822

**U.S. Department of Energy  
Budget Page**  
(See reverse for Instructions)

Year 2

ORGANIZATION <b>Lawrence Livermore National Laboratory</b>				Budget Page No: <u>    2    </u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Caroline Bono</b>				Requested Duration: <u>    12    </u> (Months) Year 2	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested
			CAL	ACAD	SUMR
					by Applicant
					by DOE
1.	Caroline Bono		6.00		\$54,643
2.					
3.					
4.					
5.					
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE) TSM 110-119				
7.	( ) TOTAL SENIOR PERSONNEL (1-6)		6.00		\$54,643
B. ( ) OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1.	( ) POST DOCTORAL ASSOCIATES				
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER				
TOTAL SALARIES AND WAGES (A+B)					\$54,643
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					\$23,223
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$77,866
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL					\$5,000
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL					\$5,000
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					\$4,250
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					\$500
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					\$750
5. SUBCONTRACTS					
6. OTHER					\$2,247
TOTAL OTHER DIRECT COSTS					\$7,747
H. TOTAL DIRECT COSTS (A THROUGH G)					\$90,613
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS					\$83,545
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$174,158
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					\$174,158



Year 3

ORGANIZATION <b>Lawrence Livermore National Laboratory</b>				Budget Page No: <u>3</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Caroline Bono</b>				Requested Duration: <u>12</u> (Months) Year 3	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested
			CAL	ACAD	SUMR
					by Applicant
					by DOE
1.	Caroline Bono		6.00		\$56,282
2.					
3.					
4.					
5.					
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE) TSM 110-119				
7.	( ) TOTAL SENIOR PERSONNEL (1-6)		6.00		\$56,282
B. ( ) OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1.	( ) POST DOCTORAL ASSOCIATES				
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER				
TOTAL SALARIES AND WAGES (A+B)					\$56,282
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					\$23,920
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$80,202
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL			1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)		\$5,000
			2. FOREIGN		
TOTAL TRAVEL					\$5,000
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					\$4,250
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					\$500
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					\$750
5. SUBCONTRACTS					
6. OTHER					\$2,247
TOTAL OTHER DIRECT COSTS					\$7,747
H. TOTAL DIRECT COSTS (A THROUGH G)					\$92,949
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS					\$86,163
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$179,112
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					\$179,112

Years 1 - 3

ORGANIZATION <b>Lawrence Livermore National Laboratory</b>				Budget Page No: <u>4</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Caroline Bono</b>				Requested Duration: <u>36</u> (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)				Summary - All Years	
	DOE Funded Person-mos.			Funds Requested	Funds Granted
	CAL	ACAD	SUMR	by Applicant	by DOE
1. <b>Caroline Bono</b>	18.00			\$163,791	
2.					
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE) TSM 110-119					
7. ( ) TOTAL SENIOR PERSONNEL (1-6)	18.00			\$163,791	
B. ( ) OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				\$163,791	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				\$69,611	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				\$233,402	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL				\$15,000	
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL				\$15,000	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				\$12,750	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				\$1,500	
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES				\$2,250	
5. SUBCONTRACTS					
6. OTHER				\$6,741	
TOTAL OTHER DIRECT COSTS				\$23,241	
H. TOTAL DIRECT COSTS (A THROUGH G)				\$271,643	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS				\$250,449	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				\$522,092	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				\$522,092	

# **A Science Application Partnership (SAP) on Local Refinement Methods for Atmospheric Modeling Budget Justification**

## **A. Senior Personnel**

Caroline Bono will develop and implement new numerical algorithms that will be used to create a prototype for an atmospheric dynamical core that allows for adaptive mesh refinement and would be suitable for use in a production climate simulation code.

## **B. Other Personnel**

None.

## **C. Fringe Benefits**

The Laboratory's Payroll Burden Rate is 42.5% and is applied to the non-leave standard salary of all Laboratory employees, including overtime. PostDocs are charged a 35% Payroll Burden, and students are charged 9.5%.

## **D. Equipment**

None planned.

## **E. Travel**

The anticipated travel is 3 trips to the University of Michigan per year to work with Prof. Christiane Jablonowski who is part of our team, and 1 trip for a conference per year. Total estimated travel will be \$15,000.

## **F. Trainee/Participant Costs**

N/A.

## **G. Other Costs**

- 1.) Standard computer hardware and software will be purchased as needed for the project. Total estimated cost is \$12,750.
- 2.) Publication costs for technical review and release of publishing project results is anticipated at \$1,500.
- 4.) Computer services, as needed on the project, are estimated at \$2,250.
- 6.) Office space is estimated at \$6,741.

## **H. Total Direct Costs**

\$271,643

## **I. Indirect Costs**

Total Indirect Costs are estimated at \$250,449. LLNL rate amounts and their definitions are explained in Attachment A. Note that rates are applied in a specified order and not all taxes apply to each direct cost.

## Attachment A

### Lawrence Livermore National Laboratory Current FY2006 Rates

<b>Indirect Cost Pool</b>	<b>Rate (%)</b>	<b>Allocation Base/Rate Determination</b>
<u>Organization Personnel Charge (OPC):</u> Computation - Associate Director's Office	19.09%	Distribution of specific Organization's personnel management costs to users of the Organization Personnel Charge accounts. The rates vary by the Organization providing the service.
<u>Program Management Charge (PMC):</u> Computation - Associate Director's Office Computation - Program	4.50% 8.10%	A distribution of costs associated with managing and administering direct funded Programs within a Directorate. PMC is allocated on a value-added cost input base to Direct Operating, LDRD, Capital Equipment, and Construction accounts under the Programs' administration. The value-added base consists of the Programs' total cost input base less direct materials, subcontracts, and the Electricity Recharge. Supplemental Labor is included in the base.
<u>General &amp; Administrative (G&amp;A):</u>	31.50%	G&A is allocated on a value-added base, which is total operating costs less direct materials, subcontracts, and the Electricity Recharge. Supplemental Labor is included in the base. G&A is applied to Direct Operating, Capital Equipment and Construction accounts.
<u>Strategic Mission Support (SMS):</u>	7.00%	SMS costs include institutional strategic planning, institutional capabilities, outreach, and special employees. Applied to direct operating, WFO, and capital equipment accounts using a value-added base.
<u>Institutional General Purpose Equipment (IGPE):</u>	0.80%	The IGPE allocation is for capital equipment of a general use or institutional nature that benefits multiple cost objectives and is required for general-purpose site-wide needs. It is allocated on a total-cost base, and is not applied to DOE major items of equipment, general plant projects, line item construction or Work for Others - DOE.
<u>Institutional General Plant Projects</u>	0.65%	The IGPP allocation is for new construction projects that cost less than \$5M and are of a general institutional nature benefiting multiple cost objectives and required for general-purpose site-wide needs.
<u>Laboratory Directed Research &amp; Development (LDRD):</u> Operating Calculation - An assessment applied to Laboratory operating costs to support exploratory research and development.	6.38%	Rate is applied against total capital equipment (excluding line items) and operating costs, excluding Federal Administrative Charge.

**Cover Page**

Scientific Discovery through Advanced Computing  
DE-FG02-06ER06-04

**A Science Application Partnership (SAP) on  
Local Refinement Methods for Atmospheric  
Modeling**

For the period September 1, 2006 – August 31, 2009

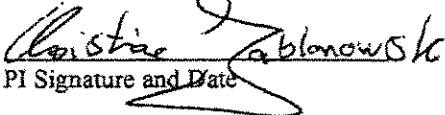
Principal Investigator

Christiane Jablonowski, Assistant Professor  
Atmospheric, Oceanic, and Space Science  
University of Michigan  
Space Research Building  
2455 Hayward St.  
Ann Arbor, MI 48109-2143  
734-763-6238 (Voice)  
734-763-0437 (Fax)  
cjablono@umich.edu

Official Signing for Institution

Janes R. Randolph, Senior Associate Director  
Division of Research Development and Administration  
The Regents of The University of Michigan  
3003 South State St.  
Wolverine Tower, Room 1056  
Ann Arbor, MI 48109-1274  
734-647-4852  
734-763-4053

Christiane Jablonowski

 2/27/2006  
PI Signature and Date

Official Name

  
Official Signature and Date

Requested Funding:      Year 1: \$147,765  
                                    Year 2: \$149,997  
                                    Year 3: \$150,000  
Total Funding Requested: \$447,762

Use of Human Subjects: No  
Use of Vertebrate Animals: No

**APPLICATION FOR FEDERAL ASSISTANCE  
SF 424 (R&R)**

<b>2. DATE SUBMITTED</b> [ ]	<b>Applicant Identifier</b> [ ]
<b>3. DATE RECEIVED BY STATE</b> [ ]	<b>State Application Identifier</b> [ ]
<b>4. Federal Identifier</b> [ ]	

**1. \* TYPE OF SUBMISSION**

Pre-application  Application  
 Changed/Corrected Application

**5. APPLICANT INFORMATION** \* Organizational DUNS: 0731335710000

\* Legal Name: The Regents of The University of Michigan

Department: Atmospheric, Oceanic Space Sci Division: [ ]

\* Street1: 3003 S. State St. Street2: [ ]

\* City: Ann Arbor County: [ ] \* State: MI \* ZIP Code: 48109-1274

\* Country: USA

Person to be contacted on matters involving this application

Prefix: \* First Name: Kate Middle Name: [ ] \* Last Name: Koorhan Suffix: [ ]

\* Phone Number: 734-647-4852 Fax Number: 734-763-4053 Email: kkoorhan@umich.edu

**6. \* EMPLOYER IDENTIFICATION (EIN) or (TIN):**  
38-6006309

**7. \* TYPE OF APPLICANT:**  
F: State-Controlled Institution of Higher Education

**8. \* TYPE OF APPLICATION:**  New  
 Resubmission  Renewal  Continuation  Revision

Other (Specify):  
**Small Business Organization Type**  
 Women Owned  Socially and Economically Disadvantaged

If Revision, mark appropriate box(es).  
 A. Increase Award  B. Decrease Award  C. Increase Duration  
 D. Decrease Duration  E. Other (specify)

**9. \* NAME OF FEDERAL AGENCY:**  
Chicago Service Center

\* Is this application being submitted to other agencies? Yes  No   
What other Agencies?

**10. CATALOG OF FEDERAL DOMESTIC ASSISTANCE NUMBER:**  
81.049  
TITLE: Office of Science Financial Assistance Program

**11. \* DESCRIPTIVE TITLE OF APPLICANT'S PROJECT:**  
A Science Application Partnership (SAP) on Local Refinement Methods for Atmospheric Modeling

**12. \* AREAS AFFECTED BY PROJECT (cities, counties, states, etc.)**  
n/a

**13. PROPOSED PROJECT:**  
\* Start Date: 09/01/2006 \* Ending Date: 08/31/2009

**14. CONGRESSIONAL DISTRICTS OF:**  
a. \* Applicant: 15 b. \* Project: 15

**15. PROJECT DIRECTOR/PRINCIPAL INVESTIGATOR CONTACT INFORMATION**

Prefix: \* First Name: Christiane Middle Name: [ ] \* Last Name: Jablonowski Suffix: [ ]

Position/Title: Assistant Professor \* Organization Name: The Regents of The University of Michigan

Department: Atmospheric, Oceanic Space Sci Division: [ ]

\* Street1: 3003 S. State St. Street2: [ ]

\* City: Ann Arbor County: [ ] \* State: MI \* ZIP Code: 48109-1274

\* Country: USA

\* Phone Number: 734-763-6238 Fax Number: 734-763-0437 \* Email: cjablono@umich.edu

OMB Number: 4040-0001  
Expiration Date: 04/30/2008

16. ESTIMATED PROJECT FUNDING		17. * IS APPLICATION SUBJECT TO REVIEW BY STATE EXECUTIVE ORDER 12372 PROCESS?	
a. * Total Estimated Project Funding	447,762.00	a. YES	<input checked="" type="checkbox"/> THIS PREAPPLICATION/APPLICATION WAS MADE AVAILABLE TO THE STATE EXECUTIVE ORDER 12372 PROCESS FOR REVIEW ON:
b. * Total Federal & Non-Federal Funds	447,762.00		DATE: <input type="text"/>
c. * Estimated Program Income	0.00	b. NO	<input type="checkbox"/> PROGRAM IS NOT COVERED BY E.O. 12372; OR <input type="checkbox"/> PROGRAM HAS NOT BEEN SELECTED BY STATE FOR REVIEW

18. By signing this application, I certify (1) to the statements contained in the list of certifications\* and (2) that the statements herein are true, complete and accurate to the best of my knowledge. I also provide the required assurances \* and agree to comply with any resulting terms if I accept an award. I am aware that any false, fictitious, or fraudulent statements or claims may subject me to criminal, civil, or administrative penalties. (U.S. Code, Title 18, Section 1001)

\* I agree

\* The list of certifications and assurances, or an Internet site where you may obtain this list, is contained in the announcement or agency specific instructions.

19. Authorized Representative

Prefix:  \* First Name:  Middle Name:  \* Last Name:  Suffix:

\* Position/Title:  \* Organization:

Department:  Division:

\* Street1:  Street2:

\* City:  County:  \* State:  \* ZIP Code:

\* Country:

\* Phone Number:  Fax Number:  \* Email:

\* Signature of Authorized Representative  \* Date Signed

20. Pre-application

## UNIVERSITY OF MICHIGAN COSTING FACTORS

for

### **A Science Application Partnership (SAP) on Local Refinement Methods for Atmospheric Modeling**

The attached preliminary costing estimates are based on a number of assumptions and rationales as follows:

#### Salaries, Wages, and Benefits

Approximately \$80,280 of salary support, an average of 2.8 months per year, over three years is included for the principal investigator to supervise and direct project activities and participate in the evaluations and analyses. Salary of \$109,568 is included for one postdoctoral research fellow at 75% appointment over the three years to participate in the research activities. Salaries are increased at the standard inflation rate of 4% in the second and third year. Benefits totaling \$24,084 for the principal investigator and \$32,870 for the research fellow are calculated at 30% of all salaries and wages consistent with the policies established and published by University of Michigan.

#### Materials and Services

A project of this size and duration will require the purchase of specific supplies and services to support its research efforts. They include such items as shipping (\$184), duplication fees (\$370), toll charges (\$375), networking support and computer maintenance (\$9,138), and general research supplies (\$1,498) where all expenditures are of direct benefit to the successful completion of the project goals and can be specifically accounted for on this project. It is expected that research supplies, duplication, copy services, shipping (Fed. Ex.) and toll charges will be necessary due to data analysis involved with this research along with the communication necessary with the sponsor and collaborators. Network support and maintenance is calculated as a University approved recharge at the rate of \$1.49 per labor hour charged to this project. A total amount of \$7,492 has been budgeted for publication of the results of this research at the end of each of the three years. The purchase of reference books for an estimated amount of \$300 is necessary due to the information needed on atmospheric dynamics and General Circulation Models and also the numerical aspects of climate modeling. The books will be primarily used as a reference for the modeling effort and as an educational tool for the postdoctoral researcher.

#### Travel

University of Michigan policy reimburses travel and living expenses on a reasonable and actual basis upon receipt of itemized reports. Per Diem rates are not used. However, for estimating purposes, established rates from the Federal Travel Regulations are used. Due to the collaboration necessary with the participants at LLNL and LBNL we have budgeted three trips per year for the principal investigator and the research fellow to Berkeley and Lawrence Livermore. Travel is budgeted for five days each trip and



includes airfare, subsistence, and ground transportation. The dates of this travel will be decided as the research progresses.

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Subcontracts

This project has no subcontract requirements

Equipment

This project has no equipment requirements

Total Direct Costs (TDC)

Total Direct Costs is the sum of all direct project costs and includes the categories of salaries, benefits, tuition, materials and services, travel, equipment and/or equipment fabrication, and sub-contracts where applicable to the proposed program.

Modified Total Direct Costs (MTDC)

Modified Total Direct Costs is the cost basis used to calculate the indirect cost for a project. The MTDC is the TDC less the sum of tuition, equipment, and sub-contracts where applicable to the proposed program.

Indirect Costs (IC)

The current University of Michigan approved indirect cost rate for on-campus sponsored research is 52% of MTDC.

Total Project Costs

The total project cost is equivalent to the sum of TDC + IC + cost sharing where applicable to the proposed program. For this program total project cost is \$447,762.

## **Description of Facilities and Resources**

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### **Lawrence Berkeley National Laboratory**

LBNL has access to leading-edge computing platforms and services through NERSC as well as several departmental clusters. An IBM RS/6000 SP, makes up the heart of NERSC's computer hardware capability. NERSC's 6080-processor IBM RS/6000 SP has 380 16-CPU POWER3+ SMP nodes with a peak performance of 150 teraflop/s, making it one of the most powerful unclassified supercomputer in the world. Each node has a common pool of between 16 and 64 gigabytes of memory, and the system has 44 terabytes of disk space. Additional capabilities are provided by two special-purpose servers: a cluster of four PCs for numerical and statistical processing, and a dedicated Silicon Graphics computer for scientific visualization from remote locations. NERSC's research in data-intensive computing is grounded in their operation of a major production facility, the PDSF (Parallel Distributed Systems Facility). The PDSF is a 390-processor Linux cluster used by large-scale high energy and nuclear physics investigations for detector simulation, data analysis, and software development. The PDSF's 48 disk vaults provide a total 35 TB of data storage.

The NERSC IBM p575 POWER 5 system, named Bassi, is a distributed memory computer with 888 processors available to run scientific computing applications. Each Bassi processor has a theoretical peak performance of 7.6 GFlops. The processors are distributed among 111 compute nodes with 8 processors per node. Processors on each node have a shared memory pool of 32 GBytes. The compute nodes are connected to each other with a high-bandwidth, low latency switching network. The disk storage system is a distributed, parallel I/O system called GPFS. Additional nodes serve exclusively as GPFS servers. Bassi's network switch is the IBM "Federation" HPS switch which is connected to a two-link network adapter on each node.

Jacquard is a 640-CPU Opteron cluster running a Linux operating system. Jacquard has 320 dual-processor nodes available for scientific calculations. There are additional I/O and service nodes. Each processor runs at a clock speed of 2.2GHz, and has a theoretical peak performance of 4.4 GFlop/s. Processors on each node share 4GB of memory, which is being upgraded to 6GB. The nodes are interconnected with a high-speed InfiniBand network. Shared file storage is provided by a GPFS file system.

In addition to the NERSC resources, the High Performance Computing Research Department (HPCRD) has computational facilities available for research activities. The Harmonic cluster is a general computational cluster, with 32 nodes, each with two 866 MHz Intel Pentium III processors and 1 GB RAM and Myrinet interconnect for low latency node communication. Another cluster for general computational activities is a 16 CPU Opteron cluster with 2.4 GHz processors and a Quadrics interconnect. Other smaller clusters dedicated to nanoscience and astronomy calculations are also available. The Future Technologies Group within HPCRD also has a heterogeneous computing research cluster composed of 34 Intel(R) PII400 single cpu nodes, and 4 2-way SMP nodes consisting of 2.8GHz Xeon cpus with HyperThreading, all running Linux. Each of the PII nodes has from 128 to 256MB of memory. The faster Xeon nodes have 4 Gbytes of memory. The cluster of PII nodes is connected via GigaNet network. The faster nodes are connected with 4X InfiniBand and Myrinet 2000. The FTG cluster is primarily used as a research testbed for system software development.

Access to the LBNL computational facilities from anywhere in the U.S. or the world is available through ESnet, which provides OC-48 bandwidth to NERSC, OC-192 bandwidth on major backbone links, and OC-48 links over much of the rest of its coverage area. In the near future there are plans to upgrade the connectivity between ESnet and NERSC to OC-192.

LBNL's high-speed networking testbed is capable of routing and switching traffic up to 20 gigabits per second. The testbed includes network equipment with a switching capacity of 1.2 terabits per second, multi-port 10-gigabit Ethernet, as well as Spirent Smartbits traffic generation equipment that can be used to provide background loads for Internet emulation.

## **Lawrence Livermore National Laboratory**

The Center for Applied Scientific Computing (CASC) is the organizational home of applied mathematics and computer science research at LLNL (<http://www.llnl.gov/CASC>). CASC has about one hundred scientific staff members and all have ready access to the supercomputing resources administered by Livermore Computing (LC) (<http://www.llnl.gov/computing>), which is the computer center for LLNL. In addition to maintaining desktop workstations for staff and visiting researchers, LC maintains various large-scale computing platforms, including the 2304 and 4096 processor MCR and Thunder Linux clusters and the 131,072 processor BlueGene/L platform. These production computers provide users with a rich tool environment that includes high-performance compilers, debuggers, analyzers, editors, and locally developed custom libraries and application packages for software development. Access to such resources is provided by an LLNL Multiprogrammatic and Institutional Computing Initiative and therefore does not directly affect the requested budget for this proposal.

## **University of Michigan**

The computational resources at the University of Michigan include MacIntosh laptops, Linux workstations and parallel Linux cluster systems at the University of Michigan Center for Advanced Computing. They will be used for the model development, short tests and for documentation purposes. We will also apply for large-scale computing resources at the DOE facilities in Oak Ridge, Berkeley or Livermore for long-term, high-resolution model runs.

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## RESUME

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### Phillip Colella

- Office Address** Computational Research Division, Applied Numerical Analysis Group  
MS 50A1148, Lawrence Berkeley National Laboratory  
Berkeley, CA 94720  
Phone: (510) 486-5412  
FAX: (510) 495-2505  
E-mail: PColella@lbl.gov
- Education** *Ph.D.*, Applied Mathematics, 1979, University of California at Berkeley  
*M.A.*, Applied Mathematics, 1976, University of California at Berkeley  
*A.B.*, Applied Mathematics, 1974, University of California at Berkeley
- Recent Professional Experience** *Senior Staff Scientist and Group Leader*, 1996 to Present, Applied Numerical Analysis Group, Lawrence Berkeley National Laboratory. *Associate Professor*, 1989 to 1992; *Professor*, 1992 to 1995; *Professor in Residence*, 1995 to 1998, Mechanical Engineering Department, University of California at Berkeley.
- Honors** 1989, Presidential Young Investigator Award; 1998, IEEE Sidney Fernbach Award for High-Performance Computing; 2003, ACM-SIAM Prize for Computational Science and Engineering; 2004, elected to the National Academy of Sciences.

### Specific or Technical Accomplishments:

- Developed high-resolution and adaptive numerical algorithms for partial differential equations, including higher-order Godunov methods for hyperbolic conservation laws, block-structured adaptive mesh refinement, and Cartesian grid embedded boundary methods for problems with complex boundary geometries.
- Developed numerical simulation capabilities for a variety of applications in science and engineering, including shock hydrodynamics, combustion, astrophysics, solid mechanics, plasma physics, environmental fluid dynamics, and bioengineering.
- Participated in the design of high-performance software infrastructure for scientific computing, including software libraries (BoxLib, Chombo), and programming languages (FIDIL, Titanium).
- Led a number of multi-disciplinary and / or multi-institutional algorithm and software development projects in high-performance computing, including: the DOE HPCCP Computational Fluid Dynamics and Combustion Dynamics Project (1992-1997); a NASA ESS Computational Technologies project on adaptive mesh refinement (<http://davis.lbl.gov/NASA>) (2001-2005); and the DOE SciDAC Applied Partial Differential Equations Integrated Software Infrastructure Center (APDEC) (<http://davis.lbl.gov/APDEC>) (2001-2006).
- Led the development of spatial modeling capabilities in BioSpice for the DARPA BioComp program.
- Supervised or co-supervised 16 Ph. D. students and 11 postdoctoral researchers. Currently supervising a group of nine staff members.

### Recent Publications:

1. G. Balls and **P. Colella**, "A finite-difference domain-decomposition methods for solving Poisson's equation using local corrections", J. Comput. Phys. 180, p. 25-53 (2002)

## RESUME

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2. M. Barad and **P. Colella**, "A fourth-order accurate adaptive mesh refinement method for Poisson's equation", *J. Comput. Phys.* 209, p. 1-18 (2005).
3. **P. Colella**, D. T. Graves, B. Keen, and D. Modiano, "A Cartesian grid embedded boundary method for hyperbolic conservation laws", *J. Comput. Phys.* 211, p. 347-366 (2006).
4. R. Crockett, **P. Colella**, R. T. Fisher, R. I. Klein, and C. M. McKee, "An unsplit, cell-centered Godunov method for ideal MHD" *J. Comput. Phys.* 203, p. 422-448 (March, 2005).
5. C. Gatti-Bono and **P. Colella**, "An anelastic allspeed projection method for gravitationally stratified flows", *J. Comput. Phys.* in press.
6. P. McCorquodale, **P. Colella**, D. P. Grote, and J.-L. Vay, "A node-centered local refinement algorithm for Poisson's equation in complex geometries", *J. Comput. Phys.* 201, p. 34-60 (November, 2004).
7. P. McCorquodale, **P. Colella**, G. Balls, and S. B. Baden "A scalable parallel Poisson solver with infinite domain boundary conditions", to appear in the Proceedings, the 7th Workshop on High Performance Scientific and Engineering Computing, Oslo, Norway, June 14-17, 2005.
8. D. F. Martin, **P. Colella**, M. Anghel, and F. Alexander, "Adaptive mesh refinement for multiscale nonequilibrium physics", *Computers in Science and Engineering.* 7, p. 24-31 (2005).
9. G. H. Miller and **P. Colella**, "A conservative three-dimensional Eulerian method for coupled solid-fluid shock capturing", *J. Comput. Phys.*, 183, p. 26-82 (2002).
10. R. Samtaney, **P. Colella**, S. Jardin, and D. F. Martin, "3D Adaptive Mesh Refinement simulations of pellet injection in tokamaks", *Comput. Phys. Comm.* 164, p. 220-228 (2004).
11. P. Schwartz, M. Barad, **P. Colella**, and T. J. Ligocki, "A Cartesian grid embedded boundary method for the heat equation and Poisson's equation in three dimensions", *J. Comput. Phys.* 211, p. 531-550 (2006).
12. P. Schwartz, D. Adalsteinsson, **P. Colella**, A. P. Arkin, M. Onsum, "Numerical computation of diffusion on a surface", *Proc. Nat. Acad. Sci.* 102, p. 11151-11156 (2005).
13. D. Trebotich, **P. Colella**, and G. H. Miller, "A stable and convergent scheme for viscoelastic Flow in contraction channels", *J. Comput. Phys.* 205, p. 315-342 (2005).
14. J.L. Vay, **P. Colella**, P. McCorquodale, B. Van Straalen, A. Friedman, D.P. Grote, "Mesh refinement for particle-in-cell plasma simulations: Applications to and benefits for heavy ion fusion", *Laser and Particle Beams*, 20, p.569-575, (2002).
15. J.-L. Vay, **P. Colella**, A. Friedman, D. P. Grote, P. McCorquodale, D. B. Serafini, "Implementations of Mesh Refinement Schemes for Particle-In-Cell Plasma simulations", *Comput. Phys. Commun.* 164, p. 297-305 (December 2004).
16. J.-L. Vay, **P. Colella**, J. Kwan, P. McCorquodale, D. B. Serafini, D. P. Grote, G. Westenkow, J. C. Adam, A. Heron, and I. Haber, "Application of adaptive mesh refinement to particle-in-cell simulations of plasmas and beams", *Phys. of Plasmas* 11, p. 2928-2934 (May 2004).

# CAROLINE GATTI-BONO

## OFFICE ADDRESS

---

Center for Applied Scientific Computing  
Applied Mathematics Group  
Lawrence Livermore National Laboratory  
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Livermore, CA 94551

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## EDUCATION

---

**Ph.D. in Mechanical Engineering and Scientific Computing**, University of Michigan, 2002  
**M.S. in Mechanical Engineering**, University of Michigan, 1999  
**Diplôme d'Ingénieur**, Ecole Nationale Supérieure de Techniques Avancées, Paris, France, 1999

Areas of Research and Study: Computational fluid dynamics, numerical methods in scientific computing, modeling of dynamic systems, advanced mathematics, computational dynamics, fluid mechanics

## HONORS

---

- Luis Alvarez Post-Doctoral Fellowship, Lawrence Berkeley National Laboratory, 2003
- Rackham Pre-Doctoral Fellowship, University of Michigan, 2001
- Mechanical Engineering Departmental Fellowship, University of Michigan, 1998

## RECENT PROFESSIONAL EXPERIENCE

---

02/05-present    **Lawrence Livermore National Laboratory**, Livermore, CA  
Post-doctoral researcher in the **Center for Applied Scientific Computing**  
06/02-02/05    **Lawrence Berkeley National Laboratory**, Berkeley, CA  
Post-doctoral researcher in the **Applied Numerical Algorithms Group**

## TECHNICAL ACCOMPLISHMENTS SINCE JUNE 2002

---

- Developed and implemented a fully conservative 1D algorithm to track sharp moving interfaces in compressible media
- Developed and implemented an algorithm to model atmospheric flows over mountain ranges using Cartesian grid embedded boundary methods on anisotropic grids
- Developed method to filter fast gravity modes, releasing classical time step restriction imposed by fast atmospheric dynamics

## JOURNAL PUBLICATIONS

---

- **Caroline Gatti-Bono**, P. Colella, "A Filtering Method for Gravitationally Stratified Flows", LBNL-57161.
- **Caroline Gatti-Bono**, P. Colella, "An Anelastic Allspeed Projection Method for Gravitationally Stratified Flows", (accepted for publication by the *Journal of Computational Physics*).
- **Caroline Gatti-Bono**, N.C. Perkins (2004) "Effect of Loop Shape on the Drag-Induced Lift of a Fly Line", *ASME Journal of Applied Mechanics*, Vol. 71, No. 5, pp. 745-747.
- **Caroline Gatti-Bono**, N.C. Perkins (2004) "Numerical Model for the Dynamics of a Coupled Fly Line/Fly Rod System and Experimental Validation", *Journal of Sound and Vibration*, Vol. 272, No. 3-5, pp. 773-791.
- **Caroline Gatti-Bono**, N.C. Perkins (2004) "Numerical Simulations of Cable/Seabed Interactions", *International Journal of Offshore and Polar Engineering*, Vol. 14, No. 2, pp. 118-124.
- **Caroline Gatti-Bono**, N.C. Perkins (2003) "Comparison of Numerical and Analytical Solutions for Fly Casting Dynamics", *Journal of Sports Engineering*, Vol. 6, No. 1, pp. 165-176.
- **Caroline Gatti-Bono**, N.C. Perkins (2002) "Dynamic Analysis of Loop Formation in Cables Under Compression", *International Journal of Offshore and Polar Engineering*, Vol. 12, No. 3, pp. 217-222.
- **Caroline Gatti-Bono**, N.C. Perkins (2002) "Physical and Numerical Modeling of the Dynamic Behavior of a Fly Line", *Journal of Sound and Vibration*, Vol. 255, No. 3, pp. 555-577.

## SELECTED OTHER PUBLICATIONS AND PRESENTATIONS

---

- **Caroline Gatti-Bono**, P. Colella, G. Miller, D. Trebotich (2005) "A One-Dimensional Conservative Method for Front-Tracking in a Compressible Medium", *58<sup>th</sup> Annual Meeting of the Division of Fluid Dynamics*, APS
- **Caroline Gatti-Bono** (2004) "A Non-Hydrostatic Model to Simulate Atmospheric Flows in the Presence of Orography", *Fifth Bay Area Scientific Computing Day*

Christiane Jablonowski  
University of Michigan  
Department of Atmospheric, Oceanic and Space Sciences  
2455 Hayward St.  
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E-mail: [cjablono@umich.edu](mailto:cjablono@umich.edu)  
Phone: 248 346 4986

## CURRICULUM VITAE -- Christiane Jablonowski

### PROFESSIONAL PREPARATION

1994 BSc., Physics, Aachen University of Technology, Germany  
1998 MSc., Meteorology, University of Bonn, Germany  
2004 Ph.D. in Atmospheric and Space Sciences and Scientific Computing,  
University of Michigan, Ann Arbor, MI  
2004 - 2006 Postdoctoral Fellow, Advanced Study Program and Scientific Computing Division,  
National Center for Atmospheric Research (NCAR), Boulder, CO

### APPOINTMENTS

9/2006 – Assistant Professor of Atmospheric Science, University of Michigan, Ann Arbor  
3/2006 – 8/2006 Research Assistant at the University of Michigan, Ann Arbor, MI and Visiting  
Scientist at the Geophysical Fluid Dynamics Laboratory, Princeton, NJ  
2/2004 – 2/2006 Postdoctoral Fellow, National Center for Atmospheric Research, Boulder, CO  
8/2003 Visiting Scientist, Lawrence Livermore National Laboratory, Livermore, CA  
5/1999 – 12/2003 Graduate Student Assistant, Atmospheric Science, University of Michigan  
9/1998 – 4/1999 Graduate Student Instructor, Atmospheric Science, University of Michigan  
11/1997 – 2/1998 Consultant, European Centre for Medium-Range Weather Forecasts, Reading, UK

### KEY PUBLICATIONS

C. Jablonowski, M. Herzog, J. E. Penner, R. C. Oehmke, Q. F. Stout and B. van Leer (2006), **Adaptive Grids in Weather and Climate Modeling: Test of the Dynamical Core**, *Mon. Wea. Rev.*, submitted

C. Jablonowski and D. L. Williamson (2006), **A Baroclinic Instability Test Case for Atmospheric Model Dynamical Cores**, *Quarterly Journal of the Royal Meteorological Society*, submitted

C. Jablonowski, M. Herzog, J. E. Penner, R. C. Oehmke, Q. F. Stout, B. van Leer and K. G. Powell (2006), **Block-Structured Adaptive Grids on the Sphere: Advection Experiments**, *Mon. Wea. Rev.*, accepted

C. Jablonowski (2004), **Adaptive Grids in Weather and Climate Modeling**, Ph.D. dissertation, University of Michigan, Ann Arbor, Department of Atmospheric, Oceanic & Space Sciences, 292 pp.

### SCIENTIFIC ACCOMPLISHMENTS AND SYNERGISTIC ACTIVITIES

- Expert in Adaptive Mesh Refinement (AMR) techniques for atmospheric General Circulation Models (GCMs), developer of an adaptive version of the hydrostatic Lin-Rood Finite Volume dynamical core
- Expert in evaluation methods for dynamical cores of GCMs, model intercomparisons
- Experienced in working with an interdisciplinary team consisting of atmospheric scientists, computer scientists, mathematicians and aerospace engineers from the University of Michigan Research area: Adaptive Mesh Refinements for Weather and Climate Models
- Lecturer of several tutorials on *Parallel Computing 101* at the renowned Computer Science Conference *SuperComputing in 2000, 2001, 2004, 2005*
- Lecturer of a newly developed tutorial on NCAR's Finite Volume Dynamical Core

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## RESUME

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### Daniel Martin

- Office Address** Computational Research Division, Applied Numerical Analysis Group  
MS 50A1148, Lawrence Berkeley National Laboratory  
Berkeley, CA 94720  
Phone: (510) 495-2852  
FAX: (510) 495-2505  
E-mail: [dmartin@hpcrd.lbl.gov](mailto:dmartin@hpcrd.lbl.gov)
- Education** *Ph.D.*, Mechanical Engineering, 1998, University of California at Berkeley  
*B.S.*, Mechanical Engineering, 1991, University of Florida
- Recent Professional Experience** *Math/Statistician Scientist Engineer*, 2001 to Present, Applied Numerical Algorithms Group, Lawrence Berkeley National Laboratory.  
*Postdoctoral Researcher*, 1998 to 2001.

### Specific or Technical Accomplishments:

- Lead Developer for the NASA Computational Technologies (CT) adaptive mesh refinement (AMR) effort in the Applied Numerical Algorithms Group (ANAG), comprising of algorithm and software development activities for NASA microgravity research capabilities, including multifluid and suspended-particles in incompressible flow.
- Supervised code performance improvement effort as part of NASA CT program.
- Developed and implemented AMR algorithms for the incompressible Navier-Stokes equations in fluid dynamics and for the Time-Dependent Ginzberg-Landau equations in nonequilibrium physics.
- Current member of the development team for the Chombo framework for solving partial differential equations with AMR

### Relevant Recent Publications:

1. **D. Martin** and P. Colella, "A Cell-Centered Adaptive Projection Method for the Incompressible Euler Equations", *J. Comput. Phys.*, **163**, p. 271 (2000).
2. R. Samtaney, S. Jardin, P. Colella, and **D. Martin**, "3D Adaptive Mesh Refinement Simulations of Pellet Injection in Tokamaks", *Computers Physics Communications*, **164**, p. 220 (2004). (also Princeton Plasma Physics Laboratory Report PPPL-3891)
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## **Open Source Policy Statement**

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Lawrence Berkeley National Laboratory (Berkeley Lab) has been a leader among U.S. national laboratories in open source software and has a proven record as a leader in open source distribution of publicly-funded software. Berkeley Lab technology transfer representatives worked closely with DOE legal counsel in the development of DOE's open source policy. Berkeley Lab has been publicly recognized by DOE's Chief Patent Counsel as a leader in implementing open source distribution that is effective and a model for other laboratories to follow.

For software developed under funding arising from this proposal, Berkeley Lab intends that the source code is fully and freely available for use and modification throughout the scientific computing community by using the pre-approved open source process, consistent with open source policy guidance issued by DOE's OASCR and ASCI in May 2003.

Berkeley Lab has released scores of different software codes as "open source" from varied scientific disciplines, resulting in tens of thousands of downloads each year (e.g., over 30,000 no-cost open source downloads from Berkeley Lab web sites in FY2005 alone). Berkeley Lab uses a variety of distribution mechanisms, tailored to the particulars of the target audience, including Berkeley Lab web sites, Sourceforge.org web sites, on-site workshops, and collaborations with other research and industrial organizations. We intend to use a similar array of distribution channels for software developed under this funding.

Berkeley Lab uses the well-known and well-accepted open source "BSD" license as its default open source license. Our experience has shown that academics and industry favor the BSD license since it has 'no strings attached' and allows end users to use, modify and redistribute code in any manner that they see fit (in contrast to other more restrictive open source licenses).

## **Carbon Data Assimilation and Parameter Estimation Using Local Ensemble Transform Kalman Filter (LETKF)**

**Program Area:** Scientific Application Partnership: Computer Science

**Principal Investigator:** Eugenia Kalnay (University of Maryland)

**Senior Personnel:** Inez Fung (UC – Berkeley), Michael Wehner (LBNL)

**Scientific Application Partner:** A Scalable and Extensible Earth System Model for Climate Change Science (PI - John B. Drake, Oak Ridge National Laboratory)

**Participating Institutions:** U. Maryland, U.C.-Berkeley, Lawrence Berkeley National Laboratory (LBNL)

**Projected Funding Request:** FY07 - \$711K, FY08 - \$719K, FY09 - \$726K, Total \$2156K for three years.

## 1. ABSTRACT:

The goal of the proposed work is to develop a carbon data assimilation system to synthesize all meteorological and carbon observations in a single dynamical framework to derive new estimates of the contemporary carbon sources and sinks at high spatial resolution, and to improve the representation of carbon processes in the DOE-NCAR coupled carbon-climate models. The proposed work will be carried out by a team comprising UMD scientists (expert in data assimilation) and UCB scientists (expert in the carbon cycle and carbon-climate modeling) working in collaboration with modelers and computer scientists from LBNL. In the first phase (first 3 years) we plan to couple the carbon-climate model CAM3-CASA' already implemented on DOE computers with the accurate and parallel Local Ensemble Transform Kalman Filter (LETKF) data assimilation available from UMD, and perform simultaneous assimilations of simulated meteorological and CO<sub>2</sub> data. In this phase we will develop an end-to-end system, including observation operators that convert model variables into synthetic meteorological and CO<sub>2</sub> observations. The data assimilation of meteorological and carbon simulated observations with the fvCAM3-CASA'/LETKF system for the test periods will provide a clear estimate of the ability of the system to estimate CO<sub>2</sub> concentrations, surface fluxes, carbon cycle parameters such as Light Use Efficiency (LUE), and their uncertainty. The system will be ready for carrying out data assimilation of real observations, using in situ, aircraft and satellite data.

## 2. EXECUTIVE SUMMARY

We propose to take advantage of three scientific advancements to create, for the first time, a carbon data assimilation system that includes carbon cycle parameter estimations, and estimations of uncertainty. In recent years a realistic global atmosphere-ocean-land model in the DOE-NCAR CCSM framework has been coupled to interactive terrestrial and oceanic carbon cycles to project the co-evolution of CO<sub>2</sub> and climate (Doney et al. 2006; Fung et al 2005). Previous SciDAC efforts have added the terrestrial carbon cycle CASA' to CAM3 with finite volume, spectral and semi-lagrangian versions for experiments contributing to the WRCP-IGBP Coupled Carbon Cycle Climate Model Intercomparison Project (C4MIP) (Friedlingstein et al. 2006). At the same time, the University of Maryland has developed an advanced Ensemble Kalman Filtering (EnKF) system that is model independent, accurate and computationally very efficient and parallel, and that provides an estimate of the uncertainty of the analysis (Ott et al, 2004, Hunt et al, 2004, Szunyogh et al, 2005, Hunt, 2005). The third development is the maturity of carbon-relevant observations beyond the ~100 CO<sub>2</sub> mixing ratios in the marine boundary layer at remote locations around the globe. The observations include DOE's *in situ* measurements of terrestrial carbon dynamics (AmeriFlux and FACE programs, Running et al. 2001; Norby et al. 2005), aircraft data from COBRA (Gerbig et al. 2003), *in situ* and aircraft data from the forthcoming North American Carbon Program (NACP), and the forthcoming launch of O-C-O in the NASA A-train (<http://oco.jpl.nasa.gov/>) and of the Japanese Greenhouse gases Observing Satellite (GOSat, [http://www.jaxa.jp/missions/projects/sat/eos/gosat/index\\_e.html](http://www.jaxa.jp/missions/projects/sat/eos/gosat/index_e.html)) that will be measuring total column daytime CO<sub>2</sub> throughout the globe. This makes it possible, for the first time, to perform data assimilation of the carbon cycle *in conjunction with* conventional meteorological data assimilation to synthesize all carbon and meteorological observations into a single framework. The main goal of this project will be to estimate the distribution of CO<sub>2</sub> in space and time with much more accuracy than possible before and to provide reliable data-based information about CO<sub>2</sub> distributions and CO<sub>2</sub> sources and sinks for testing models and informing policy makers.

**IN THIS PROPOSAL, WHERE UMD AND UCB WILL COLLABORATE WITH MODELERS AND COMPUTER SCIENTISTS FROM LBL, WE FIRST PLAN TO COUPLE THE CAM3-CASA' MODEL WITH THE LOCAL ENSEMBLE TRANSFORM KALMAN FILTER (LETKF) DATA ASSIMILATION (BOTH ALREADY DEVELOPED) AND PERFORM ASSIMILATIONS OF SIMULATED DATA. THIS REQUIRES DEVELOPING THE "OBSERVATION OPERATORS" THAT TRANSFORM SAMPLED FORECAST MODEL VARIABLES INTO SYNTHETIC OBSERVATIONS (ALSO REQUIRED FOR THE ASSIMILATION OF ACTUAL OBSERVATIONS) AND WILL ALLOW TESTING AN END-TO-END SYSTEM. AT THE END OF 3 YEARS WE WILL HAVE A COMPLETELY DEVELOPED SYSTEM READY FOR ASSIMILATION OF THE ACTUAL *IN SITU*, AIRCRAFT AND SATELLITE OBSERVATIONS. THE SIMULATION PHASE WILL ALLOW US TO DEMONSTRATE THE FEASIBILITY OF THE PROJECT, AND QUANTIFY THE DEGREE TO WHICH I THE AVAILABLE MEASUREMENTS, COMBINED WITH THE CO<sub>2</sub> MODEL CAN IDENTIFY THE GEOGRAPHICAL AND TEMPORAL (DIURNAL AND SEASONAL) CHARACTERISTICS OF THE CARBON CYCLE, AS WELL AS THE OPTIMAL ESTIMATION OF A FEW CRUCIAL ECOSYSTEM PARAMETERS, SUCH AS THE LIGHT USE EFFICIENCY (LUE) THAT DEPENDS ON THE TYPE OF VEGETATION (E.G., STILL ET AL. 2004). IT WILL ALSO TEST THE ABILITY OF THE SYSTEM TO DISTINGUISH THE CHARACTERISTICS OF THE CARBON CYCLE BETWEEN DRY AND WET PERIODS. AT THE END OF THIS PHASE WE WILL HAVE COMPARED THE FVCAM3-CASA'/LETKF OUTPUT WITH REAL METEOROLOGICAL OBSERVATIONS FROM THE NCEP-DOE REANALYSIS 2, DEVELOPED AND TESTED AN END-TO-END SYSTEM READY TO USE WITH REAL CARBON AND METEOROLOGICAL OBSERVATIONS (INCLUDING OCO AND GOSAT, WHICH WILL BECOME AVAILABLE AT THAT TIME), AND DOCUMENTED ITS POTENTIAL WITH SIMULATED OBSERVATIONS. THIS SYSTEM SHOULD BE ABLE TO PROVIDE NOT ONLY THE BEST ESTIMATE OF THE 4D DISTRIBUTION OF CO<sub>2</sub>, BUT ALSO AN ATMOSPHERIC REANALYSIS MUCH MORE**

**COMPREHENSIVE THAN EITHER THE NCEP-DOE REANALYSIS 2 OR THE ERA40, AND FOR THE FIRST TIME, AN ESTIMATE OF UNCERTAINTIES AND OF CRUCIAL CARBON CYCLE PARAMETERS. LINKAGE TO JOHN DRAKE'S (ORNL) SA PROPOSAL, "A SCALABLE AND EXTENSIBLE EARTH SYSTEM MODEL FOR CLIMATE CHANGE SCIENCE" WILL COMPLEMENT THE DEVELOPMENT OF THE BIOGEOCHEMICAL ASPECTS OF THE CCSM.**

### 3. BACKGROUND AND RECENT ACCOMPLISHMENTS:

The contemporary increase in CO<sub>2</sub> in the atmosphere is approximately half the CO<sub>2</sub> emitted by fossil fuel combustion. The land and oceans have acted as repositories (sinks) for the remainder of the fossil fuel CO<sub>2</sub>, plus the CO<sub>2</sub> released as a result of land use modification. The key to predicting future levels of atmospheric CO<sub>2</sub> and the timing and magnitude of climate change is not only prediction of the anthropogenic carbon sources, but also of the biogeochemical processes that determine the changing magnitudes and locations of the carbon sinks. These processes determine the rate of carbon exchange between the atmosphere, land and oceans, as well as the stability and longevity of carbon storage in each of these reservoirs in a changing environment.

Inferences about the magnitudes and locations of the contemporary carbon sinks have relied on a combination of “top-down” and “bottom-up” methods, each with its own advantages and disadvantages. “Top-down” methods, mathematically an inverse problem, infer the CO<sub>2</sub> surface fluxes (carbon sources and sinks) from the geographic and temporal variations in atmospheric CO<sub>2</sub> concentrations (Tans et al. 1990). Because the CO<sub>2</sub> monitoring sites are sparse (~100 globally) and are deliberately sited in remote coastal or marine boundary layers where CO<sub>2</sub> concentrations are less variable than vegetated areas, “top-down” methods yield only broad regional information about the land sinks and how these sinks vary in response to interannual and longer-term climate perturbations (Bousquet et al. 2000; Gurney et al. 2004). “Bottom-up” methods integrate continuous in-situ observations of net ecosystem CO<sub>2</sub> exchange (e.g. Running et al. 1999; Law et al. 2002) and episodic aircraft observations of atmospheric CO<sub>2</sub> concentrations (e.g. Gerbig et al. 2003a, 2003b) to yield local estimates of carbon sources and sinks and their sensitivity to interannual climate variations. Because of the heterogeneity of the landscape, there is no clear way to extrapolate the in-situ observations to continental scale.

The uncertainty in our current understanding is illustrated by the new class of carbon-climate models used to project the co-evolution of CO<sub>2</sub> and climate to 2100A.D. in response to a specified fossil fuel emission rate (Cox et al. 2001, Friedlingstein et al. 2003; Matthews et al. 2005; Thompson et al 2004; Zeng et al. 2004; Govindasamy et al. 2005; Fung et al. 2005). Even after accounting for the variations in physical climate sensitivity among the models, there is a large range in the sensitivity of the terrestrial and oceanic carbon storage to climate change, as well as in the magnitudes of the carbon feedbacks to the climate system (Friedlingstein et al. 2006).

The goal of the proposed work is to synthesize all carbon observations in a single dynamical framework in order to derive global estimates of the contemporary carbon sources and sinks, and to improve the representation of carbon processes in coupled carbon-climate models. We propose to take advantage of three recent scientific and computational advancements to create a carbon data assimilation system that includes carbon cycle parameter estimations, as well as estimations of uncertainty.

In recent years a realistic global atmosphere-ocean-land model in the DOE-NCAR CCSM framework has been coupled to interactive terrestrial and oceanic carbon cycles to project the co-evolution of CO<sub>2</sub> and climate (Doney et al. 2006; Fung et al 2005). Previous SciDAC efforts have added the terrestrial carbon cycle CASA’ to CAM3 with finite volume, spectral and semi-lagrangian versions for experiments contributing to the WRCP-IGBP Coupled Carbon Cycle Climate Model Intercomparison Project (C4MIP) (<http://www.c4mip.cnrs-gif.fr/protocol.html>)).

At the same time, the University of Maryland has developed an advanced Ensemble Kalman Filtering (EnKF) system that is accurate and computationally completely parallel and very efficient, that can

assimilate observations simultaneously, and provides an estimate of the uncertainty of the analysis of all the variables (Ott et al, 2002, 2004, Hunt et al, 2004, Szunyogh et al, 2005, Hunt, 2005). This breakthrough in data assimilation has been the result of 5 years of research by an interdisciplinary group of experts in atmospheric sciences (Profs. Kalnay and Szunyogh), nonlinear dynamics (Profs. Hunt, Sauer, Ott and Yorke), and computer science (Prof. Kostelich). The new method, known as Local Ensemble Transform Kalman Filter (LETKF) is recognized as being as accurate as other Ensemble Square Root Filters (Tippett et al. 2003, Bishop et al. 2001, Anderson 2000, Whitaker and Hamill, 2002) but much more suitable to parallelization and the assimilation of large amounts of data (Hamill, 2006, pers. comm., Houtekamer, 2006, pers. comm.). It has also been extended to 4-dimensions (Hunt et al, 2004) thus allowing the assimilation of observations at their correct observation time. The LETKF is advantageous compared to the other advanced method (4D-Var) in several important aspects (Kalnay et al, 2006): It is simpler to code and maintain because it is model independent, it does not require the use of the model linear tangent and adjoint models (thus bypassing the tedious derivation of adjoints for every model upgrade), and, most importantly, it evolves the forecast error covariance and provides the analysis error covariance. Because of its parallelism, it is also more efficient than 4D-Var.

The third development is the maturity of carbon-relevant observations beyond the ~100 CO<sub>2</sub> flask measurements of mixing ratios in the marine boundary layer at remote locations around the globe. The observations include DOE's in situ measurements of terrestrial carbon dynamics (AmeriFlux and FACE programs (Running et al. 2001; Hendry et al. 1999), aircraft data (Gerbig et al. 2003; Sawa et al. 2004), in situ and aircraft data from the forthcoming North American Carbon Program (NACP), and the forthcoming launch of O-C-O (Crisp et al. 2004) in the NASA A train (<http://oco.jpl.nasa.gov/>) and of the Japanese Greenhouse gases Observing Satellite (GOSat, [www.jaxa.jp/missions/projects-sat/eos/gosat/index\\_e.html](http://www.jaxa.jp/missions/projects-sat/eos/gosat/index_e.html)) that will be measuring total column daytime CO<sub>2</sub> throughout the globe. Measurements of CO on MOPPITT and CO<sub>2</sub> and CH<sub>4</sub> on Sciamachy can be assimilated to separate anthropogenic from ecosystem fluxes of CO<sub>2</sub> (e.g. Arellano et al. 2004; Buchwitz et al. 2005a, 2005b). The AQUA high resolution infrared sounder AIRS (and its successor IASI) also provide information on upper troposphere and stratospheric CO<sub>2</sub>, CO and CH<sub>4</sub>, and will be considered as a possible source of concentrations (Chedin et al. 2003; Engelen and Stephens, 2004; Crevoisier et al, 2005). Since the AIRS channels are strongly sensitive to temperature and moisture, only within a data assimilation system that contains detailed information on temperature and moisture constrained by all available data sources as well as by a short range forecast is it possible to obtain accurate CO<sub>2</sub> information (Engelen et al, 2004).

These three developments make it possible, for the first time, to perform data assimilation of the carbon cycle *in conjunction* with conventional meteorological data assimilation to synthesize all carbon and meteorological observations into a single framework. The assimilation system will at the same time use the observations to optimally estimate the biogeochemical parameters (and their uncertainties) and hence improve the representation of carbon processes inside the carbon-climate model. In this way, the improved carbon-climate model provides a justified framework for extrapolating the sparse and asynchronous observations into synoptic distributions. The main goal of this project will be to estimate the distribution of CO<sub>2</sub> in space and time with much more accuracy than possible before and to provide reliable data-based information about CO<sub>2</sub> distributions and CO<sub>2</sub> sources and sinks for testing models and informing policy makers.

Previous atmospheric transport inversion studies have estimated CO<sub>2</sub> concentrations by relating observed atmospheric CO<sub>2</sub> concentrations in the planetary boundary layer at ~100 remote coastal sites to surface fluxes by means of atmospheric transport models (Tans et al. 1990; Enting, 2002; Gurney et al. 2004; Michalak et al. 2005; and references within Peters et al., 2005). The system of

equations involved in these studies is solved by large matrix inversions, and the largest computational requirement is the construction of the observation operators relating the unknown surface fluxes to the CO<sub>2</sub> atmospheric measurements. Furthermore, the problem is under-determined and the solution is non-unique, and there is little information about CO<sub>2</sub> variations above the boundary layer. The inversion approach has been extended beyond the surface CO<sub>2</sub> measurements to include column CO<sub>2</sub> data anticipated from the OCO satellite (Rayner and O'Brien 2001) and intensive field campaigns (Peylin et al. 2005). Because of the size of the matrices, the fluxes are solved for either at a resolution much coarser than that of the satellite information itself (Rayner and O'Brien 2001) or at high-resolution for a short duration (Peylin et al. 2005).

A new class of carbon data assimilation models employing approaches from numerical weather prediction has emerged recently to synthesize existing remote boundary layer CO<sub>2</sub> observations (Peters et al. 2005), or upper tropospheric CO<sub>2</sub> observations from AIRS (Chevallier et al. 2005; Engelen et al. 2004), or anticipated column CO<sub>2</sub> observations from the satellite OCO (Baker et al. 2005). The central models are either an existing atmospheric tracer transport model with specified circulation statistics (Chevallier et al. 2005) or the ECMWF data assimilation system for numerical weather prediction (Engelen et al. 2004). Different assimilation approaches are employed, ranging from a steepest descent (Baker et al. 2005) to 4D VAR approach (Engelen et al. 2004). 4DVAR is not easily up-scalable, as it requires the derivation of an adjoint and linearized observations operators specific to the chosen atmospheric model and the chosen set of observations.

Peters et al. (2005), in a very recent pioneering study, tested an approach that is closer (but still significantly different) to the one we are proposing. They took advantage of the Ensemble Square Root Filter (EnSRF) of Whitaker and Hamill (2002) developed for numerical weather prediction (NWP) and performed a simulation where they assimilated weekly CO<sub>2</sub> pseudo-observations. The pseudo-observations were obtained from a "nature" run where they allowed for about 10 weeks of surface fluxes to interact with the observations. Because of the similarities and difference between Peters et al (2005) System for Ensemble Assimilation of Tracers in the Atmosphere (SEAT-A) and our proposed method (LETKF), we describe the SEAT-A in some detail. Their model state consists of 10 successive CO<sub>2</sub> *surface fluxes* ( $f_{t-10}, f_{t-9}, \dots, f_{t-0}$ ). The forecast model (for the ensemble mean fluxes) is persistence ( $f_{t+1}^b = f_t^a$ ). The observation operator that transforms the state variables (fluxes) into observed CO<sub>2</sub> concentrations is the TM5 transport model. The TM5 is a linear transport model driven by ERA-40 reanalysis winds, and integrates forward the forecast CO<sub>2</sub> concentrations for each ensemble member at t-10, forced by the surface fluxes until time zero ( $H(f) = \text{CO}_2^b$ ). At this time the new observed CO<sub>2</sub> concentrations are compared with the ensemble mean forecasted concentrations, and the EnSRF equations are used to update the ensemble mean 10-week fluxes. The ensemble flux perturbations for t=0 are created by random perturbations obtained from a Gaussian, fixed background error covariance  $P^b$ . They estimate the spin-up time as about twice the number of weeks used in the lagged analysis (20 weeks). As done in NWP, the covariance is localized to avoid long-distance sampling errors in the correlation. The net result of the SEAT-A system is that weekly CO<sub>2</sub> concentration observations provide improved estimations of the previous weeks surface fluxes, up to 10 weeks before current time. Beyond this 10-week lag, the surface fluxes and the ensemble perturbations are not updated any further.

Parallel to the development of models and approaches for assimilating/inverting atmospheric CO<sub>2</sub> data is the assimilation systems for estimating ecosystem parameters from measured net CO<sub>2</sub> fluxes and boundary layer CO<sub>2</sub> concentrations (e.g. Vukicevic et al. 2001; Still et al. 2004; Braswell et al. 2005; Rayner et al. 2005; Williams et al. 2005; Kaminski et al. 2002). The central model in some of these studies is an ecosystem dynamics model. Like the studies above, these studies employ a variety of approaches, from Bayesian inversions (Braswell et al. 2005) to Ensemble Kalman Filters (Williams et



al. 2005).

Here we propose, by contrast, to do a “reanalysis” of the atmosphere, including standard atmospheric variables ( $u, v, T, q, p_s$ ) as well as CO<sub>2</sub>, and estimate the 4-dimensional CO<sub>2</sub> distribution and surface fluxes. The model will be the coupled atmosphere-ecosystem climate model fvCAM3-CASA’, and the data assimilation system is the Local Ensemble Transform Kalman Filter (LETKF). The prognostic variables indicated above, augmented by the surface flux proxies or ecosystem parameters that we also want to estimate, constitute the model state. Since the CO<sub>2</sub> transport forced by the surface fluxes is accurately estimated during the integration of the coupled atmospheric model (rather than a linear transport model), the observation operator is simply the interpolation of the CO<sub>2</sub> concentration forecast to the observation location, at the time of the observation (not a weekly average). In the next sections we discuss the LETKF approach and its advantages (and computational cost), as well as the differences with SEAT-A in more detail.

### Recent accomplishments:

The carbon data assimilation system in the proposal will combine the CAM3-CASA’, a prognostic carbon-climate model developed in the NCAR-DOE CCSM framework, with the Local Ensemble Transform Kalman Filter (LETKF), a demonstrated approach for numerical weather prediction, to synthesize all atmospheric and terrestrial carbon observations into a single framework. The schematic figure 1 indicates that the LETKF is essentially a black box, model independent. It requires a forecast model  $M(\mathbf{x})$ , in this proposal CAM3-CASA’, and the observation operator  $H(\mathbf{x})$  that transforms model variables into synthetic observations. Given an ensemble of forecasts and the corresponding observations, the LETKF creates an ensemble of analyses, whose mean is the best estimate, and whose covariance is the analysis error covariance. These analyses are the initial condition for the next analysis cycle. In the next two sections we describe the model we plan to use and the LETKF algorithm.

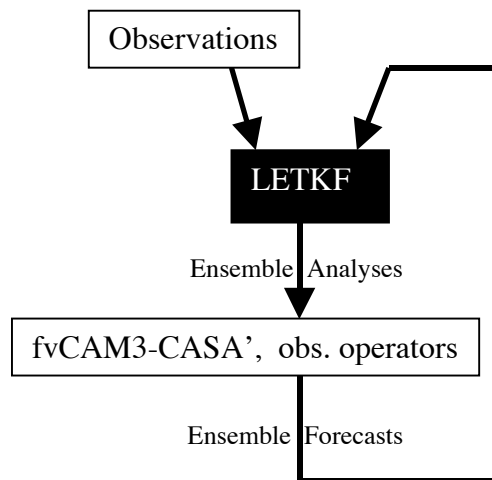


Figure 1: Schematic of the LETKF analysis cycle. Given an input of  $K$  ensemble 6-hour forecasts and the corresponding “forecasted observations” obtained applying the observation operators to the ensemble forecasts, and the actual observations, the LETKF creates a new analysis ensemble, giving the initial conditions for the next 6-hour forecast. The analysis ensemble average is the best estimate of the state, and the analysis ensemble spread provides the best estimate of the uncertainty.

#### 1) Prognostic Carbon-Climate Model

We have chosen CAM3-CASA’ with finite volume dynamic core (henceforth referred to as fvCAM3-CASA’) to prototype the development of the carbon data assimilation system because the coupling of carbon and climate codes has been implemented, and the model is developed within the CCSM

framework. Software developed and lessons learned using CAM3-CASA' can be readily transferred to future CCSM coupled carbon-climate models and to include oceanic hydrographic and carbon observations.

CAM3 is the 6<sup>th</sup> generation atmospheric general circulation model developed by the climate community (Collins et al. 2006). It includes the Community Land Model (CLM3, Dickinson et al. 2006) and a thermodynamic sea ice model (CSIM5). Important for this application is the new option for finite volume dynamical core (Lin 2004) in addition to the Eulerian spectral, semi-Lagrangian methods for approximating the dynamical equations. The finite volume dynamic core is mass-conserving, and is particularly suited for the advection of tracers (Rasch et al. 2006). CASA', like its predecessor CASA (Randerson et al. 1997), calculates the photosynthetic uptake of CO<sub>2</sub> from the atmosphere, and follows the fate of the carbon through three live vegetation carbon pools (leaves, root and wood) and nine dead soil carbon pools and the accompanying respiratory release of CO<sub>2</sub> to the atmosphere. The rates of carbon transfer among the pools are sensitivity to climate and the assumed biochemical composition of the pools. The coupling of CASA' to the atmosphere is via net carbon fluxes (also termed net ecosystem exchange, NEE) associated with photosynthesis and respiration:

$$\bar{F}_{net} = NEE = GPP - R_a - R_h$$

Here,  $F_{net}$  is the net carbon flux from the atmosphere; GPP is gross primary productivity;  $R_a$  is autotrophic (plant) respiration, while  $R_h$  is heterotrophic (microbial) respiration associated with decomposition. In the coupling of CASA' to CSM1.4, an early generation NCAR climate model (Doney et al. 2006; Fung et al., 2005), CASA' has been modified to start with GPP calculated by CCM3-LSM (the atmospheric and land modules of CSM1.4), hence coupling the carbon and water cycles. Also, the predicted leaf carbon inventory is translated into a prognostic leaf area index, hence further coupling the carbon and energy cycles. CASA' has been ported to the CAM3-CLM3 framework, and is running at ORNL (Hoffman et al. 2005). It is one of several CCSM models participating in the Coupled Carbon Cycle Climate Model Intercomparison Project (C<sup>4</sup>MIP) jointly sponsored by the World Climate Research Programme (WCRP) and the International Geosphere-Biosphere Programme (IGBP).

## 2) Description of the LETKF, recent progress with the GFS, fvGCM and Earth Simulator models

Numerical Weather Prediction (NWP) research on Ensemble Kalman Filtering (EnKF), a computationally feasible alternative to 4D-Var and the Extended Kalman Filter started with Evensen (1994) and Houtekamer and Mitchell (1998). Their methods can be classified as *perturbed observations* EnKF, and are essentially ensembles of data assimilation systems. A second type of EnKF is a class of *square root* filters (Anderson, 2001, Whitaker and Hamill, 2002, Bishop et al, 2001, see review of Tippett et al, 2003), which consist of a single analysis based on the ensemble mean, and where the analysis perturbations are obtained from the square root of the Kalman Filter analysis error covariance. Whitaker and Hamill (2002) showed that square root filters are more accurate than perturbed observation filters because they avoid the sampling errors introduced by perturbing the observations with random errors.

The three square root filters discussed by Tippett et al (2003) assimilate observations *sequentially* (as suggested by Houtekamer and Mitchell, 1998), which increases efficiency by avoiding the inversion of large matrices. At the University of Maryland Ott et al. (2002, 2004) introduced an alternative square root filter where efficiency is achieved by computing the Kalman Filter analysis at each grid point based on the ensemble forecasts within a local patch or cube of a few grid points. The Kalman Filter equations are solved using as basis the singular vectors of the ensemble in the local patch. This

method, known as Local Ensemble Kalman Filter (LEKF) allows processing all the observations within the cube simultaneously, and since the analysis at each grid point is done independently from other grid points, it is completely parallel. With an approach similar to Bishop et al (2001) but performed locally as in Ott et al. (2004), Hunt (2005) and Harlim and Hunt (2005) developed the Local Ensemble Transform Kalman Filter (LETKF), which uses as a non-orthogonal basis the local ensemble forecasts. Since it does not require performing singular value decompositions (SVD) at each grid point the LETKF is about 5 times faster than the original LEKF but gives essentially identical results. Hunt et al (2004) extended EnKF to 4 dimensions, allowing the assimilation of asynchronous observations. This method (4D-EnKF) expresses the observation as a linear combination of the ensemble perturbations at the time of the observation. The same linear combination of ensemble members can then be used to move the observational increment forward (or backward) in time to the analysis time. This simple method gives the Ensemble Kalman Filter the ability of 4D-Var to assimilate observations at their right time, but without iterations; and it allows using future observations when available.

The LETKF has been coupled and tested with several atmospheric global systems with excellent results. Szunyogh et al (2005) used the NCEP Reanalysis model (with resolution T62/L28) and showed that it is accurate and efficient. Liu et al (2006) coupled it with the NASA/NOAA finite volume GCM (fvGCM) and compared it with a 3D-Var using the same simulated observations, showing that the LETKF is much more accurate (Fig. 2). Miyoshi (2006, pers. comm.) has coupled it with the Japan Earth Simulator T159/L48 model with excellent results.

The LETKF with the NCEP GFS model is currently being tested and tuned using *real* observations. Preliminary results are extremely encouraging. Figure 3 shows the results of two data assimilations were run in parallel using exactly the same observations including *all operationally assimilated observations for January 2004 with the exception of satellite radiances*. They both used the same T62/L28 model (the resolution used in the NCEP-DOE Reanalysis), but one data assimilation is made with the current Spectral Statistical Interpolation (SSI), which is the NCEP operational implementation of 3D-Var (shown in the figure as NCEP Benchmark), and the other one with our LETK system. 24-hour forecasts were carried out every 6 hours starting from initial conditions from the two analyses. The 1-day forecasts were verified against the NCEP high-resolution operational analysis using all observations. The figure shows the estimated analysis rms error for the temperature in the SH Extratropics for the last 15 days of January 2004. It can be seen that the LETK analysis (leading to the forecast) is more accurate throughout atmosphere with the exception of the near surface layer below 750 hPa. The superiority of the LETKF is especially striking in the upper troposphere and the stratosphere, where the operational scheme has obvious difficulties. This result was obtained with minimal tuning of the LETKF system and we expect further significant improvements from a careful tuning of the scheme, as well as from the extension to 4DLETKF.

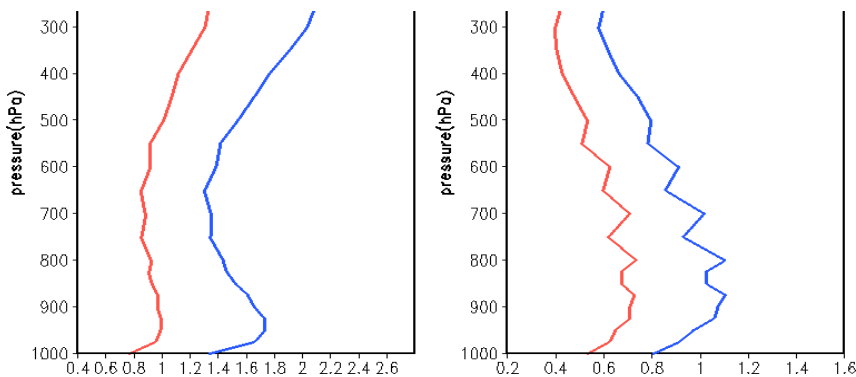


Figure 2: Comparison of the globally averaged RMS errors for the zonal wind (left) and scaled temperature (right) using PSAS (a 3D-Var scheme, in blue) and the LETKF (red). The observations used by both systems are the same simulated rawinsondes.

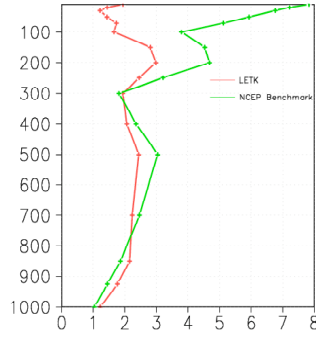


Figure 3: Comparison of the rms 1-day forecast error made from a data assimilation based on the LETKF (red) and on the operational NCEP SSI (green) in the SH extratropics. Both systems used the same model (T62/L28) and the same observations for January 2004 (all the observations used operationally with the exception of satellite radiances). The forecasts were verified against the high resolution NCEP analysis.

If we compare the LETKF with the EnSRF used in the SEAT-A system of Peters et al (2005), the main difference is that the EnSRF assimilates one observation at a time, which reduces the size of the matrix equations, whereas the LETKF assimilates all observations in the neighborhood of a grid point simultaneously, and is completely parallel since analyses at different grid points can be carried out simultaneously in different processors.

## 2.1 Description of the LETKF

The Extended Kalman Filter (EKF, e.g., Ide et al, 1997) consists of a forecast step,

$$\mathbf{x}_n^b = M_n(\mathbf{x}_{n-1}^a) \quad (1a)$$

$$\mathbf{B}_n = \mathbf{M}_n \mathbf{A}_{n-1} \mathbf{M}_n^T + \mathbf{Q}_n \quad (1b)$$

and an analysis step,

$$\mathbf{x}_n^a = \mathbf{x}_n^b + \mathbf{K}_n (\mathbf{y}_n - H_n \mathbf{x}_n^b) \quad (2a)$$

$$\mathbf{A}_n = (\mathbf{I} - \mathbf{K}_n \mathbf{H}) \mathbf{B}_n \quad (2b)$$

where  $\mathbf{K}_n$  is the Kalman gain matrix given by two equivalent formulations,

$$\mathbf{K}_n = \mathbf{B}_n \mathbf{H}^T (\mathbf{R} + \mathbf{H} \mathbf{B}_n \mathbf{H}^T)^{-1} = (\mathbf{B}_n^{-1} + \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H})^{-1} \mathbf{H}^T \mathbf{R}^{-1}, \quad (3)$$

and  $\mathbf{A}_n$  is the new analysis error covariance. Here  $n$  denotes the analysis step,  $\mathbf{x}_n$  is the state vector,  $H_n$  is the (nonlinear) observation operator at time  $t_n$  that maps model variables to observation variables  $\mathbf{y}_n$ .  $M_n$  is the nonlinear model that provides the forecast or background  $\mathbf{x}_n^b$  at step  $n$  starting from the previous analysis  $\mathbf{x}_{n-1}^a$ ,  $\mathbf{M}_n$  and  $\mathbf{M}_n^T$  are the linear tangent and adjoint models,  $\mathbf{B}_n$  is the background error covariance at the time of the analysis, and  $\mathbf{Q}_n$  is the covariance of the model errors. The update of the background error covariance (1b) requires the linear tangent and adjoint models, and makes EKF computationally unfeasible for any realistic model.

Ensemble Kalman Filter (EnKF) is similar to EKF, the main difference being that an ensemble of  $K$  forecasts

$$\mathbf{x}_{n,k}^b = M_n(\mathbf{x}_{n-1,k}^a), k = 1 \dots K \quad (4a)$$

replaces (1a) and (1b) and is used to estimate the background error covariance  $\mathbf{B}_n$ . Defining the forecast ensemble mean as  $\bar{\mathbf{x}}_n^b = \frac{1}{K} \sum_{k=1}^K \mathbf{x}_{n,k}^b$ , and  $\mathbf{E}_n^b$  as the  $M \times K$  matrix whose columns are the  $K$  ensemble perturbations  $\mathbf{x}_{n,k}^b \square \bar{\mathbf{x}}_n^b$ , and  $M$  is the dimension of the state vector, then

$$\mathbf{B}_n = \frac{1}{K} \sum_{k=1}^K \mathbf{E}_n^b \mathbf{E}_n^{bT}. \quad (4b)$$

The analysis ensemble mean increment  $\bar{\mathbf{x}}_n^a \square \bar{\mathbf{x}}_n^b$  can be obtained from (2a) with

$$\mathbf{K}_n = \mathbf{B}_n \mathbf{H}^T [\mathbf{H} \mathbf{B}_n \mathbf{H}^T + \mathbf{R}]^{-1} = \mathbf{E}_n^b [(\mathbf{H} \mathbf{E}_n^b)^T \mathbf{R}^{-1} (\mathbf{H} \mathbf{E}_n^b) + (K \square 1) \mathbf{I}]^{-1} (\mathbf{H} \mathbf{E}_n^b)^T \mathbf{R}^{-1} \quad (5)$$

where the matrix inversion is performed in the  $K \times K$  space of the ensemble perturbations.

The Ensemble Transform Kalman Filter (ETKF) approach to obtain the analysis perturbations (Bishop et al, 2001, Hunt, 2005) is based on:

$$\frac{1}{K} \sum_{k=1}^K \mathbf{E}_n^a \mathbf{E}_n^{aT} = \mathbf{A}_n = \mathbf{E}_n^b \left[ (K \square 1) \mathbf{I} + (\mathbf{H} \mathbf{E}_n^b)^T \mathbf{R}^{-1} (\mathbf{H} \mathbf{E}_n^b) \right]^{-1} \mathbf{E}_n^{bT} = \mathbf{E}_n^b \hat{\mathbf{A}}_n \mathbf{E}_n^{bT} \quad (6a)$$

where  $\hat{\mathbf{A}}_n$ , a  $K \times K$  matrix, represents the new analysis covariance in the  $K$  space of the ensemble forecasts. The new analysis perturbations are then obtained from

$$\mathbf{E}_n^a = \mathbf{E}_n^b \left[ (K \square 1) \hat{\mathbf{A}}_n \right]^{1/2}. \quad (6b)$$

Note that  $\mathbf{H} \mathbf{E}_n^b$ ;  $H \mathbf{x}_{n,k}^b \square H \bar{\mathbf{x}}_n^b$  and, since  $\mathbf{H}$  always appears multiplying a perturbation vector or matrix, in EnKF it is possible to use the full nonlinear observation operator, without the need for the Jacobian or adjoint (e.g., Szunyogh et al, 2005, Appendix).

Because the size of the ensemble ( $\sim 100$ ) is much smaller than dimension of the model (about  $10^7$  for NWP models) the computation of (2a), and (4)-(6) done in the ensemble space becomes computationally feasible. In the LETKF an additional important measure is taken to increase efficiency: after performing the ensemble forecasts (4a) globally, the analysis at each grid point is performed *locally* within a ‘‘cube’’ or 3D patch of grid points surrounding the central grid point. The results are not strongly sensitive to the size of the local patch, which typically is about 1000 km by several layers for a 6 hour analysis cycle (Szunyogh et al, 2005). This localization allows assimilating all the observations simultaneously (rather than one at a time as in EnSRF) and makes the LETKF algorithm completely parallel.

### 3) Computational cost and advantages of the proposed LETKF approach

#### 3.1 Computational costs

Compared with the SEAT-A approach, the proposed LETKF CO2 assimilation has a much larger (but computationally very feasible) cost, and holds the potential of providing more detailed and accurate descriptions of the 4D field of CO2 concentrations and surface fluxes. Because of its parallelism, the LETKF has an excellent computational performance. For example, Szunyogh et al (2005) found that using a simple cluster of 25 PCs, it was possible to carry out a 40 member LETKF 6 hour assimilation with over 2 million observations and the NCEP GFS model in about 5 minutes. Adding a single additional tracer for CO2 only increases the number of analysis/forecast 3-dimensional variables at each grid point from 4 (u, v, T, q) to 5, and adds an additional 2D field of surface fluxes of CO2. Timing experiments with CAM3.0 on bassi.nersc.gov, a 1024 processor IBM Power 5 indicate that a single realization can be integrated on 16 processors (two nodes) at a rate of 2.5 simulated years per compute day using a medium resolution of T85/L27. The (embarrassingly parallel) scaling of the ensemble would indicate that the 40 members of the CAM3/CASA’ portion of the calculation could

be obtained at the same rate on 640 Power 5 processors, a relatively modest portion of modern supercomputing systems. The (also embarrassingly parallel) LETKF portion of the simulation should impact this computational rate only minimally as it will also be mapped to all 640 processors, although the observations I/O will have some impact. Concurrent execution of the entire system is readily achievable by use of the Multi-Program Handshake (MPH) protocol developed at LBNL. If larger computing systems are available, the processor count could be doubled or quadrupled with minor impact on parallel efficiency at this resolution. Higher resolution configurations of the CAM/CASA model (e.g T170 or finite volume dynamics at  $0.5^\circ \times 0.625^\circ$ ) permit even larger processor counts. (Oliker, et al, 2005). We will aim for an aggressive production rate of 1-6 months of Reanalysis per day depending on the resolution of the model.

### 3.2 Accuracy

Most previous inversion estimations of CO<sub>2</sub> have used monthly averaged boundary layer observations and a single realization of winds and circulation statistics obtained from an independent reanalysis, whose accuracy is not considered. In reality, the reanalysis winds have significant uncertainties, and the CO<sub>2</sub> transports are affected by these uncertainties, a factor generally ignored in previous approaches, including the SEAT-A method. The studies that deal with transport uncertainties consider multiple realizations of the circulation from a range of atmospheric GCM's whose simulations are not continuously updated with observations, thus overestimating transport uncertainties (Peylin et al. 2002; Gurney et al. 2003). In our system we plan to assimilate simultaneously the standard atmospheric observations (including winds and temperatures) and the CO<sub>2</sub> observations at their correct observational time, taking advantage also of new satellite OCO and GOSat continuous observations. In principle, the results should be more accurate and more informative about carbon processes because of the lack of restricting assumptions.

The estimation of surface fluxes of CO<sub>2</sub> and their uncertainties within the LETKF is akin to the estimation of a model forcing such as surface evaporation from the assimilated humidity field (or a bias). We have already experience already in such an approach (Baek et al, 2006, Li et al, 2006) and we are confident that such estimation will be relatively optimal, although it may require to increase the number of ensemble members or retune the size of the LETKF local cubes.

## 4. RESEARCH DESIGN AND METHODS:

In this proposal, where UMD and UCB will collaborate with modelers and computer scientists from LBL, we first plan to couple the CAM3-CASA' model with the Local Ensemble Transform Kalman Filter (LETKF) data assimilation, *both already developed*, and perform assimilations of simulated data. This requires developing the "observation operators" that transform sampled forecast model variables into synthetic "forecasted" observations (also required for the assimilation of actual observations) and will allow testing an end-to-end system. We estimate that the tasks involved in this first phase will take about 2-3 years, at the end of which we will have a completely developed system ready for assimilation of the actual *in situ*, aircraft and satellite observations. The simulation phase will allow us to test whether the project is feasible, i.e., whether the available measurements, combined with the CO<sub>2</sub> model can identify the geographical and temporal (diurnal and seasonal) characteristics of the carbon cycle, as well as the optimal estimation of a few crucial parameters, such as the Light Use Efficiency (LUE) that depends on the type of vegetation (e.g., Still et al. 2004). It will also test the ability of the system to distinguish the characteristics of the carbon cycle between dry and wet periods.

In the second phase of the project (assuming continued support from DOE) we will carry out several years of real data assimilation, using in situ and the newly available OCO and GoSat data. We will apply the same system developed and tested with simulated data but using real observations, including several years of satellite CO<sub>2</sub> measurements that will be available at that time.

## **A. Detailed Project Description**

The tasks we propose to carry out in the first 3 years of this project are (with lead institution first):

### ***1A) Couple the UMD LETKF data assimilation system with the CAM3 model, adapt observation operators, and test the system by assimilating meteorological observations provided by UMD (LBL and UMD)***

After the implementation, the test will be equivalent to running the NCEP-DOE Reanalysis (Kanamitsu et al, 2002) for a period of 1-2 years, using the same observations but replacing the NCEP model with the CAM3 model, and the 3D-Var data assimilation with the LETKF.

### ***1B) Implement MPH (Multiprogramming handshaking) for ensemble runs facilitating 4D LETKF (LBL and UMD).***

MPH will permit simultaneous execution of all realizations in the ensemble of CAM3 simulations permitting both rapid problem turnaround and the ability to exploit thousands of individual processors.

### ***2) Analyze the CAM3-CASA' model run in the AMIP configuration using an appropriate version of the CAM3. Select two distinct 3-year periods ("drought" like 1998-2003, and a "normal" or "wet" period) used to create simulated observations. (UCB, ORNL, LBL).***

In the atmospheric CO<sub>2</sub> record, the largest variations in the CO<sub>2</sub> growth rate are associated with wet and dry periods, and are higher during droughts (e.g. Angert et al. 2005; Ciais et al. 2005). The results of C4MIP, the coupled carbon-climate model intercomparison project (Friedlingstein et al. 2006) show that ecosystem responses to moisture variability is a dominant cause of divergence in the modeled CO<sub>2</sub> abundance and climate, after accounting for the differences in the physical climate models. The CAM3-CASA' code is participating in "Phase 1" of the C4MIP, with specified sea surface temperatures, fossil fuel emissions, land use changes, and air-sea CO<sub>2</sub> exchange for the period 1800 to 2000 (<http://www.c4mip.cnrs-gif.fr/protocol.html>). The experiment is being carried out by Forrest Hoffman at ORNL. The fvCAM3-CASA' code will be run using the same experimental protocol for two distinct periods ("drought" like 1998-2003, and a "wet" period 1993-1997), using the results of CAM3-CASA' for 1993 and 1998 as initial conditions. The modeled carbon output (especially surface and column CO<sub>2</sub> concentrations, and photosynthetic and respiratory fluxes) for the last years of these periods (like 1997 and like 2003) will be saved in conjunction with the standard meteorological output (temperature, humidity, all energy fluxes) at least every 3 hours so as to resolve the diurnal cycle. These periods are chosen as "extremes" to challenge the CAM3-CASA' model, especially to determine whether the model captures the sensitivity of carbon processes to temperature and moisture perturbations. As there are meteorological and (limited) carbon observations for these periods, these simulations also establish the baseline against which improvements from the carbon data assimilation system can be ascertained.

### ***3) Assemble all relevant observations, including both standard atmospheric observations (wind, temperature, humidity, pressure and satellite radiances) such as those available from the NCEP-DOE Reanalysis 2, and the CO<sub>2</sub> observations mentioned above. (UCB (CO<sub>2</sub>), LBL (Met data), UMD (Met data)).***

#### **Meteorological observations**

As indicated above, the bulk of the meteorological observations will be the observations used already in the NCEP-DOE Reanalysis. In addition, we plan to assimilate (for the short test periods) AIRS radiances, an instrument that has been designed primarily for temperature and moisture retrievals, but which has been shown to provide significant information about CO<sub>2</sub> and other gases, when the temperature and humidity are accurately estimated.

### **Carbon Observations**

Since the establishment of CO<sub>2</sub> monitoring at Mauna Loa Observatory in 1957, there are several classes of carbon observations ready for assimilation into a carbon data assimilation system.

The first class includes now-routine measurements of the concentration of CO<sub>2</sub> in air samples collected in the planetary boundary layer at over 100 stations around the world. The air samples are collected at three types of stations:

- (a) *in situ* monitoring stations (Mauna Loa, Hawaii; Point Barrow, Alaska; America Samoa; South Pole; Cape Grim, Tasmania) where air is sampled continuously and CO<sub>2</sub> is measured at the observatories. The data are available hourly.
- (b) flask sampling network (over 100 cooperative stations mainly at remote coastal locations around the world), where air samples are collected ~twice per week, and the flasks are sent to a central facility for analysis of the concentrations of CO<sub>2</sub> and other trace gases. The data are available bi-weekly.
- (c) continental tower sites where continuous variations in CO<sub>2</sub> vertical profiles are measured up to heights of ~400m in the planetary boundary layer (Bakwin et al. 1998; Davis et al. 2003).

The second class includes CO<sub>2</sub> vertical profiles and transects from episodic aircraft research campaigns (e.g. Gerbig et al. 2003; Machida et al. 2002; Sawa et al. 2004), as well as pseudo-regular CO<sub>2</sub> at altitude from scheduled flights (e.g. Matseuda et al. 2002). These observations represent Lagrangian snapshots that may capture a weather front or a biomass burning event rather than the climatology.

The third class of atmospheric CO<sub>2</sub> observations come from space-borne instruments. Depending on the instrument design, the measurements are either column integrals (e.g. OCO, GoSAT), or weighted towards the upper troposphere (e.g. AIRS). OCO and GoSAT will provide global but asynchronous coverage with satellite re-visit typically 3-16 days, depending on the satellite orbit.

In addition to atmospheric CO<sub>2</sub> observations, FLUXNET, a global network of ~200 micrometeorological tower sites (<http://daac.ornl.gov/FLUXNET/>), use eddy covariance methods to provide continuous measurements of the net fluxes of CO<sub>2</sub>, water and energy at a height of ~ 5-10m (Baldocchi et al. 2001; Law et al. 2002). The net fluxes by themselves do not discriminate among the processes that alter CO<sub>2</sub> fluxes. However the application of ecosystem models and relationships has led to the determination of the temporal variations in ecosystem respiration, gross ecosystem production (GEP), as well as ecosystem parameters such as Light Use Efficiency (LUE) at each site (e.g. Braswell et al. 2005). A first task of the proposed work is to assemble all the observations into a single framework.

***4) Create for each of the observed state variables (of task 3) the corresponding observation operator and the corresponding simulated observation (with observational errors) from the nature run (task 2) for the dry and wet periods. Create simulated observations corresponding to OCO, GOSAT and in situ observations. (UMD (CO<sub>2</sub>, Met), UCB (CO<sub>2</sub>), LBL (Met)). Implement the observation operators into LETKF (LBL, UMD, UCB).***

An essential component of any data assimilation system (including 3D-Var, 4D-Var and Ensemble Kalman Filter) is the observation operators  $H$  that, given a model forecast ( $\mathbf{x}^b$ ), create a "forecasted" (synthetic) observation  $\mathbf{y}^b = H(\mathbf{x}^b)$ . For rawinsonde observations, for example, this is simply a special



interpolation of the model temperature, humidity and wind to the location of the rawinsonde. For OCO or other satellite radiance observations, it involves the radiative transfer model that creates (from the vertical distribution of model variables and instrument specifications) the radiance that would be observed. For most meteorological observations the observation operators already exist (e.g., at NCEP, NESDIS, NASA and ECMWF), and have to be adapted to the structure of our model. However, for others, we will have to work with the team of instrument developers (e.g., OCO). To start, we shall include in  $\{\mathbf{x}^b\}$  the global 3-D distribution of atmospheric CO<sub>2</sub>. The observation operators  $H(\mathbf{x}^b)$  for each three classes of CO<sub>2</sub> mixing ratio as discussed above, including column CO<sub>2</sub> mixing ratios retrieved from OCO radiances, are straightforward, and like those for temperature and humidity, involve only interpolation to the space and time of the observations. Construction of the operators to transform the modeled radiances into CO<sub>2</sub> concentrations, as Engelen et al. (2004) did for AIRS, is beyond the scope of this three-year proposal.

The most challenging part of our project is how to include flux tower observations into the carbon data assimilation system. Including in the observations  $\{y_n\}$  carbon fluxes from the flux tower measurements may not be meaningful, because the landscape is known to be heterogeneous, the boundary layer flow not readily predictable, and the ground-based measurements may or may not be representative of the fluxes in a model gridbox. And so a large error covariance  $\mathbf{A}_n$  associated with the analyzed surface fluxes may not be informative about the model representation or about the real magnitude of the fluxes at model resolution. Instead, we plan to explore a strategy employed in ecosystem studies where the observations  $y_n$  represent ecosystem parameters (rather than fluxes) from the flux tower observations (e.g. Williams et al. 2005; Braswell et al. 2005). For example, light-use-efficiency (LUE), an ecosystem-specific parameter that varies with the ambient climate, can be derived from incident photosynthetically active radiation (PAR) and the derived GEP. Similarly  $Q_{10}$ , which expresses respiration variations in terms of temperature variations, can be calculated readily from the flux tower measurements.  $H(\mathbf{x}^b)$  can be derived using the same procedure, as the fvCAM3-CASA' output  $\{\mathbf{x}^b\}$  includes the relevant carbon fluxes and climate parameters. Because CASA' is more complex than a two-parameter representation, the "analyzed" LUE and  $Q_{10}$  are not readily applied to update the representation in CASA' every assimilation time step. Nevertheless inclusion of LUE and  $Q_{10}$  in the analysis (equations 2a and 2b) will contribute to the innovation of the CO<sub>2</sub> analyzed field itself. Furthermore, the "analyzed" LUE and  $Q_{10}$  yields critical information for assessing the realism CASA' processes and their consistency with the atmospheric CO<sub>2</sub> as well as flux tower observations.

This will pave the way for exploring the appropriate ecosystem parameters from CASA' that could be included directly in the analysis, so that the innovation could be introduced to the CO<sub>2</sub> fluxes themselves, as was done by Rayner et al. (2005) using the model BETHY. This is probably the most complex component of our project. One advantage of our project is that (unlike 3D-Var and 4D-Var), the LETKF does not require the development of a linear tangent (Jacobian) and adjoint of the observation operator. Also, the algorithm, once set up, can be readily applied to other ecosystem models coupled to CAM3, and would guide the improvements of future coupled carbon-climate models.

### ***5) Test the extension to time-continuous data (4DLETLF) (UMD, LBL, UCB).***

As indicated before, LETKF has been extended to 4 dimensions, allow the assimilation of observations at their right observation time (the main advantage of 4D-Var). This code is being developed at UMD, and should be well tested by the start of the project. Nevertheless, it may require considerable development to ensure it remains efficient in the DOE supercomputers (e.g., using MPH, multiprocessing handshake).

**6) Perform data assimilation of the conventional atmospheric observations and the CO<sub>2</sub> observations using the LETKF (and/or 4DLETKF) and model forecasts for both the wet and dry periods (LBL, UMD, UCB). This will require submitting a request to INCITE for substantial computational resources at LBNL NERSC and/or ORNL CCS. Data storage capabilities of NERSC are essential for this production task.**

After testing the end-to-end system developed in tasks 1-5, we will carry out data assimilation of the simulated observations for two different years (as indicated in Task 4). There are several purposes for this important exercise: a) Complete testing and debugging, for which a simulation (where truth is known) is very helpful. b) Verify the feasibility of the project, including the ability to estimate the CO<sub>2</sub> concentrations and fluxes. c) Estimate the spin-up time for the system, and, very importantly, d) optimize the production code and input/output flow.

**7) Use the assimilated data to assess the representation of carbon processes and parameter estimation within a simulation where we know the truth (task 2) and we have used synthetic data to observe it (tasks 4 and 6). (UCB, UMD, LBL).**

This task will indicate the extent to which we have succeeded in this project, and whether the system is ready for the assimilation of real observations for the estimation of the carbon cycle. A first product of the carbon data assimilation proposed here is global analyzed fields of atmospheric CO<sub>2</sub> that are consistent with both the available CO<sub>2</sub> observations from remote monitoring sites, aircraft and satellites as well as with ecosystem parameters derived from flux towers. The analyzed CO<sub>2</sub> will contain the detailed spatial and temporal variations lost when the CO<sub>2</sub> are reconstructed from broad regional fluxes obtained by inversion procedure. Surface CO<sub>2</sub> fluxes can be derived immediately as the residual required for CO<sub>2</sub> conservation at each gridbox. In this first step, an analysis of the discrepancy between the calculated surface CO<sub>2</sub> fluxes and that directly calculated by fvCAM3-CASA', and the temporal evolution of the discrepancy, will be an important metric of the fvCAM3-CASA'. A companion analysis is that of the ecosystem parameters across vegetation and climate space and the error covariance  $\mathbf{A}_n$  associated with these parameters.

At the end of the three-year proposal period we will have a tested end-to-end system ready to use with real observations and a fairly good idea of the strengths of the system, its problems, the accuracy that we can expect and the changes that should be made. If we get continued support from DOE we will start with the second phase (years 4-6), where we will perform several years of carbon data reanalysis using standard atmospheric data and in situ and satellite carbon data (including OCO and GOSat available by that time). This will provide not only the best estimate of the 4D distribution of CO<sub>2</sub>, but also an atmospheric reanalysis much more comprehensive than either the NCEP-DOE Reanalysis 2 or the ERA40, and for the first time, an estimate of uncertainties and of crucial carbon cycle parameters. The only system comparable to ours will be the European GEMS, using 4D-Var (Engelen et al, 2004). We plan to compare our results with them and exchange information on what has been successful in both systems.

## **B. Project schedules, milestones and deliverables**

The tasks and responsibilities are described in detail in Section 4A.

### Project schedule:

Tasks 1A, 1B and 2 will be completed in the first year.

Tasks 3, 4 and 5 will be completed in the second year

Tasks 6 and 7 will be completed in the third year.

Milestones, Deliverables and Performance Metrics (organizations listed in order of responsibility)

End of first year:

- Documented and tested fvCAM3 coupled with LETKF on DOE supercomputer (LBNL and UMD). Metric: One month run with simulated observations from an fvCAM3 run.
- Meteorological observations used in a 5 year period of the NCEP-DOE Reanalysis 2 and corresponding observation operator for the same observations on the fvCAM3 model (UMD, LBNL, UCB). Metric: One month comparison of synthetic observations obtained from the fvCAM3 model and real observations. Observation count for all classes of observations.
- 20 years of an AMIP “Nature run” with the coupled fvCAM3-CASA’ model on DOE supercomputers. Selection of two 2-year test periods (UCB, LBNL). Metric: Output showing carbon cycle summaries for two contrasting periods.

End of second year:

- Implementation of MPH to control simultaneous execution of the ensemble (LBNL). Metric: Documentation of the LETKF performance with and without MPH.
- 5 years of fvCAM3/LETKF Reanalysis using the same observations as NCEP-DOE Reanalysis 2 (LBNL and UMD). Metric: Report comparing fvCAM3/LETKF and NCEP-DOE reanalyses, with appropriate performance metrics such as rms fit of 6 hour forecasts to observations.
- Simulated meteorological observations and observation operators for the two test periods from the Nature test periods (UMD and UCB). Metric: One month comparison of synthetic observations obtained from the fvCAM3-CASA’ model and “nature” observations.
- Simulated carbon observations (including atmospheric CO<sub>2</sub> concentrations and surface fluxes, from current and future instruments such as OCO and GoSAT) and corresponding observation operators for the two test periods from the Nature test periods (UCB and UMD). Metric: Comparison of fields observations obtained from the fvCAM3-CASA’ model and “nature” observations for two contrasting periods.

End of third year:

- Documented and tested fvCAM3-CASA’ coupled with LETKF on DOE supercomputer (UMD, UCB and LBNL). Metric: Report on the computational performance of the system.
- Data assimilation of meteorological and carbon simulated observations with the fvCAM3-CASA’/LETKF system for the test periods (LBNL, UMD, UCB). Metric: Report submitted on the results of the data assimilation of simulated carbon and meteorological observations, strengths and weaknesses (UCB, UMD, LBNL)
- Collection of meteorological and carbon observations for the period 2005-2009 including OCO and GoSAT as available (UCB, UMD, LBNL). Metric: Observation count for all classes of observations. Comparison between real and synthetic observations.
- End-to-end system ready to assimilate real carbon and meteorological observations on DOE supercomputer (UMD, LBNL, UCB). Metric: One month test with real meteorological observations and a selection of available carbon observations. Test includes quality control of observations based on the ratio of observation minus ensemble mean of the forecasts and the forecast spread.

### **C. Work assignments:**

All the tasks will be carried out collaboratively, with each of the three institutions taking the lead responsibility of each task according to their area of expertise. The responsibilities are indicated within each task and deliverable.

## 5. BUDGET EXPLANATION

### **University of Maryland, College Park: PI E. Kalnay**

**Personnel.** Funds are requested to support the PI at 0.5 month/yr.

Support is requested for one post-doctoral fellow and one graduate student to couple and test the LETKF with fvCAM3-CASA', and work with Profs. Szunyogh and Kostelich (for whom we request support for 3.5 months/year and 2 months/year respectively) in the development, implementation, testing and production of all the elements of the system.

**Equipment.** We plan acquire a server with disk space analyze and preprocess the real observations.

**Domestic Travel.** The PI and Prof. Szunyogh will travel to Berkeley for team meetings once a year, and the postdoc and graduate student will spend extended periods at LBNL.

**Publication** We anticipate presenting papers at the AMS, and publishing one paper on each of the last two years in GRL/JGR.

**Materials and Supplies** Included in materials and supplies costs are software licenses and hardware maintenance contracts, and computer supplies (back-up tapes, printer cartridges).

### **University of California, Berkeley: I. Fung**

**Personnel.** Funds are requested to support the PI at 0.1 FTE/yr.

Support is requested for one post-doctoral fellow and one graduate student at UC Berkeley to create the synthetic observations from the CAM3-CASA' runs for the wet and dry periods and to compile the carbon observations. They will also work with the UMD team to develop the carbon observations operators, and integrate them into the carbon data assimilation. They will interpret the assimilated data in terms of the magnitudes, locations and uncertainties of the carbon sources and sinks. 5 months support per year is requested for the senior programmer/analyst Jasmin John to work closely with UMD and LBNL teams in the coupling the CAM3-CASA' code to the LTEKF code, executing the runs and managing the large volumes of output.

**Graduate Student Fees Remission and Out-of-State Fees.** Given the California state budget, tuition has risen dramatically, as have fees for non-resident students. The fees for 2005-2006 are \$3,728.45 per term for California residents. Non-resident tuition fees are \$7,347 per term, thus totaling charges of \$11,197.95 per term for non-residents.

**Equipment.** We plan to purchase 4 PC's for interfacing to the supercomputers at NERSC and ORNL. The equipment cannot be purchased with indirect funds because sec.J.16 of A-21 states that, "b. The following rules of allowability shall apply to equipment and other capital expenditures... (4) Capital expenditures are unallowable as F&A costs".

**Domestic Travel.** The PI, postdoc and graduate student will travel to University of Maryland for team meetings once a year, and the PI will participate in SciDAC meetings at ORNL or Washington DC once a year. We estimate a cost of \$1250 for each trip

(Air-fare rt \$500; Hotel and perdiem 4 days @150/day=\$600; local transport \$150), thus totaling \$1250 each trip and \$5000 for 4 trips.

**Publication** We anticipate sharing publication costs with other grants. The costs of "typical" papers in the AGU journals are: \$1730 for Geophys. Res. Letters (4 pages (@\$170 + 2 color plates); \$650 for Global Biogeochemical Cycles (no page charges 4 Color plates + Color integrated in on-line PDF); \$1370 for JGR (8 pages @\$90 + 4 Color plates + Color integrated in on-line PDF).

**Materials and Supplies** Included in materials and supplies costs are software licenses and hardware maintenance contracts, and computer supplies (back-up tapes, printer cartridges).

### **Lawrence Berkeley National Laboratory: M. Wehner**

Cost estimates have been presented in this proposal to be comparable to other research institution's proposals. At Lawrence Berkeley National Laboratory (LBNL), actual costs will be collected and

reported in accordance with the Department of Energy (DOE) guidelines. Total cost presented in this proposal and actual cost totals will be equivalent.

Michael F Wehner – Career (0.1 FTE/yr) Dr. Wehner will manage the LBNL portion of project and supervise the junior scientists in this project. He will also facilitate the coordination of the project to the SciDAC Scientific Application “A Scalable and Extensible Earth System Model for Climate Change Science”

Yu-Heng Tseng – Career (.65 FTE/yr) Dr. Tseng will be responsible for the overall incorporation of the CAM/CASA model into the LETKF system. He will also be responsible for the integration of the model on DOE supercomputing platforms as well as the analysis of results.

Helen (Yun) He – Career (.1 FTE/yr) Dr. He will be responsible for the implementation of the MPH package allowing the code to exploit large numbers of processors through concurrent execution of ensemble members.

## **LBNL DIRECT COSTS**

### **SENIOR PERSONNEL – ITEM A.1-6**

The salary figure listed for Senior Personnel is an estimate based on the current actual salary for an employee in her/his division plus 3% per year for FY06 through FY10 for inflation.

### **FRINGE BENEFITS – ITEM C**

Fringe Benefits for LBNL employees are estimated to be the following percent calculated on labor costs:

Career Employees – FY06 24%; FY07 24.9%; FY08 25%; FY09 25.9%, FY10 26.7%

### **TRAVEL – ITEMS E.1 AND E.2**

The senior staff members plan to attend domestic and/or foreign technical conferences/workshops in the areas of research covered by this proposal. Total cost includes plane fare, housing, meals and other allowable costs under government per diem rules.

### **OTHER DIRECT COSTS – ITEM G.6**

The estimated cost of telephone, space, computer usage, etc., calculated on person-months directly associated with the project.

## **LBNL INDIRECT COSTS – Item I**

### **ORGANIZATIONAL BURDEN**

Use of organizational burden pools in LBNL Computing Sciences (CS) Division is the approved method for collection and distribution of indirect costs associated with personnel. These pools are established to collect costs associated with personnel engaged in a single operation or several closely related operations. The objective is to establish uniformity and compatibility in recording, distributing, and reporting organizational burden. The types of costs which can be charged to these pools are labor and labor-related costs of secretaries, division administration and general materials/service costs such as environmental, safety, and health, finance and budget provided for the general benefit of a division. The estimated LBNL CS CRD Organizational Burden rate is 17.6% and is calculated on all CRD research salaries.

Other LBNL on-site indirect estimated costs are as follows:

Procurement Burden – 8.4% calculated on all procurements and electricity

Travel – 14% calculated on all travel

General & Administrative General Rate – 46.3% calculated on all costs

LDRD Rate – 2.9% calculated on operating and equipment costs

## 6. MANAGEMENT PLAN

This SAP proposal is a collaborative effort between the University of Maryland (PI: Eugenia Kalnay); University of California, Berkeley (co-PI: Inez Fung); and the Lawrence Berkeley National Laboratory (co-PI: Michael Wehner). The proposal takes advantage of the unique expertise at these institutions in data assimilation (U MD), carbon cycle science and carbon-climate modeling (UC Berkeley), and large-scale computing (LBNL).

The DOE is a significant partner to the NSF's NCAR CCSM project. Through the BER Climate Change Prediction Program and the SciDAC 1 project "Collaborative Design and Development of the Community Climate System Model for Terascale Computers", substantial DOE investments in CCSM have yielded a flexible state of the art coupled climate system model. The database of CCSM integrations is by far the largest and most complete in the IPCC AR4 archive of climate model simulations at PCMDI in LLNL. We expect to collaborate closely with the consortium of DOE laboratories involved with the SciDAC 2 scientific application "A Scalable and Extensible Earth System Model for Climate Change Science" While this proposal focuses on CAM3-CLM3-CASA' and could exist as a stand-alone project, the methodology and software developed here is readily adapted to newer versions of the carbon-climate model as well as to an expanded suite of observations. The enhancements to the carbon components of the model will complement the development of the biogeochemical aspects of the CCSM. We also expect to work closely with PCMDI throughout this project in the development of model evaluation tools. No formal consortium agreement is necessary.

This proposal is multi-institutional collaborative enterprise. The PI and the co-PIs have long experience in scientific and computational aspects of general circulation models and their applications. The goal of the project is to prototype a totally new carbon data assimilation system that takes advantage of the new developments in mathematics of data assimilation, advances in computers and computer science, and maturing observations of the carbon cycle. The strategy for guiding the management plan is to build a team that truly learns and works together, and produce a new generation of young researchers who are multi-disciplinary, and yet grounded in a particular "home" discipline. Kalnay has the overall responsibility for setting the research agenda, coordinating the research projects, maintaining the schedule for results dissemination, and for interfacing with the DOE SciDAC program office. She will act as the initial point of contact or representative for the project, and will deputize the co-PI's as required. Each investigator will lead at least one of the development/analysis efforts, outlined in Section 4C on Work Assignments. We anticipate that the whole team will jointly analyze the series of sensitivity experiments.

The investigators will communicate among themselves to solve day-to-day problems, make use of other expertise within the projects, and hold mini-group meetings on specialized topics as required. The PI and co-PI's will confer with DOE and with SciDAC 2 Consortium on a regular basis. This SAP team will meet every 6 months, with host responsibilities rotating among UMD and UC Berkeley/LBNL. These meetings will concentrate on the collaborative areas within tasks, and will be used to identify bottlenecks and scientific and computational opportunities. Codes and datasets will be shared among the team members as well as with other SciDAC and CCSM collaborative projects.

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### A.3.3. CURRICULUM VITA

#### Curriculum vitae: Eugenia Kalnay

Born October 1, 1942 in Buenos Aires, Argentina

U.S. Citizenship (1978)

#### Address:

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#### Education:

Ph.D., 1971, Department of Meteorology, Massachusetts Institute of Technology

(Advisor: Prof. Jule G. Charney).

Licenciatura en Ciencias Meteorológicas, 1965 University of Buenos Aires, Argentina.

Primary School Teacher, 1959, Lenguas Vivas High School, Buenos Aires, Argentina.

#### Work Experience:

- Jul02- Distinguished University Professor, Dept. of Meteorology, U. of Maryland
- Jul99-Jun02 Professor and Chair, Department of Meteorology, University of Maryland
- Jan97-Jun99 National Centers for Environmental Prediction, Senior Scientist, and Robert E. Lowry Chair Professor at the School of Meteorology, Oklahoma University
- Aug97-Dec97 National Centers for Environmental Prediction, Senior Scientist.
- 1987-Jul 97 Director, Environmental Modeling Center, (formerly Development Division), National Centers for Environmental Prediction, ES-4 and NCEP Deputy for Science
- 1984-1986 Head, Global Modeling and Simulation Branch, Goddard Laboratory for Atmospheres, NASA/GSFC, GS-15
- 1979-1984 Senior Research Meteorologist, Goddard Laboratory for Atmospheric Sciences, Modeling and Simulation Facility, NASA/GSFC, GS-15
- 1977-1978 Associate Professor, Department of Meteorology, Massachusetts Institute of Technology
- 1975-1977 Assistant Professor, Department of Meteorology, Massachusetts Institute of Technology
- 1973-1974 Research Associate, Department of Meteorology, Massachusetts Institute of Technology
- 1971-1973 Assistant Professor, Laboratorio Dinámica de la Atmósfera, Universidad de la República, Montevideo, Uruguay,
- 1967-1971 Research Assistant, Department of Meteorology, Massachusetts Institute of Technology
- 1965-1966 Research Assistant, Department of Meteorology, University of Buenos Aires
- 1961-1963 Teaching Assistant, Departments of Meteorology, Physics and Mathematics, University de Buenos Aires, Argentina

#### Awards:

Fellow of the American Geophysical Union (2005)  
Kalnay and Cai (2004) selected as one of the top 100 science news by Discovery Magazine  
Member of the Argentine Academy of Exact and Natural Sciences (2003)  
Distinguished University Professor at the University of Maryland (2001)  
Foreign member of the Academia Europaea (2000)  
Robert E. Lowry endowed chair at the University of Oklahoma, 1998-99.  
Dept of Commerce Gold Medal for Reanalysis project (1997).  
Senior Executive Service Presidential Rank Award (1996)  
Member of the National Academy of Engineering (1996)  
American Meteorological Society Jule G. Charney award (1995)  
Dept of Commerce Gold Medal awarded to the Development Division headed by Kalnay (1993)  
Department of Commerce Silver Medal (1990)  
Fellow of American Meteorological Society (1982)  
NASA Medal for Exceptional Scientific Achievement (1981)  
Highest GPA among 1965 graduates of the School of Sciences, U. of Buenos Aires, Argentina  
1st place in 1960 scholarships competition from the National Meteorological Service, Argentina

### **Research Area Experience:**

From 1979 to 1986 Eugenia Kalnay worked in and later directed, the Global Modeling and Simulation Branch, at NASA/GSFC. She developed the accurate and efficient “NASA Fourth Order Global Model” which for more than 15 years was the core of many data assimilation and forecasting experiments as well as climate studies. From 1987 to 1997, Dr. Kalnay was the Director of the Environmental Modeling Center (EMC/NCEP/NWS). Major improvements in the operational models' forecast skill and many successful projects such as ensemble forecasting, 3-D and 4-D variational data assimilation, advanced quality control, coastal ocean forecasting, GCIP research with the Eta model, seasonal and interannual dynamical predictions, were carried out during those years. She directed the NCEP/NCAR 50-year Reanalysis project, creating the most widely used data set in the geophysical sciences, and with Zoltan Toth developed the breeding method for ensemble forecasting implemented in 1992 at NCEP.

Current research interests of Dr. Kalnay are in predictability and ensemble forecasting, numerical weather prediction and data assimilation. With the Chaos Group (Profs. Ott, Hunt, Yorke, and Drs. Szunyogh and Patil) she discovered the intermittent low dimensionality of the atmospheric attractor, whose application resulted in an efficient Local Ensemble Kalman Filtering. With Dr. Ming Cai and S-C. Yang she is studying the leading Lyapunov vectors of the coupled ocean-atmosphere system for several. She introduced the method of backward integration of atmospheric models used in several novel applications such as Inverse 3D-VAR, and targeted observations. She is the author (with Zoltan Toth, Ross Hoffman and Wesley Ebisuzaki) of widely used ensemble methods known as Breeding, Lagged Averaged Forecasting (LAF) and Scaled LAF. She has also papers on atmospheric dynamics and convection, numerical methods, and the atmosphere of Venus, and recently developed with M. Cai a method to estimate that land-surface use changes are responsible for about half of the observed decrease in the trends in the surface diurnal temperature range over the US

published in Nature. Her book “Atmospheric Modeling, Data Assimilation, and Predictability” was published in 2003 by Cambridge University Press and is on its third printing. She has over 100 peer-reviewed papers.

**Graduate Students and Postocs:**

M.S: Bill Grant, Carlos Cardelino and Larry Marx at MIT.

Ph.D: Steven Brenner (MIT), Carolyn Reynolds (PSU), Zhao-Xia Pu (Langzhou U.), Carolina Vera (U. Buenos Aires), Malaquias Peña (U MD), Sim Aberson (U MD), Matteo Corazza (U. Genoa), DJ Patil (U MD), Shu-Chih Yang (U MD), Pablo Grunman (U MD), Takemasa Miyoshi (U MD), Chris Danforth (U MD).

Postdoctoral advisees: Zoltan Toth, Alvin Bayliss, David Hoitsma, Ross Hoffman, Amnon Dalcher, Richard Wobus, Song-you Hong, Zhao-xia Pu, Istvan Szunyogh, Shu-Chih Yang, Dirceu Herdies, Jose Aravequia.

Current students:, Hong Li, Junjie Liu, Debra Baker, Ji-Sun Kang, all in doctoral programs in a MS/PhD program.

**Recent Refereed Publications:**

Kalnay, Eugenia, Park, Seon Ki, Pu, Zhao-Xia, Gao, Jidong. 2000: Application of the Quasi-Inverse Method to Data Assimilation. *Monthly Weather Review*: Vol. 128, No. 3, pp. 864–875.

Pu, Zhao-Xia and Eugenia Kalnay, 2000: Targeting observations with the quasi-inverse linear and adjoint NCEP global models: performance during FASTEX. *JQRMS*, 125, 3329-3337.

Falkovich, Alexander, E. Kalnay, S. Lord and Mukut Mathur, 2000: A new method of observed rainfall assimilation in forecast models. *J. Applied Met.* 39, 1282-1298.

Shukla, J., J. Andersson, D. Baumhefner, C. Brankovic, Y. Chang, E. Kalnay, L. Marx, T. Palmer, D. Paolino, J. Ploshay, S. Schubert, M. Suarez and J. Tribbia, 2000: Dynamical Seasonal Prediction. *Bull. Amer. Meteor. Soc.*, 81, 2593-2606.

Hong, Song-you and E. Kalnay, 2000: Origin and maintenance of the Oklahoma-Texas drought of 1998. *Nature*, 842-845.

Patil, DJ, Brian Hunt, Eugenia Kalnay, James A Yorke and Edward Ott, 2001: Using Bred Vectors to Establish Local Low Dimensionality of Atmospheric Dynamics. *Phys. Review Letters*, 86, 5878-5881.

Hou, D., E. Kalnay, and K.K. Droegemeier, 2001: Objective verification of the SAMEX '98 ensemble forecasts. *Mon. Wea. Rev.* , 129, 73-91.

Kistler, R., E. Kalnay, and co-authors, 2001: The NCEP/NCAR 50-year Reanalysis: Monthly means CDROM and documentation. *Bull. Am. Met. Soc.*, 82, 247-267.

Hong, Song-you and Eugenia Kalnay, 2002: The 1998 Oklahoma-Texas Drought: Mechanistic Experiments with NCEP Global and Regional Models. *J. of Climate*, 15, 945-963.

Kalnay, E. and M. Cai, 2003: Impact of urbanization and land-use change on climate. *Nature*, 423, 528-531.

Cai, Ming, E. Kalnay and Z. Toth, 2003: Bred Vectors of the Zebiak-Cane Model and Their Application to ENSO Predictions. *J. of Climate*, 16, 40-56.

Corazza, M., E. Kalnay, D. J. Patil, R. Morss, I. Szunyogh, B. R. Hunt, E. Ott, and M. Cai, 2003: Use of the breeding technique to estimate the structure of the analysis “errors of the day”. *Nonlinear Processes in Geophysics*, 10, 233-243.

Chase, T.N., J.A. Knaff, R.A. Pielke Sr. and E. Kalnay, 2003: Changes in global monsoon circulations since 1950. *Natural Hazards*, 29, 229-254.

Pielke, Roger A., E. Kalnay, and co-authors, 2003: The USWRP Workshop on the Weather Research Needs of the Private Sector. *Bulletin of the American Meteorological Society*: Vol. 84, No. 7, pp. 934–934.

Ott, Edward, B. R. Hunt, I. Szunyogh, A. Zimin, E. Kostelich, M. Corazza, E. Kalnay, D.J. Patil, and J. A. Yorke, 2002: A Local Ensemble Kalman Filter for Atmospheric Data Assimilation. Posted <http://arXiv.org/abs/physics/0203058>.

Peña, M., E. Kalnay and M. Cai, 2003: Statistics of coupled ocean and atmosphere intraseasonal anomalies in Reanalysis and AMIP data. *Nonlinear Processes in Geophysics, European Geophysical Society*, 10, 245-251.

Seon-ki Park and E. Kalnay, 2004: Inverse three-dimensional variational data assimilation for an advection-diffusion problem: Impact of diffusion and hybrid application. *Geophysical Research Letters*, Vol. 31, L04102, 5pp.

Vukicevic, T., Kalnay, E., Vonder Haar, T. 2004: The Need for a National Data Assimilation Education Program. *Bulletin of the American Meteorological Society*: Vol. 85, No. 1, pp. 48–49.

Evans, Erin, Nadia Bhatti, Jacki Kinney, Lisa Pann, Malaquias Peña, Shu-Chih Yang, Eugenia Kalnay, and James Hansen, 2004: RISE undergraduates find Lorenz’s model regime changes predictable. *Bulletin of the American Meteorological Society*: Vol. 85, No. 4, pp. 520–524.

E. Ott, B.R. Hunt, I. Szunyogh, A.V. Zimin, E.J. Kostelich, M. Corazza, E. Kalnay, D.J. Patil, and J.A. Yorke, 2004: A Local Ensemble Kalman Filter for Atmospheric Data Assimilation. *Tellus* 56A, pp 415-428.

B.R. Hunt, E. Kalnay, E.J. Kostelich, E. Ott, D.J. Patil, T. Sauer, I. Szunyogh, J.A. Yorke, and A.V. Zimin, 2004: Four-Dimensional Ensemble Kalman Filtering. *Tellus* 56A, 273-277.

Peña, Malaquías, Cai, Ming, Kalnay, Eugenia. 2004: Life Span of Subseasonal Coupled Anomalies. *Journal of Climate*: Vol. 17, No. 7, pp. 1597–1604.

Peña, M. and E. Kalnay, 2004: Separating fast and slow modes in coupled chaotic systems. *Nonlinear Processes in Geophysics*, vol 19, 319-327.

Szunyogh, E.J. Kostelich, G. Gyarmati, D.J. Patil, B.R. Hunt, E. Kalnay, E. Ott and J.A. Yorke, 2005: Assessing a Local Ensemble Kalman Filter: Perfect Model Experiments with the NCEP Global Model. *Tellus*, **57A**. 528-545.

Yang, S-C, M. Cai, E Kalnay, M. Rienecker, G. Yuan and Z. Toth, 2005: ENSO bred vectors in coupled ocean-atmosphere General Circulation Models, *J. of Climate*, in press.

Cai, M. and E. Kalnay, 2005: Can Reanalysis have anthropogenic trends without model forcing? *J. of Climate*, in press.

Yang, Shu-Chih, Debra Baker, Hong Li, Katy Cordes, Morgan Huff, Geetika Nagpal, Ena Okereke, Josue Villafañe, Eugenia Kalnay and Greg Duane, 2006: Data assimilation as synchronization of truth and model: experiments with the three variable Lorenz model. *J. Atmos. Sci.*, in press.

Marzban, C., S. Sandgathe, E. Kalnay, 2005: MOS, Perfect Prog, and Reanalysis Data. *Monthly Weather Review*, Vol.134, pp 657-663.

Kalnay, E., Hunt, B., Ott, E., and Szunyogh, I. **2005**. Ensemble forecasting and data assimilation: two problems with the same solution? In Palmer, T.N. and Hagedorn, R., editors, *Predictability of Weather and Climate*. Cambridge University Press. (in press).

Harlim, J., M. Oczkowski, JA Yorke, E Kalnay and B R Hunt, 2005: Convex error growth patterns in a global weather model. PRL, in press.

Kalnay, E., Ming Cai, Hong Li and Jayakar Tobin, 2006: Estimation of the Impact of Land-Surface Forcings on Temperature Trends in Eastern United States. *JGR* (in press).

Lim, Young-Kwon, Ming Cai, Eugenia Kalnay and Liming Zhou, 2005: Observational evidence of sensitivity of surface climate changes to land surface changes and urbanization. *GRL*, in press.

Kalnay, E., Hong Li, Takemasa Miyoshi, Shu-Chih Yang and Joaquim Ballabrera, 2006: 4D-Var or EnKF? Submitted to *Physica D*.

**Books:**

Chapters in about 10 books.

Kalnay, Eugenia, 2003: *Atmospheric Modeling, Data Assimilation and Predictability*. Cambridge University Press, 341pp., on its third printing within two years. Translated to Chinese, to be published in 2005.

INEZ Y. FUNG  
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University of California, Berkeley  
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**Education:**

1971: S.B. (Applied Mathematics), Massachusetts Institute of Technology

1977: Sc.D. (Meteorology), Massachusetts Institute of Technology

**Professional Employment:**

1998-: University of California, Berkeley

Professor, Department of Earth and Planetary Science,

Department of Environmental Science, Policy and Management

Richard and Rhoda Goldman Distinguished Professor for the Physical Sciences, 1997-2002

1998-2005: Director, Berkeley Atmospheric Sciences Center

2005-: Director, Berkeley Institute of the Environment

**Synergistic Activities Relevant to this Proposal**

2000-2004: Member, Scientific Steering Committee, US Interagency Carbon Cycle Program; 1998-

2004 co-Chair (with S.C. Doney), Biogeochemistry Working Group (BGC WG), NCAR Community Climate System Model; 2005- co-Lead (with J. Randerson), Diagnostic Team for CCSM BGC WG;

2006: Organizer, Summer Graduate Workshop on Carbon Data Assimilation (at Mathematical Sciences Research Institute, Berkeley, CA).

**Selected Publications:**

Fung, I., S.C. Doney, K. Lindsay, and J. John (2005). Evolution of carbon sinks in a changing climate. *Proc. Nat. Acad. Sci. (USA)*, 102, 11201-11206.

Doney, S.C., K. Lindsay, I. Fung and J. John (2005). Natural Variability in a Stable, 1000 Year Global Coupled Climate-Carbon Cycle Simulation. *J Climate*, in press.

Friedlingstein, P., P. Cox, R. Betts, L. Bopp, W. von Bloh, V. Brovkin, S. Doney, M. Eby, I. Fung, B. Govindasamy, J. John, C. Jones, F. Joos, T. Kato, M. Kawamiya, W. Knorr, K. Lindsay, H. D. Matthews, T. Raddatz, P. Rayner, C. Reick, E. Roeckner, K.-G. Schnitzler, R. Schnur, K. Strassmann, S. Thompson, A. J. Weaver, C. Yoshikawa, and N. Zeng Climate-carbon cycle feedback analysis, results from the C<sup>4</sup>MIP model intercomparison. *J. Climate* (in press).

Lee, J.-E., R. Oliviera, T. Dawson and I. Fung (2005). Root functioning modifies seasonal climate. *Proc. Nat. Acad. Sci. (USA)*, 102, 17576-17581.

Angert, A., Sebastien Biraud, Celine Bonfils, Cara Henning, Wolfgang Buermann, Jorge Pinzon, Compton Tucker, Inez Fung (2005). Drier summers cancel out the CO<sub>2</sub> uptake enhancement induced by warmer springs. *Proc. Nat. Acad. Sci. (USA)*, 102, 10823-10827.

## Michael Wehner

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50F Berkeley, CA 94720-8139

Telephone: (510) 495-2527 Fax: (510) 486-5812 E-mail: mfwehner@lbl.gov

### Education

Ph.D., 1983, University of Wisconsin-Madison (Nuclear Engineering)

M.S., 1980, University of Wisconsin-Madison (Nuclear Engineering)

B.S., 1978, University of Delaware, Graduated with High Honors (Physics)

### Professional Experience

2002-present: Staff Scientist, Scientific Computing Group, Computational Research Division, Lawrence Berkeley National Laboratory, Berkeley, CA

1998-2002: Physicist, Program for Climate Modeling and Intercomparison, Lawrence Livermore National Laboratory, Livermore, CA

1991-1998: Physicist, Climate System Modeling group, A-division, Lawrence Livermore National Laboratory, Livermore, CA

1985-1991: Physicist, Code Development group, B-division, Lawrence Livermore National Laboratory, Livermore, CA

1983-1984: Post doctoral Research Associate, Nuclear Engineering Department, University of Wisconsin-Madison

### Recent Relevant Publications

1. B. D. Santer, T. M. L. Wigley, G. A. Meehl, M. F. Wehner, C. Mears, M. Schabel, F. J. Wentz, C. Ammann, J. Arblaster, T. Bettge, W. M. Washington, K.E. Taylor, J. S. Boyle, W. Brüggemann, and C. Doutriaux, Influence of Satellite Data Uncertainties on the Detection of Externally Forced Climate Change, *Science* 300 (2003) 1280-1284
2. B. D. Santer, M. F. Wehner, T. M. L. Wigley, R. Sausen, G. A. Meehl, C. Ammann, J. Arblaster, W. M. Washington, J.S. Boyle, W. Brüeggemann, Contributions of Anthropogenic and Natural Forcing to Recent Tropopause Height Changes, *Science* 301 (2003) 479-483.
3. Curt Covey, Krishna M. AcutaRao, Peter J. Gleckler, Thomas J. Phillips, Karl E. Taylor and Michael F. Wehner, Coupled ocean-atmosphere climate simulations compared with simulations using prescribed sea surface temperature: Effect of a “perfect ocean”. *Global and Planetary Change* 41 (2004) 1-14
4. N.P. Gillett, A.J. Weaver, F.W. Zwiers, and M.F. Wehner, Detection of volcanic influence on global precipitation, *Geophysical Review Letters* 31 (2004) L12217
5. N.P. Gillet, M.F. Wehner, S.F.B. Tett, Testing the linearity of the response to combined greenhouse gas and sulfate aerosol forcing, *Geophysical Review Letters* 31 (2004) L14201
6. B. D. Santer, T. M. L. Wigley, A. J. Simmons, P. Kahlberg, G. A. Kelly, S. Uppala, C. Ammann, J. S. Boyle, W. Brüggemann, C. Doutriaux, M. Fiorino, C. Mears, G. A. Meehl, R. Sausen, K.E. Taylor, W. M. Washington, M. F. Wehner and F. J. Wentz, Identification of anthropogenic climate change using a second generation analysis. *J. Geophysical Research* 109 (2004) D21104
7. M.F. Wehner, Predicted 21<sup>st</sup> century changes in seasonal extreme precipitation events in the Parallel Climate Model, *J. Climate* 17 (2004) 4281-4290
8. B.D. Santer, T.M.L. Wigley, C. Mears, F.J. Wentz, S.A. Klein, D.J. Seidel, K.E. Taylor, P.W. Thorne, M.F. Wehner, P.J. Gleckler, J.S. Boyle, W. Collins, K.W. Dixon, C. Doutriaux, M. Free, Q. Fu, J.E. Hansen, G.S. Jones, R. Ruedy, T.R. Karl, J.R. Lanzante, G.A. Meehl, V. Ramaswamy, G. Russell, and G.A. Schmidt, Amplification of Surface Temperature Trends and Variability in the Tropical Atmosphere. *Science*. 309 (2005) 1551-1556
9. Michael Wehner, “Changes in daily precipitation and surface air temperature extremes in the IPCC AR4 models.” US CLIVAR Variations, 3, (2005) pp 5-9



## **Istvan Szunyogh**

Associate Research Scientist

Institute for Physical Science and Technology,

Department of Atmospheric and Oceanic Science (formerly Department of Meteorology),

University of Maryland, College Park

College Park, MD 20742-2431

Born August 24, 1967 Budapest, HUNGARY

Hungarian Citizen

Permanent Resident of the United States

### **Education**

- Ph.D., Earth Science (Meteorology), 1994, Hungarian Committee for Scientific Qualification, Budapest, Hungary
- Diploma, Meteorology, 1991, Eotvos Lorand University, Budapest, Hungary

### **Former Employment**

- Assistant Research Scientist (2001-2005). Institute for Physical Science and Technology, and Department of Atmospheric and Oceanic Science (formerly Department of Meteorology); University of Maryland
- Visiting Scientist (1997-2001). University Corporation for Atmospheric Research, based at the Environmental Modeling Center/ National Centers for Environmental Prediction
- Postdoctoral Associate (1997). Department of Earth, Atmospheric, and Planetary Sciences, Massachusetts Institute of Technology, Cambridge, Massachusetts; based at the Environmental Modeling Center/National Centers for Environmental Prediction
- Postdoctoral Visiting Scientist (1996- 1997). Mesoscale and Micrometeorology Division, National Center for Atmospheric Research, Boulder, Colorado; based at the Environmental Modeling Center/National Centers for Environmental Prediction
- Visiting Scientist at the Program "Mathematics of the Atmosphere and Ocean Dynamics (July 1996- September 1996) Isaac Newton Institute for Mathematical Sciences, Cambridge, United Kingdom
- Magyary Zoltan Postdoctoral Fellow (September 1995- September 1996). Department of Meteorology, Eotvos Lorand University, Budapest, Hungary
- Research Scientist (September 1998- August 1999, on leave). Department of Meteorology, Eotvos Lorand University, Budapest, Hungary
- Research Associate (September 1991- August 1998, on leave after September 1995). Department of Meteorology, Eotvos Lorand University, Budapest, Hungary

### **Papers most relevant for proposed research**

- [Szunyogh, I.](#), E. J. Kostelich, G. Gyarmati, D. J. Patil, B. R. Hunt, E. Kalnay, E. Ott, and J. A. Yorke, 2005: Assessing a local ensemble Kalman filter: Perfect model experiments with the NCEP global model. *Tellus*, **57A**, 528-545.
- Oczkowski, M., [I. Szunyogh](#), and D. J. Patil, 2005: Mechanisms for the development of locally low dimensional atmospheric dynamics. *J. Atmos. Sci.*, **65**, 1135-1156.
- [Szunyogh, I.](#), Z. Toth, A. V. Zimin, S. Majumdar, and A. Persson, 2002: Propagation of the effect of targeted observations: The 2000 Winter Storm Reconnaissance program. *Month. Wea. Rev.*, **130**, 1144-1165.
- [Szunyogh, I.](#), Z. Toth, R. E. Morss, S. J. Majumdar, B. J. Etherton, and C. H. Bishop, 2000: The effect of targeted dropsonde observations during the 1999 Winter Storm Reconnaissance Program. *Month. Wea. Rev.*, **128**, 3520-3537.
- Langland, R., Z. Toth, R. Gelaro, [I. Szunyogh](#), M. Shapiro, S. Majumdar, R. Morss, G. Rohaly, C. Velden, N. Bond, C. Bishop, 1999: The North Pacific Experiment (NORPEX-98). *Bull. Am. Met. Soc.*, **80**, 1363-1384
- [Szunyogh, I.](#), Z. Toth, K. A. Emanuel, C. Bishop, C. Snyder, J. Woolen, T. Marchok and R. Morss, 1999: Ensemble-based targeting experiments during FASTEX: The impact of dropsonde data from the LEAR jet. *Quart. J. Roy. Met. Soc.* **125**, 3189-3218.

#### A4. CURRENT AND PENDING SUPPORT:

Eugenia Kalnay

Current and Pending Support as of 2/23/06

#### CURRENT

<u>Agency</u>	<u>Project Title</u>	<u>Starting Date</u>	<u>End Date</u>	<u>Total Amount</u>	<u>FTE</u>
NSF	CMG Collaborative Research CMCI: Data Assimilation by Synchronization Of Truth and Model #5-24322	9/15/2003	8/31/2006	173466	.5 mos/yr
NASA	Improving NSIPP Data Assimilation Using Ensembles of Bred Vectors #5-26909	10/1/2002	9/30/2006	450000	.5 mos/yr
NOAA	Estimation/correction of model errors #5-27890	6/1/2004	5/31/2006	113013	0 % FTE
NASA	Data Ass. Using Infrared Sounder #5-26071	5/15/2004	5/14/2007	150000	0 % FTE
NASA	Multiyear Global assimilation dataset #5-26073	7/1/2004	6/30/2007	63477	0 % FTE
NOAA	Impact of land surface changes on climate #5-27898	5/1/2004	4/30/2006	149224	0 % FTE
DOD	Improving High Resolution Weather Forecast #5-28561	10/1/2002	12/31/2005	320000	.5mos/yr
NASA	Coupled Ocean Atmosphere Breeding #5-26216	12/15/2005	12/14/2008	437984	.25 mos/yr
<b>PENDING</b>					
NSF	Cost/benefit Simulations of Networks of Water Vapor	Submitted 2/7/2005	3 yrs	74205	0 % FTE
Univ of Hawaii	Predictability of Climate Regimes	Submitted 3/1/2005	5 yrs	177137	.5 mos/yr
NASA	Application of the 4D LEKF to Reanalysis	Submitted 11/12/2004	3 yrs	751423	0 % FTE
NOAA	Use of Satellite Observations Indata	Submitted 9/28/2004	3 yrs	338392	0% FTE

	Assimilation without Jacobian or Adjoint of the Observation				
NASA	Coupled Ocean-Atmosphere Breeding	Submitted 11/2/2004	3 yrs	437984	.25 mos/yr
ARL	Assessing & Forecasting the Atmosphere in Geographically Localized Region	Submitted 5/1/2005	3 yrs	480000	.6 mos/yr
NOAA	Testing the Local Ensemble Transform Kalman Filter (LETKF) for Use in Long-term Reanalysis	Submitted 7/13/2005	3 yrs	412500	0% FTE
NASA	Ensemble Kalman Filter Data Assimilation for Martian-Weather Analysis and Forecasting	Submitted 8/4/2005	3 yrs	541478	.5 mos/yr
NOAA	Wild Fire Impact on Air Quality	Submitted 9/29/2005	3 yrs	158240	0% FTE

## **Carbon Data Assimilation and Parameter Estimation Using Local Ensemble Transform Kalman Filter (LETKF)**

**Program Area:** Scientific Application Partnership: Computer Science

**Principal Investigator:** Eugenia Kalnay (University of Maryland)

**Senior Personnel:** Inez Fung (UC – Berkeley), Michael Wehner (LBNL)

**Scientific Application Partner:** A Scalable and Extensible Earth System Model for Climate Change Science (PI - John B. Drake, Oak Ridge National Laboratory)

**Participating Institutions:** U. Maryland, U.C.-Berkeley, Lawrence Berkeley National Laboratory (LBNL)

**Projected Funding Request:** FY07 - \$711K, FY08 - \$719K, FY09 - \$726K, Total \$2156K for three years.

*PI: Inez Fung*

Location of Projects: University of California, Berkeley

Current:

Title: Characterizing the Variability of the Global Atmospheric Dust Cycle in Relation to the Geomorphology and Surface Characteristics of Dust Source Areas.

Sponsor: NASA

Period: September 15, 2004 – September 14, 2007

Amount: \$72,000 (Graduate Fellowship: Charlie Koven)

Time: none

Title: Studies of Biosphere Atmosphere Interaction with a GCM with MODIS Spectral Resolution.

Sponsor: NASA

Period: May 1, 2004 – April 30, 2007

Amount: \$1,310,000 (UCB portion: \$420,000)

Time: 1 mo/year

Title: Toward Detection and Attribution of North American Carbon Sources and Sinks.

Sponsor: NASA

Period: November 15, 2004 – November 14, 2007

Amount: \$885,796

Time: 1 mo/year

Title: Carbon Dynamics in Changing Hydrologic Regimes: Inference from Contemporary Observations and Coupled

Sponsor: USDCOM- NOAA

Period: June 1, 2005 – May 31, 2008

Amount: \$600,000

Time: 1 mo/year

Proposals related to the PI's role as co-Director of the Berkeley Institute of the Environment:

*The following grants do not include any support for the PI's research program.*

Title: Enhancing the Worldwide Capacity to Meet the Challenges of Sustainable Urban Development.

Sponsor: Gordon and Betty Moore Foundation

Period: June 6, 2005 – March 15, 2006

Amount: \$342,542

Time: none

Title: Berkeley HydroWatch Center

Sponsor: W.M. Keck Foundation

Period: January 1 2006 – December 31 2009

Amount: \$1,600,000

Time: none

*PI: Michael Wehner*

Location of Projects: Lawrence Berkeley National Laboratory

**Current**

Title: NERSC Support for the Community Climate System Model

Sponsor: DOE OBER

Period: Core funding 07/01-07/7

Amount: \$231,000

Time: 75% of annual salary

Title Interannual and Decadal-Scale Behavior of Atmospheric Temperature and Oceanic Column-Integrated Water Vapor and Surface Winds

Sponsor: NASA

Period: 07/05-07/08

Amount: \$15,000

Time: 15% of annual salary

**Pending:**

Title: A Scalable and Extensible Earth System Model for Climate Change Science (PI: J. Drake, ORNL)

Sponsor: DOE SciDAC

Period: 07/06-07/11

Amount: \$4,000,000

Time: 10% of annual salary

**NEW GRANT** *Carbon data assimilation and parameter estimations using Local Ensemble Transform Kalman Filter (LETKF)***PERIOD:** *July 1, 2006 - June 30, 2009*

	PERIOD 1	PERIOD 2	PERIOD 3	TOTAL
<b>I. PERSONNEL</b>				
P.I. - Kalnay (.5 month)	6,540	6,867	7,210	20,617
Co-PI-Szunyogh (3.5 mos)	24,215	25,425	26,697	76,337
Post doc (12/12/11 mos)	45,000	47,250	45,478	137,728
GRA 1 - (12 months)	20,800	21,840	22,932	65,572
<b>TOTAL SALARY AND WAGES</b>	<b>96,555</b>	<b>101,382</b>	<b>102,317</b>	<b>300,254</b>
<b>II. FRINGE BENEFITS</b>				
TUITION REMISSION (O/H EXEMPT)	9,432	9,904	10,399	29,734
OTHER	34,729	36,467	37,671	108,867
<b>TOTAL FRINGE BENEFITS</b>	<b>44,161</b>	<b>46,371</b>	<b>48,070</b>	<b>138,601</b>
<b>III. TRAVEL</b>				
FOREIGN	0	0	0	0
DOMESTIC	2,447	3,703	2,726	8,875
<b>TOTAL TRAVEL</b>	<b>2,447</b>	<b>3,703</b>	<b>2,726</b>	<b>8,875</b>
<b>IV. EQUIPMENT</b>				
EQUIPMENT UNDER \$5,000 EACH	0	0	0	0
EQUIP. OVER \$5,000 EACH- OH EXEMP.	0	5,100	0	5,100
<b>TOTAL EQUIPMENT</b>	<b>0</b>	<b>5,100</b>	<b>0</b>	<b>5,100</b>
<b>V. SUBCONTRACTS</b>				
FIRST 25k-SUBJ TO O/H	25,000	0	0	25,000
REMAINDER (O/H EXEMPT)	0	17,883	19,914	37,797
<b>TOTAL SUB CONTRACTS</b>	<b>25,000</b>	<b>17,883</b>	<b>19,914</b>	<b>62,797</b>
<b>VI. OTHER DIRECT COSTS</b>				
PUBLICATION COSTS	1,000	3,000	3,691	7,691
COMPUTER MAINTENANCE FEE	1,268	1,153	1,033	3,454
RESEARCH MATERIALS	1,000	500	500	2,000
<b>TOTAL OTHER DIR. COSTS</b>	<b>3,268</b>	<b>4,653</b>	<b>5,223</b>	<b>13,144</b>
<b>TOTAL DIRECT COSTS</b>	<b>171,431</b>	<b>179,091</b>	<b>178,250</b>	<b>528,772</b>
<b>VII. INDIRECT COSTS</b>				
Y1 - 3: 48.5% OF MODIFIED				
<b>TOTAL INDIRECT COSTS</b>	<b>78,569</b>	<b>70,909</b>	<b>71,750</b>	<b>221,228</b>
<b>TOTAL REQUESTED SUPPORT</b>	<b>\$250,000</b>	<b>\$250,000</b>	<b>\$250,000</b>	<b>\$750,000</b>



# Face Page

**TITLE OF PROPOSED RESEARCH:**

Carbon data assimilation and parameter estimations using Local Ensemble Transform Kalman Filter (LETKF)

**1. CATALOG OF FEDERAL DOMESTIC ASSISTANCE #**

81.049

**2. CONGRESSIONAL DISTRICT:**

Applicant Organization's District: 9th

Project Site's District: 9th

**3A. I.R.S. ENTITY IDENTIFICATION OR SSN:**

946002123

**3B. DUNS Number:**

124726725

**4. AREA OF RESEARCH OR ANNOUNCEMENT TITLE/#:**

Scientific Discovery Through Advanced Computing (SciDA)

**5. HAS THIS RESEARCH PROPOSAL BEEN SUBMITTED TO ANY OTHER FEDERAL AGENCY?**

YES  NO

PLEASE LIST \_\_\_\_\_

**6. DOE/OER PROGRAM STAFF CONTACT (if known):**

Lori Jernigan

**7. TYPE OF APPLICATION:**

New  Renewal  
 Continuation  Revision  
 Supplement

**8. ORGANIZATION TYPE:**

Local Govt.  State Govt.  
 Non-Profit  Hospital  
 Indian Tribal Govt.  Individual  
 Other  Inst. of Higher Educ.  
 For-Profit  
 Small Business  Disadvan. Business  
 Women-Owned  8(a)

**9. CURRENT DOE AWARD # (IF APPLICABLE):**

**10. WILL THIS RESEARCH INVOLVE:**

10A. Human Subjects  No  If yes  
Exemption No. \_\_\_\_\_ or  
IRB Approval Date \_\_\_\_\_  
Assurance of Compliance No: \_\_\_\_\_  
10B. Vertebrate Animals  No  If yes  
IACUC Approval Date \_\_\_\_\_ or  
Animal Welfare Assurance No: \_\_\_\_\_

**11. AMOUNT REQUESTED FROM DOE FOR ENTIRE PROJECT PERIOD \$** 750,000.00

**12. DURATION OF ENTIRE PROJECT PERIOD:**

07/01/06 to 06/30/09  
MM/DD/YY MM/DD/YY

**13. REQUESTED AWARD START DATE**

07/01/06  
MM/DD/YY

**14. IS APPLICANT DELINQUENT ON ANY FEDERAL DEBT?**

Yes (attach an explanation)  No

**15. PRINCIPAL INVESTIGATOR/PROGRAM DIRECTOR**

NAME Inez Fung

TITLE Professor

ADDRESS 399 McCone Hall

Earth and Planetary Science, UCB

Berkeley, CA 94720-4767

PHONE NUMBER (510) 643-9367

\* Inez Fung

**SIGNATURE OF PRINCIPAL INVESTIGATOR/ PROGRAM DIRECTOR**

(please type in full name if electronically submitted)

Date 2/21/06

PI/PD ASSURANCE: I agree to accept responsibility for the scientific conduct of the project and to provide the required progress reports if an award is made as a result of this submission. Willful provision of false information is a criminal offense. (U.S. Code, Title 18, Section 1001).

**16. ORGANIZATION'S NAME** Regents of the University of California, B

ADDRESS Sponsored Projects Office

336 Sproul Hall

Berkeley, CA 94720-5940

**CERTIFYING REPRESENTATIVE'S**

NAME Susan Hedley

TITLE Assistant Director

PHONE NUMBER (510) 642-8119

\*Susan Hedley

**SIGNATURE OF ORGANIZATION'S CERTIFYING REPRESENTATIVE**

(please type in full name if electronically submitted)

Date 2/21/06

CERTIFICATION and ACCEPTANCE: I certify that the statements herein are true and complete to the best of my knowledge, and accept the obligation to comply with DOE terms and conditions if an award is made as the result of this submission. A willfully false certification is a criminal offense. (U.S. Code, Title 18, Section 1001).

**NOTICE FOR HANDLING PROPOSALS**

This submission is to be used only for DOE evaluation purposes and this notice shall be affixed to any reproduction or abstract thereof. All Government and non-Government personnel handling this submission shall exercise extreme care to ensure that the information contained herein is not duplicated, used, or disclosed in whole or in part for any purpose other than evaluation without written permission except that if an award is made based on this submission, the terms of the award shall control disclosure and use. This notice does not limit the Government's right to use information contained in the submission if it is obtainable from another source without restriction. This is a Government notice, and shall not itself be construed to impose any liability upon the Government or Government personnel for any disclosure or use of data contained in this submission.

**PRIVACY ACT STATEMENT**

If applicable, you are requested, in accordance with 5 U.S.C., Sec. 562A, to voluntarily provide your Social Security Number (SSN). However, you will not be denied any right, benefit, or privilege provided by law because of a refusal to disclose your SSN. We request your SSN to aid in accurate identification, referral and review of applications for research/training support for efficient management of Office of Science grant/contract programs.



DOE F 4620.1

(04-93)

All Other Editions Are Obsolete

U.S. Department of Energy
Budget Page
(See reverse for Instructions)

OMB Control No.

1910-1400

OMB Burden Disclosure
Statement on Reverse

ORGANIZATION
Budget Page No:
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR
Requested Duration: (Months)
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates
DOE Funded Person-mos.
Funds Requested by Applicant
Funds Granted by DOE
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)
E. TRAVEL
F. TRAINEE/PARTICIPANT COSTS
G. OTHER DIRECT COSTS
H. TOTAL DIRECT COSTS (A THROUGH G)
I. INDIRECT COSTS (SPECIFY RATE AND BASE)
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES
L. TOTAL COST OF PROJECT (J+K)

DOE F 4620.1  
(04-93)  
All Other Editions Are Obsolete

**U.S. Department of Energy**  
**Budget Page**  
(See reverse for Instructions)

OMB Control No.  
1910-1400  
OMB Burden Disclosure  
Statement on Reverse

ORGANIZATION				Budget Page No: _____	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR				Requested Duration: _____ (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded		
			Person-mos.		
	CAL	ACAD	SUMR	by Applicant	by DOE
1.					
2.					
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. ( ) TOTAL SENIOR PERSONNEL (1-6)					
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)					
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL					
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL					
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS					
H. TOTAL DIRECT COSTS (A THROUGH G)					
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS					
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					

DOE F 4620.1  
(04-93)  
All Other Editions Are Obsolete

**U.S. Department of Energy**  
**Budget Page**  
(See reverse for Instructions)

OMB Control No.  
1910-1400  
OMB Burden Disclosure  
Statement on Reverse

ORGANIZATION				Budget Page No: _____	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR				Requested Duration: _____ (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded		
			Person-mos.		
			CAL	ACAD	SUMR
				by Applicant	by DOE
1.					
2.					
3.					
4.					
5.					
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)				
7.	( ) TOTAL SENIOR PERSONNEL (1-6)				
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1.	( ) POST DOCTORAL ASSOCIATES				
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER				
TOTAL SALARIES AND WAGES (A+B)					
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL					
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL					
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS					
H. TOTAL DIRECT COSTS (A THROUGH G)					
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS					
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					

**U.S. Department of Energy**  
**Budget Page**  
(See reverse for Instructions)

ORGANIZATION <b>Lawrence Berkeley National Laboratory</b>				Budget Page No: <u>1</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Michael Wehner</b>				Requested Duration: <u>12</u> (Months) Year 1	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested
			CAL	ACAD	SUMR
					by Applicant
					by DOE
1.	Michael Wehner, Computer Staff Scientist		0.10		\$12,063
2.	Yu-Heng Tseng, Computer Systems Engineer II		0.65		\$53,757
3.	Yun He, Computer Systems Engineer III		0.10		\$9,004
4.					
5.					
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE) TSM 110-119				
7.	( 3 ) TOTAL SENIOR PERSONNEL (1-6)		0.85		\$74,824
B.	( ) OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)				
1.	( ) POST DOCTORAL ASSOCIATES				
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER				
TOTAL SALARIES AND WAGES (A+B)					\$74,824
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$74,824
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					\$3,000
E. TRAVEL			1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)		\$5,000
			2. FOREIGN		
TOTAL TRAVEL					\$5,000
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					\$1,177
5. SUBCONTRACTS					
6. OTHER					\$1,588
TOTAL OTHER DIRECT COSTS					\$2,765
H. TOTAL DIRECT COSTS (A THROUGH G)					\$85,589
I. INDIRECT COSTS			Org Burden 17.6% -Base 108,857	Tvl Rate 14% - Base 5,000	
			Proc. Burden 8.4% Base 3,000	LDRD Rate 9.1% - Base 135,209	
TOTAL INDIRECT COSTS			Gen Rate 46.3% -Base 129,810	Payroll Rate (Var.) - Base 74,824	\$125,850
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$211,439
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					\$211,439

**U.S. Department of Energy**  
**Budget Page**  
(See reverse for Instructions)

ORGANIZATION <b>Lawrence Berkeley National Laboratory</b>				Budget Page No: <u>2</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Michael Wehner</b>				Requested Duration: <u>12</u> (Months) Year 2	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)				DOE Funded	
				Person-mos.	
				CAL	ACAD
				SUMR	
				Funds Requested	
				Funds Granted	
				by Applicant	
				by DOE	
1.	Michael Wehner, Computer Staff Scientist			0.10	
2.	Yu-Heng Tseng, Computer Systems Engineer II			0.65	
3.	Yun He, Computer Systems Engineer III			0.10	
4.					
5.					
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE) TSM 110-119				
7.	( 3 ) TOTAL SENIOR PERSONNEL (1-6)			0.85	
B.	( ) OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)				
1.	( ) POST DOCTORAL ASSOCIATES				
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER				
TOTAL SALARIES AND WAGES (A+B)					\$77,069
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$77,069
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					\$3,000
E. TRAVEL					\$5,000
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL					\$5,000
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					\$1,607
5. SUBCONTRACTS					
6. OTHER					\$2,273
TOTAL OTHER DIRECT COSTS					\$3,880
H. TOTAL DIRECT COSTS (A THROUGH G)					\$88,949
I. INDIRECT COSTS (SPECIFY ON THE ATTACHED PAGE)					
Contract and Base -Base 112,407 Tvl Rate 14% - Base 5,000					
Proc. Burden 8.4% Base 3,000 LDRD Rate 9.1% - Base 140,499					
TOTAL INDIRECT COSTS Gen Rate 46.3% -Base 135,001 Payroll Rate (Var.) - Base 77,069					\$130,666
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$219,615
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					\$219,615

**U.S. Department of Energy**  
**Budget Page**  
(See reverse for Instructions)

ORGANIZATION <b>Lawrence Berkeley National Laboratory</b>				Budget Page No: <u>3</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Michael Wehner</b>				Requested Duration: <u>12</u> (Months) Year 3	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested
			CAL	ACAD	SUMR
					by Applicant
					by DOE
1.	Michael Wehner, Computer Staff Scientist		0.10		\$12,797
2.	Yu-Heng Tseng, Computer Systems Engineer II		0.65		\$57,031
3.	Yun He, Computer Systems Engineer III		0.10		\$9,553
4.					
5.					
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE) TSM 110-119				
7.	( 3 ) TOTAL SENIOR PERSONNEL (1-6)		0.85		\$79,381
B.	( ) OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)				
1.	( ) POST DOCTORAL ASSOCIATES				
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER				
TOTAL SALARIES AND WAGES (A+B)					\$79,381
C.	FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$79,381
D.	PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)				
TOTAL PERMANENT EQUIPMENT					\$3,000
E.	TRAVEL		1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)		\$5,000
			2. FOREIGN		
TOTAL TRAVEL					\$5,000
F.	TRAINEE/PARTICIPANT COSTS				
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G.	OTHER DIRECT COSTS				
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					\$1,610
5. SUBCONTRACTS					
6. OTHER					\$2,277
TOTAL OTHER DIRECT COSTS					\$3,886
H.	TOTAL DIRECT COSTS (A THROUGH G)				\$91,268
I.	INDIRECT COSTS (SPECIFY BY TITLE AND RATE)-Base		116,336	Tvl Rate 14% - Base	5,000
Proc. Burden 8.4% Base			3,000	LDRD Rate 9.1% - Base	145,127
TOTAL INDIRECT COSTS			139,628	Payroll Rate (Var.) - Base	79,381
J.	TOTAL DIRECT AND INDIRECT COSTS (H+I)				\$226,809
K.	AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES				
L.	TOTAL COST OF PROJECT (J+K)				\$226,809

**Budget Page**

(See reverse for Instructions)

ORGANIZATION <b>Lawrence Berkeley National Laboratory</b>				Budget Page No: <u>4</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Michael Wehner</b>				Requested Duration: <u>36</u> (Months) Summary - All Years	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)				DOE Funded	
				Person-mos.	
				Funds Requested	
				Funds Granted	
				by Applicant	
				by DOE	
1.	Michael Wehner, Computer Staff Scientist	0.30			\$37,284
2.	Yu-Heng Tseng, Computer Systems Engineer II	1.95			\$166,159
3.	Yun He, Computer Systems Engineer III	0.30			\$27,831
4.					
5.					
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE) TSM 110-119				
7.	( 3 ) TOTAL SENIOR PERSONNEL (1-6)	2.55			\$231,275
B. ( ) OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1.	( ) POST DOCTORAL ASSOCIATES				
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER				
TOTAL SALARIES AND WAGES (A+B)				\$231,275	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				\$231,275	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT				\$9,000	
E. TRAVEL				1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)	
				\$15,000	
				2. FOREIGN	
TOTAL TRAVEL				\$15,000	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES				\$4,394	
5. SUBCONTRACTS					
6. OTHER				\$6,137	
TOTAL OTHER DIRECT COSTS				\$10,532	
H. TOTAL DIRECT COSTS (A THROUGH G)				\$265,806	
I. INDIRECT COSTS				Org Burden 17.6% -Base 337,600 Tvl Rate 14% - Base 15,000	
				Proc. Burden 8.4% Base 9,000 LDRD Rate 9.1% - Base 420,835	
TOTAL INDIRECT COSTS				Gen Rate 46.3% -Base 404,440 Payroll Rate (Var.) - Base 231,275	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				\$657,863	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				\$657,863	

### 9.1.2 Lawrence Livermore National Laboratory SAP

#### **Facilitating Climate Modeling Research by Joining Earth Science Analysis/Visualization Tools and Frameworks**

**Program Area:** Scientific Application Partnership: Computer Science

**Principal Investigator:** Dean Williams (Lawrence Livermore National Laboratory)

**Senior Personnel:** Robert S. Drach, Kyle Halliday

**Scientific Application Partner:** A Scalable and Extensible Earth System Model for Climate Change Science (PI - John B. Drake, Oak Ridge National Laboratory)

**Participating Institutions:** Lawrence Livermore National Laboratory (LLNL)

**Projected Funding Request:** \$350K per year for three years

This work was performed under the auspices of the U.S. Department of Energy by the University of California Lawrence Livermore National Laboratory under contract No.W-7405-Eng-48.

#### **Abstract**

We propose a Science Application Partnership (SAP) aligned with the science application project A Scalable and Extensible Earth System Model for Climate Change Science (SEESM) and with the Center for Enabling Technology Scaling the Earth System Grid to Petascale Data.

The objective of our project is to significantly expedite the application of advanced analysis and visualization tools on data sets that are used extensively by the climate research community. To meet this objective, we propose to work within the Scaling the Earth System Grid to Petascale Data infrastructure in order to connect open-source software tools which have particular strengths, but which are presently not in use across the entire climate community.

Our specific goals are twofold:

- to implement seamless access to the existing ESG and the proposed Scaling the Earth System Grid to Petascale Data by software tools for data manipulation, filtering, and visualization such as the widely used and supported analysis packages: CDAT, Ferret, GrADS and NCL.
- to allow these diverse tools/frameworks to be utilized in a common way within the current and future ESG framework.



## Narrative

The Earth System Grid II (ESG) is a collaboration among selected DOE laboratories and the National Center for Atmospheric Research (NCAR) that has been funded by the DOE Scientific Discovery Through Advanced Computation (SciDAC) program. Hundreds of climate researchers now utilize the ESG for data access, management, and analysis. For instance, the ESG is the current framework for dissemination of ~130 Terabytes of data from the Community Climate System Model (CCSM) and of ~30 Terabytes of data from some 23 model simulations of climate scenarios specified by the Intergovernmental Panel for Climate Change (IPCC). Seamless access of such ESG-enabled data by advanced analysis, diagnosis, and intercomparison tools will greatly facilitate interagency collaboration, and enhance researchers' ability to critically diagnose climate model simulations.

We propose a five-pronged approach to realize our goals:

- (1) We will develop an infrastructure to enable secure access/management of the ESG data holdings with any of the designated software tools; this will enable authorized users' to access ESG data holdings via their desktops from anywhere in the world.
- (2) We will integrate all these tools on each ESG federated data site, thereby allowing researchers to analyze, filter, manipulate, and visualize data in a sequence of easy steps.
- (3) We will develop the means to monitor requested data processes and to allocate limited computing resources at the ESG federated sites. (That is, we will implement needed data analysis brokering between the client analysis software and ESG servers.) We will enhance the ESG portal so as to enable user input for data analysis and diagnosis of ESG requested data.
- (4) We will work with existing diagnostic groups (e.g. PCMDI, NCAR, LANL, GFDL) to implement priority analysis, diagnostic, and intercomparison techniques in the ESG framework.
- (5) We will demonstrate the ability of scientists to capture and analyze complex data from the ESG data holdings using the climate software tools. Finally, we will put this new capability into production for applications such as the CCSM and other climate models, as well as for future model intercomparisons and the next IPCC Assessment Report (AR5).

We intend to work with the research community to implement advanced techniques for access, filtering, manipulation, and visualization of climate data within the ESG framework. We also will build upon ESG catalogs that track data replicas and associate metadata attributes with data sets. This development work will enable a user to conduct granular-level product searches and analysis within ESG--a capability that currently does not exist. Such enhancements will substantially increase the usability of the data not only by ESG, but also by other grid projects that are implemented within research communities.

Our objective addresses the Solutions Analysis and Visualization needs of the SciDAC application "A Scalable and Extensible Earth System Model for Climate Change Science" (PI - John B. Drake, Oak Ridge National Laboratory) and the ability of all users across the country to access and diagnose large climate datasets, thereby enhancing the ability of partner organizations to harness DOE's Earth science research efforts to meet national needs. We will also be facilitating a connection between three Enabling Computational Technologies: the Visualization and Analytics Centers for Enabling Technologies (CET) headed by Wes Bethel, the Analysis and Knowledge Discovery (AKD) CET headed by Tammy Kolda and the Scaling the Earth System Grid to Petascale Data headed by Dean N. Williams. We propose to deploy all Visualization CET and AKD developments via this framework. By coordinating this effort, we will efficiently distribute all new analysis and visualization techniques to the user community. By enhancing connections with the Climate Model Science Application areas, the Visualization Analytics CET and the AKD CET, within the Scaling the Earth System Grid to Petascale Data CET can reach a broader audience and improve access to important DOE climate data for analysis and study. We also propose to maintain this software for the duration of its life cycle.



# Face Page

**TITLE OF PROPOSED RESEARCH:**

Facilitating Climate Modeling Research by Joining Earth Science Analysis/Visualization Tools and Frameworks (climate SAP)

**1. CATALOG OF FEDERAL DOMESTIC ASSISTANCE #**

81.049

**2. CONGRESSIONAL DISTRICT:**

Applicant Organization's District: 10th

Project Site's District: 10th

**3A. I.R.S. ENTITY IDENTIFICATION OR SSN:**

95-6031193

**3B. DUNS Number:**

**4. AREA OF RESEARCH OR ANNOUNCEMENT TITLE#:**

SciDAC 2 Lab 06 04

**5. HAS THIS RESEARCH PROPOSAL BEEN SUBMITTED TO ANY OTHER FEDERAL AGENCY?**

YES  NO

PLEASE LIST \_\_\_\_\_

**6. DOE/OER PROGRAM STAFF CONTACT (if known):**

Fred Johnson (301) 903-3601

**7. TYPE OF APPLICATION:**

New  Renewal  
 Continuation  Revision  
 Supplement

**8. ORGANIZATION TYPE:**

Local Govt.  State Govt.  
 Non-Profit  Hospital  
 Indian Tribal Govt.  Individual  
 Other  Inst. of Higher Educ.  
 For-Profit  
 Small Business  Disadvan. Business  
 Women-Owned  8(a)

**9. CURRENT DOE AWARD # (IF APPLICABLE):**

**10. WILL THIS RESEARCH INVOLVE:**

**10A. Human Subjects**  No  If yes  
Exemption No. \_\_\_\_\_ or  
IRB Approval Date \_\_\_\_\_  
Assurance of Compliance No: \_\_\_\_\_  
**10B. Vertebrate Animals**  No  If yes  
IACUC Approval Date \_\_\_\_\_ or  
Animal Welfare Assurance No: \_\_\_\_\_

**11. AMOUNT REQUESTED FROM DOE FOR ENTIRE PROJECT PERIOD \$** 1,081,304.00

**12. DURATION OF ENTIRE PROJECT PERIOD:**

07/01/06 to 06/30/09  
MM/DD/YY MM/DD/YY

**13. REQUESTED AWARD START DATE**

07/01/06  
MM/DD/YY

**14. IS APPLICANT DELINQUENT ON ANY FEDERAL DEBT?**

Yes (attach an explanation)  No

**15. PRINCIPAL INVESTIGATOR/PROGRAM DIRECTOR**

NAME Dean Williams

TITLE Principal Investigator

ADDRESS 7000 East Avenue, L-103  
Livermore, CA 94550

PHONE NUMBER (925) 423-0145

*Dean A. Williams*  
SIGNATURE OF PRINCIPAL INVESTIGATOR/ PROGRAM DIRECTOR  
(please type in full name if electronically submitted)

Date 2-27-06

PI/PD ASSURANCE: I agree to accept responsibility for the scientific conduct of the project and to provide the required progress reports if an award is made as a result of this submission. Willful provision of false information is a criminal offense. (U.S. Code, Title 18, Section 1001).

**16. ORGANIZATION'S NAME** Regents of the University of California

ADDRESS Lawrence Livermore National Laboratory  
7000 East Avenue  
Livermore, CA 94550

CERTIFYING REPRESENTATIVE'S  
NAME Dona L. Crawford  
TITLE Computation, Associate Director  
PHONE NUMBER (925) 422-1985

*Dona L. Crawford for DL C*  
SIGNATURE OF ORGANIZATION'S CERTIFYING REPRESENTATIVE  
(please type in full name if electronically submitted)

Date 2-27-06

CERTIFICATION and ACCEPTANCE: I certify that the statements herein are true and complete to the best of my knowledge, and accept the obligation to comply with DOE terms and conditions if an award is made as the result of this submission. A willfully false certification is a criminal offense. (U.S. Code, Title 18, Section 1001).

**NOTICE FOR HANDLING PROPOSALS**

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**APPLICATION FACE PAGE  
OMB BURDEN DISCLOSURE STATEMENT**

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Washington, DC 20585**

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Washington, DC 20503**

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Statement on Reverse

Year 1

Table with columns for Organization (Lawrence Livermore National Laboratory), Principal Investigator (Dean Williams), and various budget categories (A-L) including Personnel, Fringe Benefits, Travel, and Direct Costs. Includes sub-columns for DOE Funded (CAL, ACAD, SUMR) and Funds Requested/Granted.

DOE F 4620.1

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1910-1400

OMB Burden Disclosure
Statement on Reverse

Year 2

Table with columns for Organization (Lawrence Livermore National Laboratory), Principal Investigator (Dean Williams), and various budget categories (A-L) including Personnel, Fringe Benefits, Travel, and Direct Costs. Includes sub-tables for DOE Funded Person-mos and Funds Requested/Granted.

DOE F 4620.1

(04-93)

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Budget Page
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OMB Burden Disclosure
Statement on Reverse

Year 3

Table with columns for Organization (Lawrence Livermore National Laboratory), Principal Investigator (Dean Williams), DOE Funded (Person-mos. CAL, ACAD, SUMR), Funds Requested (by Applicant), and Funds Granted (by DOE). Rows include personnel (Robert Drach, Kyle Halliday, Dean Williams), fringe benefits, travel, and other direct costs, totaling \$370,711.

DOE F 4620.1

(04-93)

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OMB Control No.

1910-1400

OMB Burden Disclosure
Statement on Reverse

Years 1 - 3

Table with columns for Organization (Lawrence Livermore National Laboratory), Principal Investigator (Dean Williams), and budget details for Years 1-3. Includes sections for Senior Personnel (A), Other Personnel (B), Fringe Benefits (C), Travel (E), Trainee/Participant Costs (F), Other Direct Costs (G), and Indirect Costs (I). Total project cost is \$1,081,304.

# **Facilitating Climate Modeling Research by Joining Earth Science Analysis/Visualization Tools and Frameworks (climate SAP) Budget Justification**

**A. Senior Personnel**

The PI Dean N. Williams will be leading and managing the overall project. He will be responsible for managing the team, providing insight to scientific requirements, emerging technologies, and corresponding with sponsors. Robert Drach will be developing a CDAT infrastructure to enable secure access/management of the ESG data holdings with any of the designated software tools. Kyle Halliday will be working with existing diagnostic groups (e.g. PCMDI, NCAR, LANL, GFDL) to implement priority analysis, diagnostic, and intercomparison techniques in the CDAT framework.

**B. Other Personnel**

N/A

**C. Fringe Benefits**

The Laboratory's Payroll Burden Rate is 42.5% and is applied to the non-leave standard salary of all Laboratory employees, including overtime. PostDocs are charged a 35% Payroll Burden, and students are charged 9.5%.

**D. Equipment**

None planned.

**E. Travel**

The anticipated travel cost to be roughly one trip per year for one person. The trip will be to visit the a major modeling center each year (i.e., NCAR, LANL, and GFDL).. Travel cost is estimated at \$7500.

**F. Trainee/Participant Costs**

N/A.

**G. Other Costs**

- 2.) Publication costs for technical review and release of publishing project results is anticipated at \$300.
- 6.) Office space is estimated at \$46,500.

**H. Total Direct Costs**

\$553,017

**I. Indirect Costs**

Total Indirect Costs are estimated at \$528,287. LLNL rate amounts and their definitions are explained in Attachment A. Note that rates are applied in a specified order and not all taxes apply to each direct cost.



### Other Support of Investigator(s)

Lawrence Livermore National Laboratory

Current and Pending Support (Effort will be adjusted if pending proposals are funded.)

#### Current Support for Dean N. Williams

Title	Source	Period	Award/Yr	Effort
Earth System Grid II	SciDAC	7/01 – 6/06	\$360 K	30%
Group Leader	NNSA	10/05 - present	\$200 K	30%
NASA OGC Grid Technologies	NASA	10/04 – 9/06	\$100 K	20%
Climate Data Analysis Tools	OBER	10/01 – 10/06	\$330 K	20%

#### Pending Support

Title	Source	Period	Award/Yr	Effort
SAP: Facilitating Climate Modeling Research by Joining Earth Science Analysis/Visualization Tools & Frameworks	SciDAC	7/06 – 6/11	\$350 K	40%
CET: Scaling the Earth System Grid to Petabyte Data	SciDAC	7/06 – 6/11	\$600 K	30%

#### Current Support for Robert S. Drach

Title	Source	Period	Award/Yr	Effort
Earth System Grid II	SciDAC	7/01 – 6/06	\$360 K	70%
Climate Data Analysis Tools	OBER	10/01 – 10/06	\$330 K	30%

#### Pending Support

Title	Source	Period	Award/Yr	Effort
SAP: Facilitating Climate Modeling Research by Joining Earth Science Analysis/Visualization Tools & Frameworks	SciDAC	7/06 – 6/11	\$350 K	20%
CET: Scaling the Earth System Grid to Petabyte Data	SciDAC	7/06 – 6/11	\$600 K	50%

#### Current Support for Kyle Halliday

Title	Source	Period	Award/Yr	Effort
NASA OGC Grid Technologies	NASA	10/04 – 9/06	\$100 K	50%
Climate Data Analysis Tools	OBER	10/01 – 10/06	\$330 K	50%

#### Pending Support

Title	Source	Period	Award/Yr	Effort
SAP: Facilitating Climate Modeling Research by Joining Earth Science Analysis/Visualization Tools & Frameworks	SciDAC	7/06 – 6/11	\$350 K	30%
CET: Scaling the Earth System Grid to Petabyte Data	SciDAC	7/06 – 6/11	\$600 K	20%

## Biographical Sketches (or resumes)

### Dean Norman Williams

Program for Climate Model Diagnosis and Intercomparison (PCMDI), Software Project Leader  
LLNL/CAR-EEBI Computing Applications, Acting Deputy Division Leader

---

### Professional Address

Lawrence Livermore National Laboratory                      Telephone: (925) 423-0145  
University of California    Fax: (925) 422-7675  
Mail Stop: L-103    E-mail: williams13@llnl.gov  
P.O. Box 808  
Livermore, California 94550

### Education

M.S. 1987, Computer Science, California State University at Chico, CA  
B.S. 1985, Applied Mathematics and Statistics, California State University at Chico, CA

### Related Current Professional Employment and Research Projects

CAR-EEBI Computing Applications Deputy Division Leader, 2005-present  
Computation Atmospheric Science Division Group Leader, 2004-present  
Earth Systems Grid, Principal Investigator, 1999-present  
Climate Data Analysis Tools, Project Lead, 1997-present  
Global Organization for Earth System Science Portal, Co-Principal Investigator, 2003-present  
UK National Environmental Research Council (NERC) DataGrid, Co-Principal Investigator, 2001-present

### Awards and Honors

Co-Chaired DOE Science Networking Workshop: A Roadmap to 2008  
Committee Organizer for DOE Data Management Roadmap to 2008  
Department of Energy (DOE) Research Summary of the Month: Application Development  
Computation Directorate Distinguished Achievement Award  
Society of Technical Communication: Technical Communication Award, Newsletters, Merit in Publication, Research Summary  
Lawrence Livermore National Laboratory Association of Black Laboratory Employees: Workforce Excellence Award

### Narrative

Dean N. Williams is currently working at Lawrence Livermore National Laboratory (LLNL) as the lead computer scientist for the Program for Climate Model Diagnosis and Intercomparison (PCMDI). He has been with PCMDI for the past 18 years designing and developing data analysis tools and visualization. He has published and co-authored several technical papers in the area of visualization and data analysis tools and has had some of his work presented in books. He is the lead developer of the Visualization and Computation System and lead developer of the Climate Data Analysis Tools. Dean was the initiator and important contributor of research proposals that received funding from the High Performance Computing and Communications (HPCC) Program in visualization and co-PI on other research projects funded by LLNL. For the past seven years, Dean has been engaged in research in computer science, focusing on high-performance and distributed computing. The goal of Dean's work is to develop metadata schemas, tools, and access mechanisms for the Earth Sciences communities.

### Current Related Web Sites

<a href="http://www.earthsystemgrid.org/">http://www.earthsystemgrid.org/</a>	-- Earth System Grid
<a href="http://cdat.sf.net">http://cdat.sf.net</a>	-- Climate Data Analysis Tools
<a href="http://go-essp.gfdl.noaa.gov">http://go-essp.gfdl.noaa.gov</a>	-- Global Organization for Earth System Science Portal
<a href="http://ndg.badc.rl.ac.uk">http://ndg.badc.rl.ac.uk</a>	-- NERC DataGrid

**Bob S. Drach**  
**Program for Climate Model Diagnosis and Intercomparison**  
**Lawrence Livermore National Laboratory**  
**drach@llnl.gov**

**Employment**

Robert Drach has worked as a computer scientist at the Lawrence Livermore National Laboratory since 1980. He currently supports the Program for Climate Model Diagnosis and Intercomparison, where he is responsible for the development of database and analysis software for climate modeling data and applications. His technical interests include scientific data management, information architecture, and scientific programming. He holds an MS in Mathematics and an MS in Industrial and Systems Engineering from Ohio University. He is a member of IEEE and ACM.

**Publications**

Bernholdt, D., S. Bharathi, D. Brown, K. Chanchio, M. Chen, A. Chervenak, L. Cinquini, B. Drach, I. Foster, P. Fox, J. Garcia, C. Kesselman, R. Markel, D. Middleton, V. Nefedova, L. Pouchard, A. Shoshani, A. Sim, G. Strand, and D. Williams, The Earth System Grid: Supporting the Next Generation of Climate Modeling Research. Proceedings of the IEEE Special Issue on Grid Computing, Vol. 93, No. 3, March 2005

Chen, L.T., R. Drach, M. Keating, S. Louis, D. Rotem, and A. Shoshani, Efficient organization and access of multi-dimensional datasets on tertiary storage systems. Information Systems Special Issue on Scientific Databases, 20(2):155-83, 1995

Drach, R., Serving Scientific Data over the Web, Computing in Science and Engineering, Vol. 2, No. 6, November/December 2000

**Kyle Halliday**  
**Lawrence Livermore National Laboratory**  
**P.O. Box 808, L-103**  
**Livermore, CA 94550**  
**halliday1@llnl.gov**

**Professional Experience**

2005 – present: Computer Scientist, Program for Climate Model Diagnosis and Intercomparison (PCMDI)

2003 – 2005: Team Leader, Computing Applications and Research (CAR) Department Web Team

Education

B.S. 2001, Computer Science, University of Virginia, Charlottesville, VA

Currently enrolled in M.S. program at California State University, Chico

**Awards and Honors**

CAR Department Peer Award, 2003

CAR Department Peer Award, 2004

Computation Directorate Noteworthy Achievement, 2003

Computation Directorate Noteworthy Achievement, 2004

Publications

Halliday, K., A. Hurst, J. Nelson, Analysis of next generation TCP. LLNL Technical Report. UCRL-TR-208615. 2004.

Kyle Halliday is currently working as a Computer Scientist in LLNL's Program for Climate Model Diagnosis and Intercomparison (PCMDI). Kyle's background is mainly in web application development, and he has applied his knowledge to PCMDI's web-based data management activities. He recently developed a Grid Service used to query the Intergovernmental Panel on Climate Change (IPCC) database, a 30 Terabyte repository of climate simulation data. He has also deployed a web content management system used to develop and store software documentation. Kyle's interests include scientific data management, distributed systems, and Grid computing.

## Description of Facilities and Resources

The Center for Applied Scientific Computing (CASC) is the organizational home of applied mathematics and computer science research at LLNL (<http://www.llnl.gov/CASC>). CASC has about one hundred scientific staff members and all have ready access to the supercomputing resources administered by Livermore Computing (LC) (<http://www.llnl.gov/computing>), which is the computer center for LLNL. In addition to maintaining desktop workstations for staff and visiting researchers, LC maintains various large-scale computing platforms, including the 2304 and 4096 processor MCR and Thunder Linux clusters and the 131,072 processor BlueGene/L platform. These production computers provide users with a rich tool environment that includes high-performance compilers, debuggers, analyzers, editors, and locally developed custom libraries and application packages for software development. Access to such resources is provided by an LLNL Multiprogrammatic and Institutional Computing Initiative and therefore does not directly affect the requested budget for this proposal.

## Appendix

Bernholdt, D., S. Bharathi, D. Brown, K. Chanchio, M. Chen, A. Chervenak, L. Cinquini, B. Drach, I. Foster, P. Fox, J. Garcia, C. Kesselman, R. Markel, D. Middleton, V. Nefedova, L. Pouchard, A. Shoshani, A. Sim, G. Strand, and D. Williams, The Earth System Grid: Supporting the Next Generation of Climate Modeling Research. Proceedings of the IEEE Special Issue on Grid Computing, Vol. 93, No. 3, March 2005

Chen, L.T., R. Drach, M. Keating, S. Louis, D. Rotem, and A. Shoshani, Efficient organization and access of multi-dimensional datasets on tertiary storage systems. Information Systems Special Issue on Scientific Databases, 20(2):155-83, 1995

Halliday, K., A. Hurst, J. Nelson, Analysis of next generation TCP. LLNL Technical Report. UCRL-TR-208615. 2004.

# Performance Engineering for the Next Generation Community Climate System Model

## A Proposal Submitted to the DOE Office of Science

Program Announcement: LAB 06-04  
Program Area: Science Application Partnership: Computer Science  
Program Office: Office of Advanced Scientific Computing Research  
Technical Contact: Dr. Anil Deane

### Applicant

<i>Institution</i>	<i>Principal Investigator</i>
Oak Ridge National Laboratory PO Box 2008, MS 6016 Oak Ridge, TN 37831-6016	Patrick H. Worley (865)574-3128 worleyph@ornl.gov
Field Work Proposal ERKJD13	

### Participating Institutions / Senior Personnel

**Lead PI: Patrick H. Worley, Oak Ridge National Laboratory**

<i>Institution</i>	<i>Senior Personnel</i>
Lawrence Livermore National Laboratory (LLNL)	Arthur Mirin
Argonne National Laboratory (ANL)	Robert Loy

### Science Application Partner / Science Liaisons

**A Scalable and Extensible Earth System Model for Climate Change Science**

**Lead Science Application PI: John B. Drake, Oak Ridge National Laboratory**

<i>Institution</i>	<i>Senior Personnel</i>
Oak Ridge National Laboratory	John Drake
Los Alamos National Laboratory	Philip Jones
Lawrence Livermore National Laboratory	Phillip Cameron-Smith
Argonne National Laboratory	Robert Jacob

**Projected Funding Request:** \$500K per year for three years.

**Cover Page**

**Title of Proposed Project:**

Performance Engineering for the Next Generation  
Community Climate System Model  
FWP # 57648

**Office of Science Program Announcement Title/#:**

Lab 06-04  
Scientific Discovery through Advanced Computing

**Name of Laboratory:**

Argonne National Laboratory

**Principal Investigator(s):**

Raymond M. Loy, Senior Software Developer  
Argonne National Laboratory  
Mathematics and Computer Science Division  
9700 So. Cass Avenue - Bld.221  
Argonne, IL 60439  
(T) 630-252-7205 (Fax) 630-252-6104  
[rloy@mcs.anl.gov](mailto:rloy@mcs.anl.gov)

**Official signing for Laboratory:**

Rick L. Stevens, Associate Laboratory Director-PBCS  
Argonne National Laboratory  
Mathematics and Computer Science Division  
9700 So. Cass Avenue - Bld.221  
Argonne, IL 60439  
(T) 630-252-3378, ( Fax) 630-252-6333  
[stevens@mcs.anl.gov](mailto:stevens@mcs.anl.gov)

**Requested funding for Argonne National Laboratory  
for Proposed Project:**

Year 1	\$	224,000
Year 2	\$	224,000
Year 3	\$	224,000
Total:	\$	<u>672,000</u>

**Duration of Entire Project Period:**

07/01/2006 to 06/30/2009

**Use of human subjects in proposed project:**

No

**Use of vertebrate animals in proposed project:**

No

**Signature of PI, Date of Signature:**

PI's electronic signature on file

March 6, 2006

**Signature of Official, Date of Signature:**



March 6, 2006

**U.S. Department of Energy**  
**Budget Page**  
(See reverse for Instructions)

ORGANIZATION <b>The University of Chicago, Operator of Argonne National Laboratory</b>				Budget Page No: <u>pg 1 of 4</u> Yr 1 of 3		
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Raymond M. Loy</b>				Requested Duration: <u>12</u> (Months) FWP # 57648		
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested	
			CAL	ACAD	SUMR	
					by Applicant	
					by DOE	
1.	Raymond M. Loy, PI		9.00			\$159,119
2.						
3.						
4.						
5.						
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7.	( 1 ) TOTAL SENIOR PERSONNEL (1-6)		9.00			\$159,119
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)						
1.	( ) POST DOCTORAL ASSOCIATES					
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3.	( ) GRADUATE STUDENTS					
4.	( ) UNDERGRADUATE STUDENTS					
5.	( ) SECRETARIAL - CLERICAL					
6.	( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)						\$159,119
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)						
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)						\$159,119
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)						
TOTAL PERMANENT EQUIPMENT						
E. TRAVEL			1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)			\$2,800
			2. FOREIGN			
TOTAL TRAVEL						\$2,800
F. TRAINEE/PARTICIPANT COSTS						
1. STIPENDS (Itemize levels, types + totals on budget justification page)						
2. TUITION & FEES						
3. TRAINEE TRAVEL						
4. OTHER (fully explain on justification page)						
TOTAL PARTICIPANTS ( ) TOTAL COST						
G. OTHER DIRECT COSTS						
1. MATERIALS AND SUPPLIES						\$2,981
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION						
3. CONSULTANT SERVICES						
4. COMPUTER (ADPE) SERVICES						
5. SUBCONTRACTS						
6. OTHER						
TOTAL OTHER DIRECT COSTS						\$2,981
H. TOTAL DIRECT COSTS (A THROUGH G)						\$164,900
I. INDIRECT COSTS (SPECIFY RATE AND BASE)						
Section H. Direct cost X Aggregate rate of: 35.840%						
TOTAL INDIRECT COSTS						\$59,100
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)						\$224,000
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES						
L. TOTAL COST OF PROJECT (J+K)						\$224,000

**U.S. Department of Energy**  
**Budget Page**  
 (See reverse for Instructions)

ORGANIZATION The University of Chicago, Operator of Argonne National Laboratory				Budget Page No: <u>2 of 4</u> Yr. 2 of 3	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Raymond M. Loy				Requested Duration: <u>12</u> (Months) FWP # 57648	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested
			CAL	ACAD	SUMR
					by Applicant
					by DOE
1. Raymond M. Loy, PI			8.80		
2.					
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. ( 1 ) TOTAL SENIOR PERSONNEL (1-6)			8.80		\$164,322
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)					\$164,322
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$164,322
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL			1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)		
			2. FOREIGN		
TOTAL TRAVEL					
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					\$578
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS					\$578
H. TOTAL DIRECT COSTS (A THROUGH G)					\$164,900
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
Section H. Direct cost X Aggregate rate of: 35.840%					
TOTAL INDIRECT COSTS					\$59,100
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$224,000
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					\$224,000



**U.S. Department of Energy**  
**Budget Page**  
(See reverse for Instructions)

ORGANIZATION <b>The University of Chicago, Operator of Argonne National Laboratory</b>				Budget Page No: <u>3 of 4</u> Yr 3 of 3	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Raymond M. Loy</b>				Requested Duration: <u>12</u> (Months) FWP # 57648	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested
			CAL	ACAD	SUMR
					by Applicant
					by DOE
1. Raymond M. Loy, PI			8.50		
2.					
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. ( 1 ) TOTAL SENIOR PERSONNEL (1-6)			8.50		\$164,530
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)					\$164,530
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$164,530
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL			1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)		
			2. FOREIGN		
TOTAL TRAVEL					
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					\$370
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS					\$370
H. TOTAL DIRECT COSTS (A THROUGH G)					\$164,900
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
Section H. Direct cost X Aggregate rate of: 35.840%					
TOTAL INDIRECT COSTS					\$59,100
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$224,000
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					\$224,000

## U.S. Department of Energy

## Budget Page

(See reverse for Instructions)

ORGANIZATION The University of Chicago, Operator of Argonne National Laboratory				Budget Page No: <u>4 of 4</u> 3-Yr. ANL Total Project	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Raymond M. Loy				Requested Duration: <u>36</u> (Months) FWP # 57648	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested
			CAL	ACAD	SUMR
					by Applicant
					by DOE
1. Raymond M. Loy, PI			26.30		
2.					
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. ( 1 ) TOTAL SENIOR PERSONNEL (1-6)			26.30		\$487,971
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)					\$487,971
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$487,971
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL			1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)		\$2,800
			2. FOREIGN		
TOTAL TRAVEL					\$2,800
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					\$3,928
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS					\$3,928
H. TOTAL DIRECT COSTS (A THROUGH G)					\$494,700
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS					\$177,300
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$672,000
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					\$672,000

**Lab 06-04: Scientific Discovery through Advanced Computing**  
**Performance Engineering for the Next Generation**  
**Community Climate System Model**

**Raymond M. Loy, PI**

**FWP # 57648**

**Budget Explanation**

**A-C Salaries and Fringe Benefits**

Argonne National Laboratory is a government-owned facility operated by the University of Chicago. As a contractor for the Department of Energy, Argonne National Laboratory must comply with DOE general policies and procedures on budgeting and accounting. The Laboratory's costing procedures are based on the assumption that all costs incurred will be recovered. The costing procedures use standard rates, which are used throughout the Laboratory on a consistent basis and uniformly applied to all work supported by the Department of Energy and other federal agencies.

Standard rates are established at the beginning of the fiscal year for each research division, and are monitored and revised as necessary. All labor costs are distributed using standard rates which are developed by the laboratory's budget office for each major payroll classification within the lab. The division-wide rates are based on pay bands ( salary ranges ) and fringe benefits (35.2% for a regular staff and clerical, and 11% for post/pre doctoral appointees), plus a factor for divisional overhead and for paid absences. Graduate and undergraduate students costs include housing allowance and fringe benefits( 7.65%). Effort is escalated each year by a rate provided by the Argonne Budget Department.

The principal investigator for this proposal is: Raymond M. Loy  
The PI's effort charged per year to this proposal is : 9.00 man-months

**E Travel**

Domestic: \$1.4 K per trip/escalate 4.5% per yr.  
Foreign: \$2.6 K per trip/escalate 4.5% per yr.

**G Other Direct Costs**

1. Materials and Supplies:  
Hardware/software maintenance, software, low-end computers (<\$5k), computer and misc.supplies.
2. Publication Costs:  
Books/literature, subscriptions, publishing costs related to research.

**I Indirect Costs**

Standard rates are also developed for Laboratory General and Administrative (G&A) expense. The procedures for distributing Laboratory G&A and program expense is applied on the basis of the total cost of the work performed. The following indirect rates are provisional and have been estimated for each fiscal year budget period:

PBCS Program Expenses @ 3.7%  
Laboratory G&A:  
Common Support @ 27.3%  
Service Centers @ 21.3%  
Equipment/Subcontracts@ 8.1%  
G&A Burden @ 2.9%

Argonne' s indirect rates are continuously reviewed and audited by  
Cognizant Federal Agency:

Martin Straka 630-252-7724 Department of Energy-Chicago Operations Office



# Face Page

**TITLE OF PROPOSED RESEARCH:**

Performance Engineering for the Next Generation Community Climate System Model

**1. CATALOG OF FEDERAL DOMESTIC ASSISTANCE #**

81.049

**2. CONGRESSIONAL DISTRICT:**

Applicant Organization's District: 10th

Project Site's District: 10th

**3A. I.R.S. ENTITY IDENTIFICATION OR SSN:**

95-6031193

**3B. DUNS Number:**

**4. AREA OF RESEARCH OR ANNOUNCEMENT TITLE/#:**

SciDAC 2 Lab 06 04

**5. HAS THIS RESEARCH PROPOSAL BEEN SUBMITTED TO ANY OTHER FEDERAL AGENCY?**

YES  NO

PLEASE LIST \_\_\_\_\_

**6. DOE/OER PROGRAM STAFF CONTACT (if known):**

Anil Deane (301) 903-1465

**7. TYPE OF APPLICATION:**

- New  Renewal  
 Continuation  Revision  
 Supplement

**8. ORGANIZATION TYPE:**

- Local Govt.  State Govt.  
 Non-Profit  Hospital  
 Indian Tribal Govt.  Individual  
 Other  Inst. of Higher Educ.  
 For-Profit  Disadvan. Business  
 Small Business  8(a)  
 Women-Owned

**9. CURRENT DOE AWARD # (IF APPLICABLE):**

**10. WILL THIS RESEARCH INVOLVE:**

- 10A. Human Subjects  No  If yes  
Exemption No. \_\_\_\_\_ or  
IRB Approval Date \_\_\_\_\_  
Assurance of Compliance No: \_\_\_\_\_  
10B. Vertebrate Animals  No  If yes  
IACUC Approval Date \_\_\_\_\_ or  
Animal Welfare Assurance No: \_\_\_\_\_

**11. AMOUNT REQUESTED FROM DOE FOR ENTIRE PROJECT PERIOD \$** 504,000.00

**12. DURATION OF ENTIRE PROJECT PERIOD:**

07/01/06 to 06/30/09  
MM/DD/YY MM/DD/YY

**13. REQUESTED AWARD START DATE**

07/01/06  
MM/DD/YY

**14. IS APPLICANT DELINQUENT ON ANY FEDERAL DEBT?**

Yes (attach an explanation)  No

**15. PRINCIPAL INVESTIGATOR/PROGRAM DIRECTOR**

NAME Arthur Mirin

TITLE Principal Investigator

ADDRESS 7000 East Avenue, L-561  
Livermore, CA 94550

PHONE NUMBER (925) 422-4020

**SIGNATURE OF PRINCIPAL INVESTIGATOR/ PROGRAM DIRECTOR**

(please type in full name if electronically submitted)

Date \_\_\_\_\_

PI/PD ASSURANCE: I agree to accept responsibility for the scientific conduct of the project and to provide the required progress reports if an award is made as a result of this submission. Willful provision of false information is a criminal offense. (U.S. Code, Title 18, Section 1001).

**16. ORGANIZATION'S NAME** Regents of the University of California

ADDRESS Lawrence Livermore National Laboratory  
7000 East Avenue  
Livermore, CA 94550

**CERTIFYING REPRESENTATIVE'S**

NAME Dona L. Crawford

TITLE Computation, Associate Director

PHONE NUMBER (925) 422-1985

**SIGNATURE OF ORGANIZATION'S CERTIFYING REPRESENTATIVE**  
(please type in full name if electronically submitted)

Date \_\_\_\_\_

CERTIFICATION and ACCEPTANCE: I certify that the statements herein are true and complete to the best of my knowledge, and accept the obligation to comply with DOE terms and conditions if an award is made as the result of this submission. A willfully false certification is a criminal offense. (U.S. Code, Title 18, Section 1001).

**NOTICE FOR HANDLING PROPOSALS**

This submission is to be used only for DOE evaluation purposes and this notice shall be affixed to any reproduction or abstract thereof. All Government and non-Government personnel handling this submission shall exercise extreme care to ensure that the information contained herein is not duplicated, used, or disclosed in whole or in part for any purpose other than evaluation without written permission except that if an award is made based on this submission, the terms of the award shall control disclosure and use. This notice does not limit the Government's right to use information contained in the submission if it is obtainable from another source without restriction. This is a Government notice, and shall not itself be construed to impose any liability upon the Government or Government personnel for any disclosure or use of data contained in this submission.

**PRIVACY ACT STATEMENT**

If applicable, you are requested, in accordance with 5 U.S.C., Sec. 562A, to voluntarily provide your Social Security Number (SSN). However, you will not be denied any right, benefit, or privilege provided by law because of a refusal to disclose your SSN. We request your SSN to aid in accurate identification, referral and review of applications for research/training support for efficient management of Office of Science grant/contract programs.

DOE F 4620.1

(04-93)

All Other Editions Are Obsolete

U.S. Department of Energy
Budget Page
(See reverse for Instructions)

OMB Control No.

1910-1400

OMB Burden Disclosure
Statement on Reverse

Year 1

Table with columns for Organization (Lawrence Livermore National Laboratory), Principal Investigator (Art Mirin), and various budget categories (A-L) including Personnel, Fringe Benefits, Travel, and Direct Costs. Includes sub-columns for DOE Funded (CAL, ACAD, SUMR) and Funds Requested/Granted.

DOE F 4620.1  
(04-93)  
All Other Editions Are Obsolete

**U.S. Department of Energy  
Budget Page**  
(See reverse for Instructions)

OMB Control No.  
1910-1400  
OMB Burden Disclosure  
Statement on Reverse

Year 2

ORGANIZATION <b>Lawrence Livermore National Laboratory</b>				Budget Page No: <u>2</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Art Mirin</b>				Requested Duration: <u>12</u> (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)				Year 2	
	DOE Funded Person-mos.			Funds Requested	Funds Granted
	CAL	ACAD	SUMR	by Applicant	by DOE
1.	4.32			\$53,324	
2.					
3.					
4.					
5.					
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE) TSM 110-119				
7.	4.32			\$53,324	
B. ( ) OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1.	( ) POST DOCTORAL ASSOCIATES				
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER				
TOTAL SALARIES AND WAGES (A+B)				\$53,324	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				\$22,663	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				\$75,987	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL				\$1,500	
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL				\$1,500	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				\$500	
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES				\$900	
5. SUBCONTRACTS					
6. OTHER				\$7,342	
TOTAL OTHER DIRECT COSTS				\$8,742	
H. TOTAL DIRECT COSTS (A THROUGH G)				\$86,229	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS				\$81,787	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				\$168,016	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				\$168,016	

DOE F 4620.1

(04-93)

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U.S. Department of Energy
Budget Page
(See reverse for Instructions)

OMB Control No.

1910-1400

OMB Burden Disclosure
Statement on Reverse

Year 3

Table with columns for Organization (Lawrence Livermore National Laboratory), Principal Investigator (Art Mirin), and various budget categories (A-L) including Personnel, Fringe Benefits, Travel, and Direct Costs. Includes sub-columns for DOE Funded (CAL, ACAD, SUMR) and Funds Requested/Granted.

DOE F 4620.1

(04-93)

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U.S. Department of Energy
Budget Page
(See reverse for Instructions)

OMB Control No.

1910-1400

OMB Burden Disclosure
Statement on Reverse

Years 1 - 3

Table with columns for Organization (Lawrence Livermore National Laboratory), Principal Investigator (Art Mirin), and various budget categories (A-L) including Personnel, Salaries, Fringe Benefits, Travel, and Direct/Indirect Costs. Includes sub-tables for DOE Funded Person-mos. and Funds Requested/Granted.



**Performance Engineering for the Next Generation Community  
Climate System Model  
Budget Justification**

**A. Senior Personnel**

The PI, Arthur A. Mirin, will analyze and optimize performance of the next generation Community Climate System Model. The work will include performance modeling using both analytic and artificial neural network approaches, scaling to thousands of processors, and extending to the chemistry-dominated regime, alternative meshes, and high resolution.

**B. Other Personnel**

Bronis deSupinski will act as a PERC liaison at no cost, particularly vis-a-vis the artificial neural network approach.

**C. Fringe Benefits**

The Laboratory's Payroll Burden Rate is 42.5% and is applied to the non-leave standard salary of all Laboratory employees, including overtime. PostDocs are charged a 35% Payroll Burden, and students are charged 9.5%.

**D. Equipment**

None planned.

**E. Travel**

The anticipated travel is 1-2 trips per year for one person to interact with other researchers doing related work. Travel cost is estimated at \$4,500.

**F. Trainee/Participant Costs**

N/A.

**G. Other Costs**

- 2.) Publication costs for technical review and release of publishing project results is anticipated at \$1,500.
- 4) Computer services, as needed on the project, are estimated at \$2,700.
- 6.) Office space is estimated at \$22,056.

**H. Total Direct Costs**

\$258,685

**I. Indirect Costs**

Total Indirect Costs are estimated at \$245,321. LLNL rate amounts and their definitions are explained in Attachment A. Note that rates are applied in a specified order and not all taxes apply to each direct cost.

## Attachment A

### Lawrence Livermore National Laboratory Current FY2006 Rates

Indirect Cost Pool	Rate (%)	Allocation Base/Rate Determination
<u>Organization Personnel Charge (OPC):</u> Computation - Associate Director's Office	19.09%	Distribution of specific Organization's personnel management costs to users of the Organization Personnel Charge accounts. The rates vary by the Organization providing the service.
<u>Program Management Charge (PMC):</u> Computation - Associate Director's Office Computation - Program	4.50% 8.10%	A distribution of costs associated with managing and administering direct funded Programs within a Directorate. PMC is allocated on a value-added cost input base to Direct Operating, LDRD, Capital Equipment,
<u>General &amp; Administrative (G&amp;A):</u>	31.50%	G&A is allocated on a value-added base, which is total operating costs less direct materials, subcontracts, and the Electricity Recharge. Supplemental Labor is included included in the base. G&A is applied to Direct Operating, Capital Equipment and Construction accounts.
<u>Strategic Mission Support (SMS):</u>	7.00%	SMS costs include institutional strategic planning, institutional capabilities, outreach, and special employees. Applied to direct operating, WFO, and capital equipment accounts using a value-added base.
<u>Institutional General Purpose Equipment (IGPE):</u>	0.80%	The IGPE allocation is for capital equipment of a general use or institutional nature that benefits multiple cost objectives and is required for general-purpose site-wide needs. It is allocated on a total-cost base, and is not applied to DOE major items of equipment, general plant projects, line item construction or Work for Others - DOE.
<u>Institutional General Plant Projects</u>	0.65%	The IGPP allocation is for new construction projects that cost less than \$5M and are of a general institutional nature benefiting multiple cost objectives and required for general-purpose site-wide needs.
<u>Laboratory Directed Research &amp; Development (LDRD):</u> Operating Calculation - An assessment applied to Laboratory operating costs to support exploratory research and development.	6.38%	Rate is applied against total capital equipment (excluding line items) and operating costs, excluding Federal Administrative Charge.

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## 1 Abstract

We propose a Science Application Partnership (SAP) aligned with the science application project *A Scalable and Extensible Earth System Model for Climate Change Science* (SEESM) and with the center for enabling technology *Performance Engineering Research Center* (PERC). SEESM will extend the Community Climate System Model (CCSM) to become a first-generation Earth System Model that treats the coupling between the physical, chemical, and biogeochemical processes in the climate system. It will explore new science and will run at higher resolution than today's models. Both the improved physical processes and the increase in resolution come at the cost of significant increase in computational complexity.

In order to continue to achieve the computational throughput of present-day simulations, CCSM will need to be modified to use existing computing systems more efficiently and optimized for next-generation massively parallel systems. This will require improving scalability to thousands of processors and carrying out more comprehensive performance analysis in order to attain that goal. We plan to (1) improve scalability of the atmosphere and ocean component models with respect to processor count; (2) investigate and optimize performance at high spatial resolution; (3) improve scalability of the full coupled model through improved load balance; and (4) port to and optimize on next generation high performance computing systems.

## 2 Narrative

### 2.1 Background and Significance

The goal of the DOE Climate Change Prediction Program (CCPP), including the SciDAC2 Science Application project *A Scalable and Extensible Earth System Model for Climate Change Science* (SEESM), is:

*To determine the range of possible climate changes over the 21<sup>st</sup> century and beyond through simulations using a more accurate climate system model that includes the full range of human and natural climate feedbacks with increased realism and spatial resolution.*

Over the next 5 years, SEESM intends to create a first generation Earth system model based on the Community Climate System Model (CCSM) that treats the coupling between the physical, chemical, and biogeochemical processes in the climate system. The model will include comprehensive treatments of the processes governing well-mixed greenhouse gases, natural and anthropogenic aerosols, the aerosol indirect effect and tropospheric ozone for climate change studies. It will also include improved representation of carbon and chemical processes, particularly for treatment of greenhouse gas emissions and aerosols. These improvements all come at the cost of significant increases in computation, minimally 3-5 times as costly per horizontal grid point. SEESM will also be running experiments at much higher grid resolutions, in order to validate the accuracy of the new processes and to investigate specific science questions, which involves an increase in computational cost that is at least linear in the increased size of the computational grid.

During the integration of new methods and new chemical and biogeochemical processes, the model will need to continue to perform well on the available high performance computing systems in order to maximize the length of simulations and number of ensembles that can be used for assessment products. The major assessments by the International Panel on Climate Change (IPCC) occur roughly every six years, and simulations from CCSM have been used extensively in the third and fourth IPCC reports. For the fifth assessment (AR5), the target is to use the Earth-system version of CCSM that predicts the co-evolution of physical and chemical climate. In order to complete the full suite of desired assessment runs, it will be important to achieve the same computational rate that was achieved in previous assessments. This is a very aggressive goal given the planned modifications to CCSM.

The computer resources available for computational science within the DOE Office of Science have increased dramatically with the installation of the 1024 processor Cray X1E and the 5296 processor Cray XT3 at Oak Ridge National Laboratory (ORNL), the 1024 node IBM BG/L at Argonne National Laboratory (ANL), and the 888 processor IBM POWER5 cluster and the 640 processor AMD Opteron cluster at Lawrence Berkeley National Laboratory (LBNL). This trend is expected to continue for a number of years, with the goal of installing a system with petaflop performance in 5 to 10 years. This potentially will provide the necessary resources to meet the substantial needs of SEESM, if the CCSM can take advantage of them. A petaflop system will necessarily employ tens of thousands of processors. Two major issues face the CCSM code structure as we move from systems with 1000 to 10,000 and 50,000 processors. First is parallel scalability and the second is load balancing. A number of practical issues also remain, as evidenced by the fact that the memory requirements are currently too large to be able to use systems such as the IBM BlueGene/L system.

## 2.2 Preliminary Studies

### 2.2.1 Problem Description

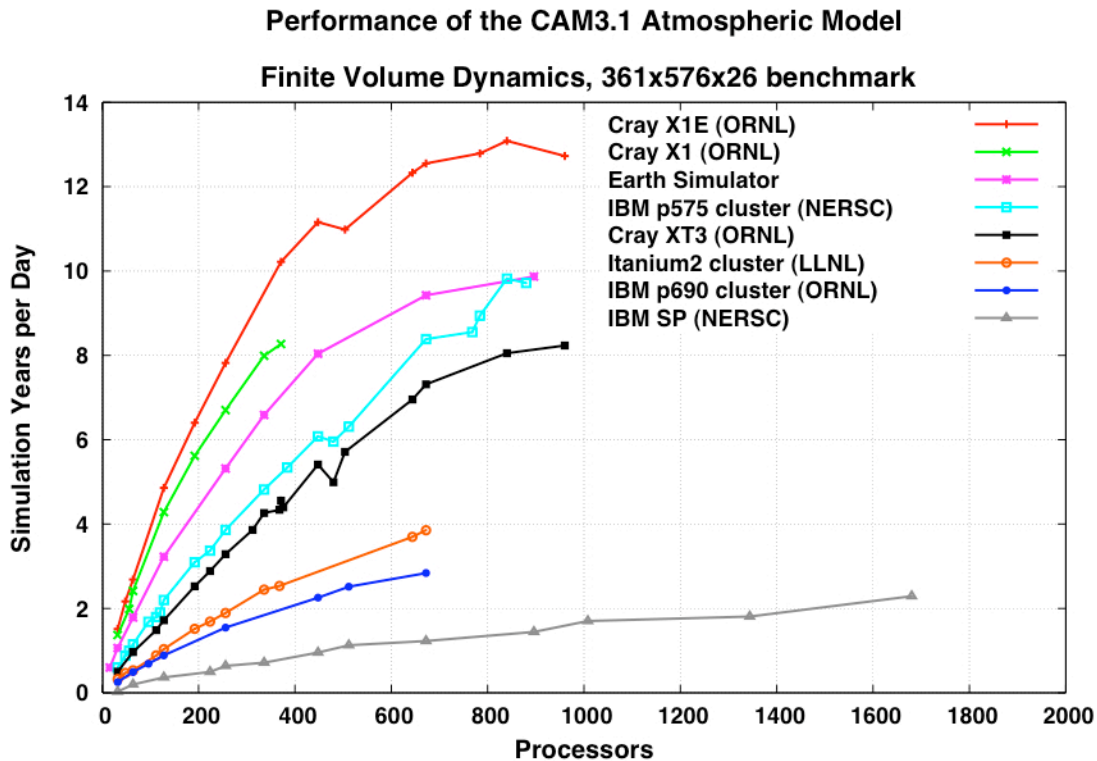
The CCSM is currently made up of atmosphere, ocean, land, and sea ice *component* models. The atmosphere component is the Community Atmosphere Model (CAM3). The ocean component is the Parallel Ocean Program (POP). The land component is the Community Land Model (CLM3). The sea ice model is the Community Sea Ice Model (CSIM4). In a coupled run these components execute concurrently (on separate processors) and communicate via a coupler component (CPL6). The atmosphere model is the most computationally expensive component currently, and is likely to become even more dominant as additional physical processes are introduced. The ocean is the second most expensive component. When allocating processors to the CCSM components, typically as many as possible are given to the atmosphere. Processors are then allocated to the other components so as to minimize the time components are idle waiting for data from the coupler. Note that the cost of a component is a function of the grid resolution used in the component. For some experiments it may be appropriate to use a much larger grid for the ocean than for the atmosphere, in which case the roles of the ocean and the atmosphere in this configuration process would switch.

The land and sea ice models and the coupler are essentially two-dimensional surface models, and, while they need to run efficiently on parallel platforms, there are intrinsic limits to their scalability. In contrast, the atmosphere and ocean models are both three-dimensional models and potentially can achieve high degrees of parallelism. To achieve the goals of SEESM, high degrees of parallelism and computational efficiency will be required of both ocean and atmosphere components.

The ocean model supports a two-dimensional domain decomposition, which allows thousands of processors to be used even for the relatively small 1-degree grid resolution (approximately 120,000 horizontal grid points and 40 vertical levels) used in current CCSM simulations. However, performance can still suffer from scaling problems due to load imbalances and the overhead of a linear system solution required at the ocean surface, that is, a two-dimensional subsystem that needs to be solved every timestep of the simulation. A new version of POP has been developed that addresses some of these issues, including a subblock algorithm to eliminate some of the load imbalances and an option to run the two-dimensional linear system solution on a subset of the processors [Jones2005]. This will be incorporated into CCSM within the current year. The efficacy of these modifications for the one-degree grid is not clear, and a careful performance analysis is required to understand the scalability of this new version of POP. As new physical processes are introduced into POP, and as the grid resolution increases, the performance characteristics of the model will change. SEESM is also developing an entirely new ocean model, one incorporating a different vertical coordinate, to replace POP.

The atmosphere model is itself made up of two major subcomponents: the physical parameterizations (*physics*) and the dynamical core (*dycore*). CAM comes with three different dycores, one of which is selected at compile-time. The current released version of CCSM uses a spectral Eulerian dycore. This dycore supports only a one-dimensional domain decomposition, severely limiting scalability. For example, at the current production resolution using ~32000 horizontal grid points, no more than 128 processors can be used in the dynamics. In contrast, a two-dimensional decomposition is supported in the physics, and many more processors can be used there. On a shared memory parallel computer (SMP), or a cluster of SMPs, OpenMP parallelism can be used to provide more processors to the physics than can be used by the dynamics. It has been shown that a two-dimensional decomposition is possible for the spectral

Eulerian dycore, but the efficiency of such an implementation is in doubt due to interprocessor communication overhead [Drake1995; Foster1997]. Experimenting with such a new implementation has been deprecated as the climate scientists are currently moving to one of the other dycores for production, a semi-Lagrangian finite-volume (FV) dynamical core [Lin2004]. The FV dycore is currently utilized with only ~13000 horizontal grid points, but more recently has been run at 1.0-degree resolution (~52000 horizontal grid points) and 0.5-degree resolution (~220000 horizontal grid points). The FV dycore can be domain-decomposed in two dimensions [Mirin2005], but the number of subdomains is limited to at most 480 at 1.0-degree resolution with 26 vertical levels, and limited to 960 for the 0.5-degree resolution with 26 vertical levels. As with the spectral Eulerian dycore, OpenMP can be used to exploit more processors in the physics than in the dynamics. This is illustrated in Fig. 1, where systems not using OpenMP can use at most 960 processors, while those supporting OpenMP can use more or, like the IBM p575 system, can use fewer MPI processes for a given number of processors and achieve better scalability.



**Fig. 1. Performance Scalability of CAM**

While the number of processors used in the full CCSM is the sum of those used in the individual component models, it is not productive to use many more processors than twice the number used by the atmosphere model. Ultimately, the scalability of the climate models has been limited by the relatively modest mesh sizes and accompanying domain decomposition methodologies. With the expected increase in the cost per horizontal grid point due to the inclusion of new physical processes, these limitations are no longer acceptable if CCSM is to make effective use of next generation petaflop systems.

The IBM BlueGene/L (BG/L) system has many architectural features in common with a number of the proposed petaflop systems. The BG/L system is optimized for bandwidth, scalability and

the ability to handle large amounts of data while consuming a fraction of the power and floor space required by today's fastest systems. Every processor on BG/L contains a two-element wide FPU, which results in 4 flops/cycle/processor. There are very high bandwidth paths between processor and memory (on a per flop basis), particularly for sequential access. The toroidal network is well suited to periodic boundary conditions, such as is found in global climate models, and a great deal of work went in to making the network partitionable. A simple kernel on the compute nodes and offloading of system services to I/O and service nodes results in less interference with running applications. The MPI library for BG/L was written to exploit hardware features and deliver high communication performance. The drawbacks of BG/L, compared to other contemporary platforms, are its relatively low clock speed (700MHz) and small per-node memory (512MB). The small memory will present particular challenges in porting CCSM to BG/L because CCSM components typically use global arrays on a single node for I/O and many of the physical processes planned for addition will also increase the per-node memory requirements.

As will be shown in the following sections, we are proposing a number of solutions to these problems. Much is still unknown however, and will remain unknown unless significant effort is made to measure and track the performance of the CCSM as the model evolves. The primary responsibility of measuring and tracking performance resides within the SEESM project, and we will work closely with the software engineers within SEESM to analyze this data and prioritize the performance aspects of model development. This Science Application Partnership (SAP), focusing as it does on scalability and on enabling the exploitation of the next generation of massively parallel systems, is a crucial component to the success of the SEESM research goals.

### 2.2.2 Collaboration and Past Accomplishments

This SAP is led by 3 researchers who have been involved in CCSM development for many years, have led analyses that have quantified the performance limitations of the current model, and have a vision of how to correct the problems.

- Patrick Worley has worked with the atmosphere model for over 15 years. He designed, implemented, and evaluated the parallel algorithms used in the spectral dynamics in CCM/MP-2D, the Computer Hardware, Advanced Mathematics and Model Physics (CHAMMP) funded massively parallel version of the Community Climate Model (CCM), the predecessor to CAM. For CAM, Worley designed and implemented the data structures and load balancing scheme used in CAM physics, supporting both efficient vectorization and increased scalability when used with OpenMP parallelism. Worley was also an active participant in the porting, performance analysis, and performance optimization of both CAM and POP on the Cray X1, X1E, XD1, and XT3, the IBM POWER4 and POWER5 clusters, and the SGI Altix. Worley is a co-chair of the CCSM Software Engineering Working Group. Worley was the liaison between the SciDAC science application projects in climate and the SciDAC Integrated Software Infrastructure Center *Performance Evaluation Research Center* and will be the coordinator of application engagement activities in the SciDAC2 Center for Enabling Technologies *Performance Engineering Research Center* (PERC).
- Arthur Mirin has worked in the area of high-performance computing for global climate modeling since the beginnings of the CHAMMP program over 15 years ago. He developed the two-dimensional domain decomposition methodology for the finite-volume dynamical core, significantly increasing the scalability of CAM with FV. He also led the vectorization of the FV dycore. He has extensive experience with communication paradigms (e.g., one-sided MPI-2, Shmem, and hybrid programming models). Mirin



coordinated the simulation and was lead author of the work that won the Gordon Bell Award for Best Performance in 1999. He has worked in large-scale computing for nearly 37 years and is presently leader of the Scientific Computing Group in the Center for Applied Scientific Computing.

- Raymond Loy has over 10 years of experience with parallel message-passing performance and load-balancing of structured, block-structured, and unstructured computations in a variety of codes including CCSM and the FLASH code from the ASC/Alliances Center for Astrophysical Thermonuclear Flashes. He is the author of Autopack, a tool for MPI-based programs. Autopack is a library providing automatic message-packing support for an application, reducing the burden on the application scientist, and easing platform-specific tuning. An early user of BG/L, he has ported several versions of POP to BG/L and has assisted in the BG/L port of other applications at several BlueGene Consortium Application Workshops. He has performed message-passing performance analysis of POP and the full CCSM on various platforms and has contributed to development of the Model Coupling Toolkit (MCT) [Larson2005], which is used in CPL6 [Craig2005]. Loy has participated in a Terascale Simulation Tools and Technologies (TSTT) working group as well as the Common Component Architecture (CCA) Forum.

All three members of the team have close working relationships with the computational scientists in SEESM, and have prior experience working with the ocean, sea ice, land, atmosphere, and coupler developers. For this SAP, the science application partners are John Drake (ORNL) for the atmosphere, Phil Jones (Los Alamos National Laboratory) for the ocean, Philip Cameron-Smith (LLNL) for the atmospheric chemistry, and Robert Jacob (ANL) for the coupler and coupler-level interactions within the full CCSM.

### 2.2.3 Purpose

The main purpose of this work is to analyze and optimize CCSM so that it can simulate tomorrow's science at the same throughput as CCSM simulates today's science. This will be accomplished through increased scalability, performance analysis and improvement, extension to new architectures, and application and exploitation of performance prediction techniques.

## 2.3 Research Design and Methods

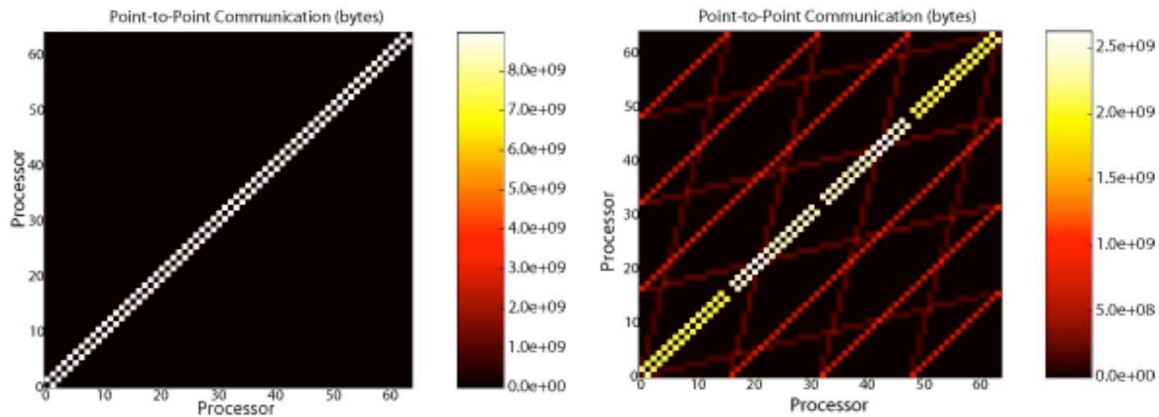
As indicated in Section 2.2.1, we are concerned with CCSM performance and scalability when introducing new physics, new problem sizes, and new architectures. Here we describe the approaches we expect to take to address these concerns. We begin with a description of approaches for the individual component models, in particular, the atmosphere. However, a number of the issues we will be facing may not become clear until the CCSM model development is more advanced, and a careful performance analysis and tracking, in coordination with internal SEESM efforts, is an important aspect of this proposal. This will require the exploitation of sophisticated tools and techniques for performance instrumentation and analysis. To this end, we plan to work with the SciDAC2 Center for Enabling Technology *Performance Engineering Research Center* (PERC).

### 2.3.1 Model Performance and Scalability

#### 2.3.1.1 CAM Scalability

#### Performance Instrumentation and Analysis

We will begin with the performance analysis and performance modeling of CAM, to determine a performance baseline before the new physical processes are introduced. As CAM evolves, we will periodically update this analysis, using it to predict or identify scalability and other performance problems early in the development process. It is important that state-of-the-art performance tools, such as IPM [IPM], MPE/Jumpshot [Chan2002], or TAU [Mohr1994, Malony2004], be used in this activity. For example, we recently used IPM to compare communication patterns in 1-D and 2-D decompositions of CAM (see Fig. 2), where the diagram shows latitudinal border communications (main diagonal), vertical geopotential communications (parallel to and offset from main diagonal) and transpose communications (diamond pattern).



**Fig. 2. Communication patterns in CAM as measured by the IPM tool.**

The results from this analysis, showing over double the traffic with the 1-D decomposition (top) versus 2-D (bottom), were in contradiction to our conventional wisdom that the transposes associated with the 2-D decomposition technique would dominate. This reinforces the importance of such tools.

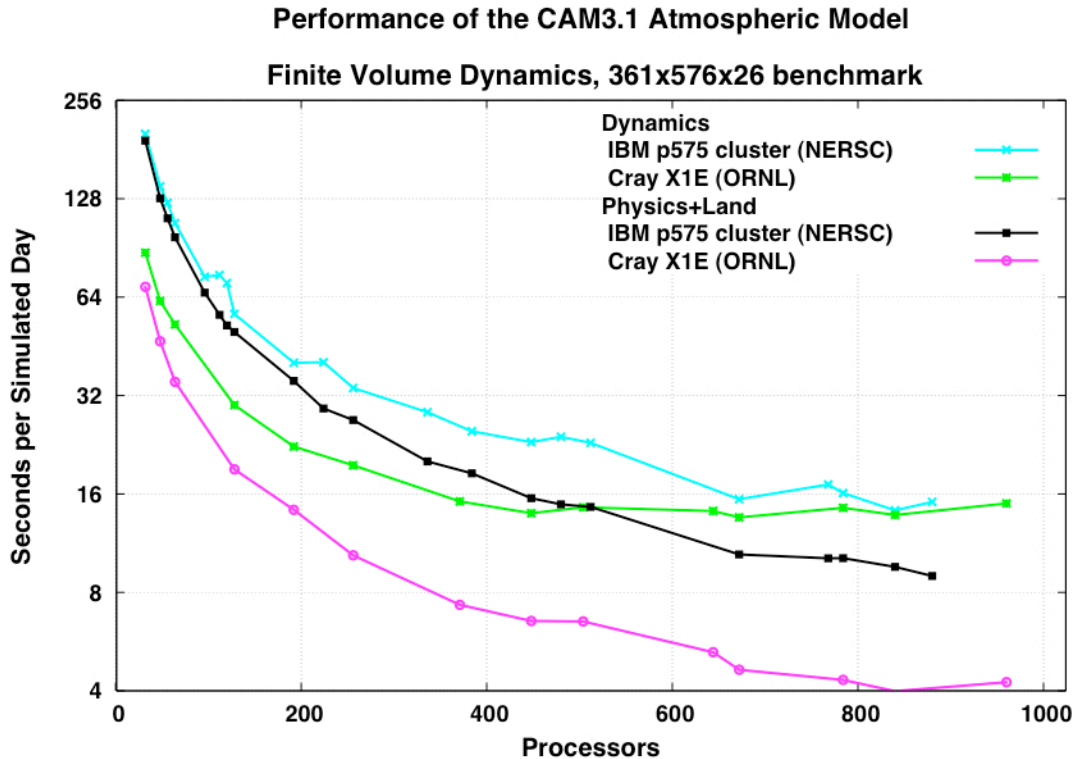
Much of the instrumentation and analysis will take place within the SEESM project. We are primarily consumers of these data, but will also advise on the process. Performance models and other prediction techniques are our primary contribution to this aspect of the work. The performance analysis process is iterative: posing questions, collecting data, analyzing data, reformulating questions. As such, performance models can be extremely useful in encapsulating current knowledge about performance and directing future experiments. In particular, the cost of the performance experiments can be high, and performance models also allow extrapolation to scenarios that cannot be easily tested, such as new problem sizes or new architectures. While performance models have proven their worth in architectural evaluations and algorithm evaluations, current modeling techniques make them less useful for development and optimization of codes as complex as CAM. As such, CAM performance modeling is a higher risk (and high payoff) activity than the other work described in this proposal. While modeling will not be the highest priority within the project, we do plan on pursuing the activity in collaboration

with our PERC colleagues at the San Diego Supercomputing Center, at Lawrence Livermore National Laboratory, and at Oak Ridge National Laboratory.

### Optimization of CAM in Chemistry-Dominated Regime

While many of the proposed modifications to the physical processes in CAM will have significant impacts on performance and scalability, here we focus on the atmospheric chemistry. The performance impact of atmospheric chemistry is better understood than that for some of the other proposed changes, and the issues and solutions are generally applicable.

Up until now, climate simulations using CAM, while modeling many important physical effects, have only marginally taken into account chemical processes. This has been due largely to the expense involved with modeling chemistry along with climate. Next-generation climate simulations require inclusion of these important chemical mechanisms. From a performance standpoint this will require analysis of regimes containing hundreds of advected constituents (instead of only a few). Also, the balance of computation involved in columnar processes (e.g., model physics, chemistry) versus the dynamical core will put us into a whole new regime, thereby requiring us to take a fresh look at parallelization methodology and scaling. For example, Fig. 3 describes the scaling of the dynamics versus the physics for the current model on the Cray X1E and on the IBM p575 cluster. Here, dynamics dominates for even small processor counts, and does not scale as well as the physics. With the introduction of atmospheric chemistry, the physics will become much more expensive.



**Fig. 3. Scalability of CAM dynamics versus physics.**

Preliminary scaling tests show that, with the current CAM model, advecting 100 tracers more than quadruples the execution time. There is a memory cost as well to store the additional 3-D tracer arrays, and that can become a limiting factor at moderate resolutions on certain

architectures. It is therefore all the more important to be able to amortize the memory costs by scaling to a very large number of processors. We propose to in effect carry out a three-dimensional decomposition of the tracer advection phase of the dycore, with the third dimension being the tracer index. Based on our experience with the multi-two-dimensional domain decomposition in the FV dycore, we expect the increased communication costs of the tracer decomposition to be manageable. The tracer advection phase also involves some border communication. We will aim to hide by communicating small groups of tracers using nonblocking primitives. We will investigate optimal sizes of those blocks to maximize the overlap with computation.

In the chemistry-dominated regime, the highest priority will be given to optimizing performance of the chemical and physical processes, which operate along vertical columns independent of one-another. Much effort has already gone into parallelizing the columnar processes using a general chunking methodology [Worley2005]. That technology generally scales well to large numbers of processes and in terms of process count should match up well with the tracer decomposition. If the current two-dimensional decomposition approach is not sufficient, much of the atmospheric chemistry is independent between grid points, not just between columns, and a full three-dimensional decomposition just for the atmospheric chemistry may be required. One concern though is with vector machines, where at fine decomposition, the work per computational process might result in inefficient vector lengths. This will need to be considered in the overall scaling strategy.

The chemistry-dominated regime also requires a different approach to load-balance. There is presently a choice of how to decompose the horizontal mesh among processes. The default choice has been to use a physics decomposition identical to that of the dynamics. However, such a decomposition is generally not load-balanced due to variations in computational work associated with solar radiation. We have also provided several alternatives that take load-balancing into account in the decomposition. These alternatives require an additional transpose between the dynamics and physics decompositions. While the communication costs associated with load balancing are typically smaller than the savings brought about by improved load-balance, the performance enhancement due to load balancing is sensitive to computer system, processor count, and problem size. For example, on the Cray X1E using the spectral Eulerian dycore and the production problem size, load balancing improves overall CAM performance by 15% for all processor counts [Worley2006]. In contrast on an IBM p690 cluster, load balancing is only useful for smaller processor counts. In the chemistry-dominated regime, however, we expect the equation to change and for load-balanced decompositions to be much superior in all situations.

Up to now the alternative decompositions have been from among several fixed choices. With the added costs of chemistry, refining the load-balance will be all the more important. We plan on generalizing the decomposition choices as well as implementing a dynamic load-balancing scheme. The dynamic decomposition choice will depend on statistics over previous time steps. We will also need to consider decomposition startup costs in determining the frequency with which to alter decompositions.

The scenario being considered involves four or five domain decompositions – two for the main dynamics (already implemented in the FV dycore), one for the tracer advection, and one or two for the chemistry and physics. We see no way to increase the process count associated with the primary dycore evolution using the currently available dycores, beyond that which will come naturally from increased computational grid resolution. Therefore, we will need to allow different phases of the evolution to use different numbers of processes. This is supported in the current

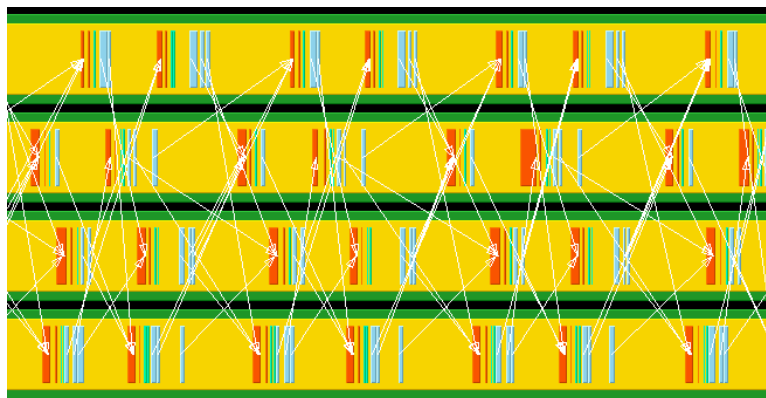
atmosphere model through the use of OpenMP parallelism. We will need to adapt and generalize this approach to also work in an MPI-only environment.

### Extension to Cubed Sphere Grid

Under the direction of S-J Lin, one of the inventors of the FV dycore, work is under way to extend the dynamical core to the cubed sphere grid [Rancic1996]. This is motivated by the well-known drawbacks of the polar singularity of the latitude/longitude grid. The cubed sphere version of the dycore is expected to be available in early CY 2007. An alternative dycore being developed using a discontinuous Galerkin (DG) discretization on the cubed sphere will also be available in CAM in the same time frame. Elimination of the polar singularity will allow decomposition in all three dimensions – latitude, longitude and vertical. We plan to collaborate with SEESM on a performance analysis and modeling of the cubed sphere version of FV and DG as soon as they become available. If, as expected, the cubed sphere implementation allows scaling to a much larger process count, we will immediately begin experiments to determine how best to exploit this scalability in the context of CAM and a chemical atmosphere.

#### 2.3.1.2 Scalability of Other Component Models

As mentioned in Section 2.2.1, a new version of the ocean model, POP 2, has recently been developed that addresses many of the known scalability and performance problems of the current production version. Until the performance of this new ocean model is carefully analyzed, it is difficult to identify what more needs to be done. However, preliminary performance instrumentation indicates that there may be an opportunity for further optimizations. For example, MPE has been used to analyze the intra-model message passing performance of POP 2.0 (see Fig. 4). Results suggest possible efficiency gains through use of Autopack [Loy2000], a message-passing library developed at ANL that transparently packs small messages into fewer larger ones for more efficient transport by MPI. Performance models of POP have been developed by two different research groups [Kerbyson2005, Snavely2003]. We will examine using these to identify performance optimization opportunities. As these models do not incorporate the new POP2 features, we will also update the models or generate a new performance model that allows us to determine performance and scalability bottlenecks.



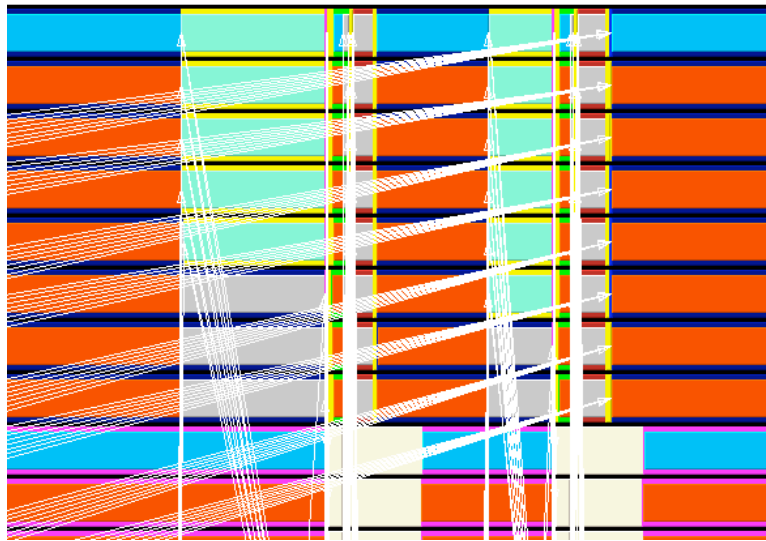
**Fig. 4. Jumpshot visualization of the POP baroclinic solver running a test case on 4 processors. The yellow background is the boundary condition calculation within the baroclinic solver (green). Colored vertical bars represent time spent in various MPI calls: MPI\_Isend() (light blue), MPI\_Irecv() (turquoise), and MPI\_Waitall() (red). Direct arrows connect MPI send and receive operations on source and target processors, respectively.**

The surface (land, ice) models will also be undergoing rapid development, and their performance will need to be tracked as well (as part of SEESM). We do not expect to focus on the surface models during the duration of this proposal but will adjust our efforts as necessary if the performance analysis indicates that they have become significant limiters to scalability, and if our expertise in modeling and parallel algorithm development are deemed by the Science Application leads to be of use.

### 2.3.1.3 CCSM Modeling and Configuration Optimization

Optimizing the allocation of processors to CCSM is very challenging. It is a combination of five separate parallel codes having an asymmetric communication pattern, with the associated communication barriers preventing optimal allocation of processors based solely on component throughput. Deciding on a CCSM configuration has been accomplished largely by trial and error.

More sophisticated approaches utilizing performance tools have been tried recently. For example, the MPE tool has been used in an attempt to gain a better understanding of the interaction between CCSM components. While MPE can automatically log all MPI activity, CCSM has been manually instrumented to provide specific information about message passing activity between the different model components, facilitating determination of the optimum load balance (see Fig. 5). This type of work will continue within SEESM, representing an improvement over past practice.



**Fig. 5. Each horizontal bar depicts the timeline of a single processor. The color indicates what state the processor is in. As shown in the example above, states may be nested. Arrows denote messages being sent between processors.**

Although MPE provides some insight into the workings of CCSM, a much more comprehensive performance modeling effort appears to be needed. Modeling the full CCSM with the goal of optimizing the configuration process has different accuracy requirements than identifying

scalability issues in the component models. The full CCSM is also much too complicated a code to model adequately within the time frame of this project using standard techniques. Instead we will use a technique undergoing development in PERC, namely that of artificial neural networks (ANNs) trained on a sampling of performance data over a parameter space [Ipek2005]. The criteria will consist of machine and configuration parameters. The idea will be to choose judicious sets of parameters at which the code will be evaluated, hoping to extrapolate results to parameter ranges of interest. B. de Supinski of LLNL, one of the pioneers of the ANN approach, has agreed to work with us at no cost. The neural network approach avoids the challenge of representing the inner workings of the code but provides little insight into those inner workings. Hence we will augment the ANN approach with data from more traditionally based performance models of the component models, to provide an integrated performance modeling capability for CCSM.

### *2.3.2 CCSM Portability and Exploitation of New Architectures*

A second focus of this proposal is preparing CCSM for porting to the next generation of massively parallel computer systems. The initial targets of the Cray X1E, Cray XT3, IBM p575 SMP cluster, and IBM BG/L cover most of the currently available architectures. Porting to the BG/L is the most challenging of these four, and a successful port to the BG/L will be the most useful preparation for future systems, requiring as it does both increased scalability and improved memory and I/O management. In the rest of this section we focus exclusively on the challenges and approaches to porting and optimizing the CCSM on the BG/L system.

#### *2.3.2.1 Porting CCSM to BG/L*

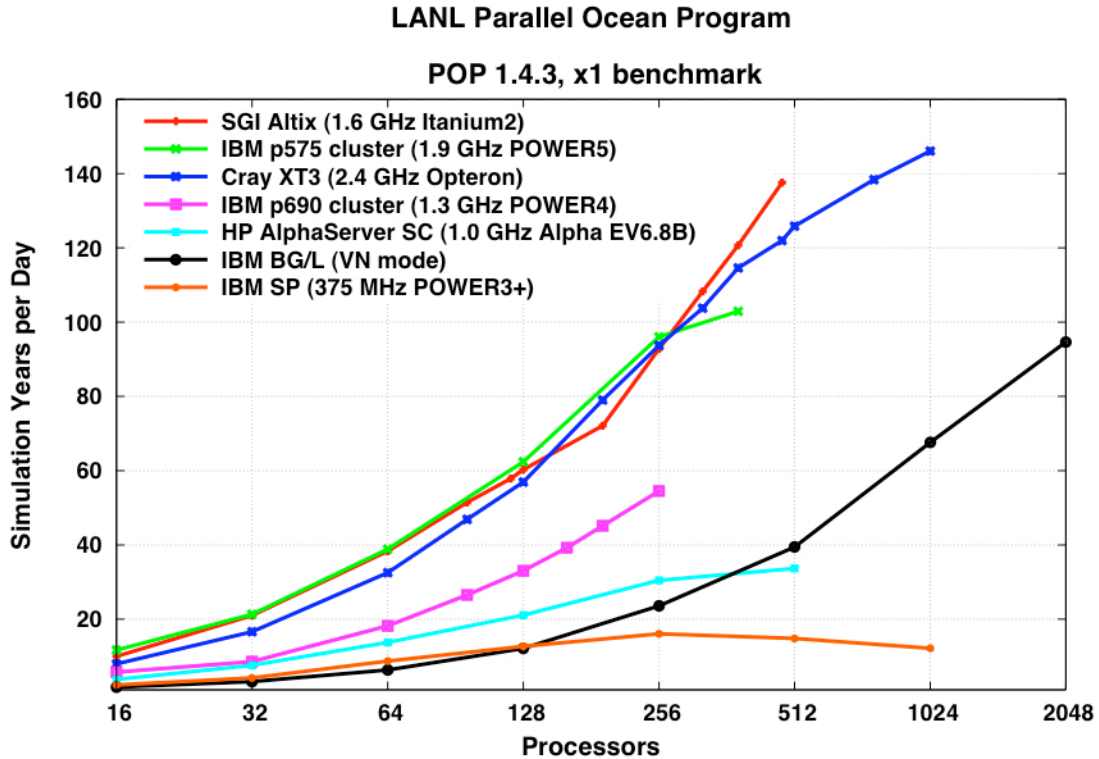
A main topic to address for the CCSM port to BlueGene/L will be global arrays associated with parallel I/O. All CCSM component models perform I/O to create large history and restart files. Binary mode file writes may be performed in parallel for POP2, though the current implementation of this feature has not been ported successfully to all target platforms. The preferred format for history output is NetCDF [NetCDF] and support in POP2 for NetCDF is currently only serial. A version of CAM that uses ZioLib [Yang2003] and Parallel NetCDF [Li2003] is available and we will transfer these capabilities to CCSM when porting to BG/L. Parallel-NetCDF will then be introduced in other components as necessary to improve scalability and performance.

Under the first SciDAC program, the Los Alamos standalone versions of POP 1.4.3 and POP 2.0 were ported to BG/L and good scaling was observed (see Fig. 6). POP2 will become the default ocean model in the development version of CCSM within this calendar year. Additional work may be required to parallelize diagnostic calculations that are added to POP by the CCSM ocean model working group.

A port of CAM/CLM has begun at the National Center for Atmospheric Research (NCAR) by programmers in the Scientific Computing Division. They found parallel I/O was necessary for CAM's binary restart files. We will join this effort and provide additional resources to ensure any required code changes are integrated with the development branches of CAM and CLM. The performance profiling and alternate parallelization schemes outlined above for CAM will be ported to BG/L as soon as they have been validated. (To ensure that the parallel algorithm work is incorporated into the production versions of the component models as soon as possible, we will

focus most of the initial development work of the non-BG/L specific modifications on the current production platforms: Cray X1E, Cray XT3, and IBM p575 cluster.)

Once the standalone versions of POP and CAM are ported, we shall port the simplest coupled system in CCSM, the coupler interacting with 4 “dead” models, to BG/L. The dead models are small parallel programs that send simple two-dimensional sine waves to the coupler for data fields. Since all modes of CCSM, full, data and dead models, use the same coupler “hub”, this system will allow us to study the performance of the hub on BG/L. The coupler’s underlying library, the Model Coupling Toolkit [Larson2005], has already been ported to BlueGene/L.



**Fig. 6. Performance of POP 1.4.3 "x1" Benchmark on the ANL BG/L. Scaling for virtual node (VN) mode is shown in comparison to other platforms.**

BG/L system software has the limitation that it can only load and run a single executable, unlike other MPP systems that can load a different MPI executable on each node of a run. While CCSM components are traditionally run in multi-executable configuration, work is currently underway by CCSM participants to produce a single-executable version of CCSM. Completion of this work will be supported by SEESM. If a single executable is not available when we are ready to try the dead-model case, we will assist this effort.

Once a single-executable, dead-model case is running on BlueGene, we will proceed to the all-data model case. Data models send real fields read from files to the coupler but perform no internal calculations other than possibly time interpolation. The data-models are currently not parallel but they are necessary when running with at least one full model (dead and full models can not be run together). The next step after the all-data model case is working will be to add



one or two full models at a time starting with the “G-case” which uses an active ocean and ice model but data land and atmosphere models. The final goal will be a fully coupled case

Once CCSM is working and scaling reasonably well on the BG/L system at ANL, we will perform enhanced scalability tests of the large LLNL BlueGene system. The purpose will be not only to better understand CCSM scaling to very large processor count, but also to understand the applicability of the BG/L architecture to a broader set of algorithms.

The next generation BlueGene system, BG/P, is expected to have increased performance over BG/L through a processor clock speedup of 20% and increased inter-node communication bandwidth. Each node will be 4-way SMP, rather than BG/L's 2-way nodes which have only limited ability for intra-node communication due to lack of cache coherency. While BG/P is expected to have approximately twice the memory per processor, compared to other massively parallel systems it remains low in its ratio of memory per processor owing to the basic design goal of balancing heat generation, package density, and clock rate. BG/P will offer the possibility of shared memory parallelism as well. We will attempt to run with hybrid parallelism provided the system support is there. We expect BG/P systems to be available near the end of this project and will port our BG/L-capable version of CCSM to this platform.

## **2.4 Consortium Arrangements**

### **2.4.1 Overall Management**

Patrick Worley is the principal investigator for the project, and will determine overall project direction and milestones. Arthur Mirin has primary responsibility for the investigation of CAM dycore scalability and CCSM configuration optimization. Raymond Loy has primary responsibility for the port of CCSM to the BG/L system. Worley has primary responsibility for CAM physics scalability and POP scalability analysis. All three researchers have prior experience working with each other, and we expect the collaboration to be close on all of these areas.

The SAP is motivated and guided by the needs of the SEESM project. Worley will discuss progress and goals at least monthly with the SEESM principal investigator John Drake (ORNL), and members of the SAP will confer with other members of SEESM as needed. In particular, Phil Jones (LANL) is the liaison between the SAP and SEESM for the ocean model, Phillip Cameron-Smith (LLNL) is the liaison between the SAP and SEESM for atmospheric chemistry, and Robert Jacob (ANL) is the liaison between the SAP and SEESM for the coupler and coupler-level interactions within the full CCSM.

Mirin and Worley are also members of SEESM, with responsibilities for the short term performance engineering needs of SEESM, as described in the SEESM proposal, and are well-positioned to determine scalability issues during future CCSM development within SEESM. Worley is the liaison between the SAP, SEESM, and the PERC center for enabling technology, Worley will provide guidance on the application of PERC technology to the CCSM, and provide knowledge of CCSM performance issues to PERC researchers. Finally, Worley is also a co-chair of the CCSM Software Engineering Work Group, which will enable the SAP to stay coordinated with the activities of other CCSM software engineering activities that impact CCSM performance and scalability.

## 2.4.2 Software Management and Software Engineering

The SAP contributions to the CCSM are via the SEESM project, and so utilize and depend on the same software management as SEESM. The follow description is from the SEESM proposal: *Mariana Vertenstein at NCAR manages access to the development team repository. Each component model is quality assured by a gatekeeper or change review board. Permission to commit changes to the development trunk is, however, a critical item for the rapid advancement of the model by researchers on this proposal. This permission was granted and exercised in SciDAC 1. The distribution outside this consortium of code under development is strictly prohibited, though researchers engaged with the CCSM Working groups have the ability to manage branches and perform simulations using the development code. Released code is publicly available and freely distributed.*

## 2.4.3 Project Plans and Milestones

The following represent project milestones by fiscal year. The lead institution for the given milestone is listed in parentheses. However in most cases, more than one institution will be contributing to the work.

### **FY06 (last 3 months)**

1. Work with SEESM to analyze current CAM performance on representative architectures. Quantify nature of scalability bottlenecks in terms of problem size, processor count, and computer system. (ORNL)
2. Characterize performance impact of additional tracers on CAM performance. (LLNL)
3. Port CAM/CLM to BG/L at ANL using NCAR port. Analyze performance and identify current bottlenecks. (ANL)

### **FY07**

1. Construct performance model of current CAM physics. (ORNL)
2. Work with SEESM to analyze load imbalances introduced by atmospheric chemistry. (ORNL)
3. Optimize physics load-balance in chemistry-dominated regime using static load balancing. (ORNL)
4. Work with SEESM to analyze performance of POP2 on Cray X1E, Cray XT3, and IBM p575 cluster. (ORNL)
5. Optimize CAM at large tracer count, including decomposition over tracers. (LLNL)
6. Optimize chemical mechanisms, including decomposition over vertical levels. (LLNL)
7. Eliminate global arrays and implement parallel I/O throughout CCSM components. (ANL)
8. Optimize CAM/CLM on BG/L. (ANL)
9. Port CICE to BG/L. (ANL)

### **FY08**

1. Update/generate POP2 performance model, compare with empirical performance characterization, and use to predict scalability. (ORNL)
2. Construct performance model of CAM physics with atmospheric chemistry. (ORNL)
3. Implement dynamic load-balance capability in chemistry-dominated regime. (ORNL)
4. Extend capability to vary process count over various phases of computation to include atmospheric chemistry and tracer advection. (LLNL)
5. Develop and implement ANN performance model for CAM and POP. (LLNL)

6. Port full CCSM to BG/L. (ANL)
7. Optimize CCSM on BG/L. (ANL)
8. Validate CCSM simulated climate on BG/L. (ANL)

#### **FY09 (first 9 months)**

1. Generate performance model for CAM, including support for varying processor count between different computational phases. Use model to predict scalability and optimal processor allocations. (ORNL)
2. Analyze and optimize DG dycore for cubed sphere grid, for both current
3. and high resolutions. (ORNL)
4. Analyze and optimize FV dycore for cubed sphere grid, for both current and high resolutions. (LLNL)
5. Develop and implement ANN performance model for full CCSM; Demonstrate CCSM configuration optimization using the model. (LLNL)
6. Update CCSM port to include new physics and new parallel algorithms. (ANL)
7. Port CCSM to BG/P. (ANL)
8. Determine optimal load balance and optimize communication performance of CCSM on BG/P. (ANL)
9. Perform extended scalability tests on LLNL BlueGene system. (LLNL)

#### **2.4.4 Other SciDAC Interactions**

As described throughout section 2.3 and again in section 2.4.1, this SAP expects to work closely with the SciDAC Center for Enabling Technology *Performance Engineering Research Center*. From PERC we expect guidance on performance tools and on performance analysis, optimization, and prediction techniques. In particular, PERC involvement will be important in the CCSM configuration optimization research. In turn, the SAP and SEESM will provide insight into the performance needs of CCSM, accelerating the development of PERC modeling and optimization technology. The SAP and performance engineering funded directly by SEESM will provide the necessary mechanism for PERC to be able to work with us.

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**U. S. Department of Energy**  
**Budget Page**  
(See reverse for Instructions)  
(Amounts in Thousands)

ORGANIZATION <b>OAK RIDGE NATIONAL LABORATORY</b>				Budget Page No: <u>    FY2006    </u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Patrick Worley</b>				Requested Duration: <u>    3    </u> (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Amounts in Whole Dollars
			CAL	ACAD	SUMR
					Funds Requested by Applicant
					Funds Granted by DOE
1.	<b>Patrick Worley</b>		1.0		10,165
2.					
3.					
4.					
5.					
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)				
7.	( 1 ) TOTAL SENIOR PERSONNEL (1-6)		1.0		10,165
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1.	( ) POST DOCTORAL ASSOCIATES				
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER (CRAFTS)				
TOTAL SALARIES AND WAGES (A+B)					10,165
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					3,558
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					13,722
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL			1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)		
			2. FOREIGN		
TOTAL TRAVEL					1,000
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER Division Organization Burden and Labor Burden					
TOTAL OTHER DIRECT COSTS					
H. TOTAL DIRECT COSTS (A THROUGH G)					
I. INDIRECT COSTS (SPECIFY RATE AND BASE) G&A 35.0%, Legacy Tax 4.8% Management Fee 2.90%					
TOTAL INDIRECT COSTS					
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					

**U. S. Department of Energy**  
**Budget Page**  
(See reverse for Instructions)  
(Amounts in Thousands)

ORGANIZATION <b>OAK RIDGE NATIONAL LABORATORY</b>			Budget Page No: <u>    FY2007    </u>		
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Patrick Worley</b>			Requested Duration: <u>    12    </u> (Months)		
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Amounts in Whole Dollars	
	CAL	ACAD	SUMR	Funds Requested by Applicant	Funds Granted by DOE
1. <b>Patrick Worley</b>	3.8			41,124	
2.					
3.					
4.					
5.					
6. (     ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. ( <b>1</b> ) TOTAL SENIOR PERSONNEL (1-6)	3.8			41,124	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (     ) POST DOCTORAL ASSOCIATES					
2. (     ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. (     ) GRADUATE STUDENTS					
4. (     ) UNDERGRADUATE STUDENTS					
5. (     ) SECRETARIAL - CLERICAL					
6. (     ) OTHER (CRAFTS)					
TOTAL SALARIES AND WAGES (A+B)				41,124	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				14,599	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				55,723	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL					
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL				3,000	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS (     ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER Division Organization Burden and Labor Burden					
TOTAL OTHER DIRECT COSTS				18,013	
TOTAL OTHER DIRECT COSTS				18,013	
H. TOTAL DIRECT COSTS (A THROUGH G)				76,737	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) G&A 34.0%, Legacy Tax 4.8% Management Fee 2.90%					
TOTAL INDIRECT COSTS				31,275	
TOTAL DIRECT AND INDIRECT COSTS (H+I)				108,012	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
TOTAL COST OF PROJECT (J+K)				108,012	

**U. S. Department of Energy  
Budget Page**  
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(Amounts in Thousands)

ORGANIZATION <b>OAK RIDGE NATIONAL LABORATORY</b>				Budget Page No: <u>    FY2008    </u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Patrick Worley</b>				Requested Duration: <u>    12    </u> (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Amounts in Whole Dollars
			CAL	ACAD	SUMR
					Funds Requested by Applicant
					Funds Granted by DOE
1.	<b>Patrick Worley</b>		3.6		40,771
2.					
3.					
4.					
5.					
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)				
7.	( 1 ) TOTAL SENIOR PERSONNEL (1-6)		3.6		40,771
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1.	( ) POST DOCTORAL ASSOCIATES				
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER (CRAFTS)				
TOTAL SALARIES AND WAGES (A+B)					40,771
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					14,678
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					55,449
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL			1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)		
			2. FOREIGN		
TOTAL TRAVEL					4,000
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER Division Organization Burden and Labor Burden					17,893
TOTAL OTHER DIRECT COSTS					17,893
H. TOTAL DIRECT COSTS (A THROUGH G)					77,342
I. INDIRECT COSTS (SPECIFY RATE AND BASE) G&A 35.0%, Legacy Tax 2.9% Management Fee 2.50%					
TOTAL INDIRECT COSTS					30,710
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					108,052
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					108,052



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(Amounts in Thousands)

ORGANIZATION <b>OAK RIDGE NATIONAL LABORATORY</b>				Budget Page No: <u>    </u> FY2009	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Patrick Worley</b>				Requested Duration: <u>    </u> 9 (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)		DOE Funded Person-mos.		Amounts in Whole Dollars	
				Funds Requested	Funds Granted
				by Applicant	by DOE
1.	<b>Patrick Worley</b>	3.5		<b>30,684</b>	
2.					
3.					
4.					
5.					
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)				
7.	( <b>3</b> ) TOTAL SENIOR PERSONNEL (1-6)	3.5		<b>30,684</b>	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1.	( ) POST DOCTORAL ASSOCIATES				
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER (CRAFTS)				
TOTAL SALARIES AND WAGES (A+B)				<b>30,684</b>	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				<b>11,046</b>	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				<b>41,731</b>	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL					
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL				<b>3,000</b>	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER Division Organization Burden and Labor Burden				<b>13,001</b>	
TOTAL OTHER DIRECT COSTS				<b>13,001</b>	
H. TOTAL DIRECT COSTS (A THROUGH G)				<b>57,731</b>	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) G&A 35.0%, Legacy Tax 2.9% Management Fee 2.50%					
TOTAL INDIRECT COSTS				<b>23,280</b>	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				<b>81,011</b>	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				<b>81,011</b>	

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Budget Page**  
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(Amounts in Thousands)

ORGANIZATION <b>OAK RIDGE NATIONAL LABORATORY</b>				Budget Page No: <u>YRS 1 - 3</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Patrick Worley</b>				Requested Duration: <u>36</u> (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Amounts in Whole Dollars
			CAL	ACAD	SUMR
					Funds Requested by Applicant
					Funds Granted by DOE
1.	<b>Patrick Worley</b>		11.9		122,744
2.					
3.					
4.					
5.					
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)				
7.	( 1 ) TOTAL SENIOR PERSONNEL (1-6)		11.9		122,744
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1.	( ) POST DOCTORAL ASSOCIATES				
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER (CRAFTS)				
TOTAL SALARIES AND WAGES (A+B)					122,744
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					43,881
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					166,625
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL			1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)		
			2. FOREIGN		
TOTAL TRAVEL					11,000
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER Division Organization Burden and Labor Burden					53,340
TOTAL OTHER DIRECT COSTS					53,340
H. TOTAL DIRECT COSTS (A THROUGH G)					230,965
I. INDIRECT COSTS (SPECIFY RATE AND BASE) G&A 35.0%, Legacy Tax 2.9% Management Fee 2.50%					
TOTAL INDIRECT COSTS					93,117
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					324,082
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					324,082

## ORNL Budget Explanation

### Budget Pages

Cost estimates presented in the "budget pages" of this proposal have been reclassified in order to be comparable to proposals submitted by other research institutions. At the Oak Ridge National Laboratory (ORNL), costs are collected and reported in accordance with approved Department of Energy (DOE) accounting guidelines. Although costs have been reclassified in this proposal, integrity has been maintained in total and between direct versus indirect costs.

### A. (1-7) Senior Personnel

The ORNL's cost accounting system utilizes wage pools based upon salary ranges. For purposes of this budget, the wage pool cost estimate is divided by the fringe benefits rate. The labor component is being reported in Item A and the fringe component is being reported in Item C.

The list of senior personnel participating in this project is as follows:

Patrick Worley is the Principal Investigator (PI) for the project. He will oversee the activities at ORNL, at Lawrence Livermore National Laboratory, and at Argonne National Laboratory, and will consult with the Science Application PI John Drake on project direction and results. Worley has primary responsibility for the work on CAM physics scalability and on POP scalability.

### C. Fringe Benefits

Fringe Benefits for ORNL employees are estimated to be 35.1% of labor costs for FY 2006, 35.5% for FY2007 and 36% for FY2008 and out years.

### D. Permanent Equipment

None

### E. (1-2) Travel

Worley will travel to meet with other members of the collaboration once in FY06, three times in FY07, four times in FY08, and three times in FY09. Estimated cost per domestic travel is \$1000 and includes plane fare, housing, meals, registration, and other allowable costs under government per diem rules.

### G.6 Other - Organization Burden Administration

Use of cost collection centers in ORNL R&D divisions is the approved method for collection and distribution of organization burden costs. These accounts are established to collect costs associated with an R&D division. The types of costs which can be charged to organization burden cost collection centers are unfunded paid hours; division administration; and general materials/service costs, including, but not limited to telecommunications, space, utilities, word processing, and copying which are not directly attributable or chargeable to R&D projects. Division Administration costs include: (i) managerial, technical, and administrative oversight; and (ii) support personnel such as facilities and operations, environmental, safety, and health, finance and budget, quality, and health physics provided for the general benefit of a division.

For ORNL staff, the labor and fringe components have been estimated and reported in items A - C. For Post-BS subcontractors, the subcontract costs have been reported in Item B.1. For ORNL staff and Post-BS subcontractors, the organization burden component has been estimated and is being reported in Item G.6.

Inclusion of these costs is necessary to provide a full accounting of estimated cost for the project period. All cost will be collected and reported in ORNL's cost accounting system.

### **I. Indirect Costs**

Full General & Administrative (G&A), Legacy Charge, and Management Fee are assessed on ORNL labor costs (Items A, C, and G.6), Materials and Supplies, and Equipment less than \$35,000 unit value. Full G&A is estimated to be 35.0% for FY2006, 34.0% for FY2007 and 36.50% for FY2008, with an estimated 3% increase each year after that for additional fiscal years. Legacy Charge is estimated to be 4.8% for each year. Management Fee is estimated to be 2.9% for FY2006, 3.2% for FY2007 and 3.5% for FY20081% each year.

Non-DOE-contractor subcontract costs are assessed Subcontract G&A and Management Fee. Subcontract G&A is estimated to be 1.1% each year. Management Fee is estimated to be 2.9% for FY2006, 3.2% for FY2007 and 3.5% for FY20081% each year.

Travel costs are assessed Travel G&A and Management Fee. Travel G&A is estimated to be 7.0% each year. Management Fee is estimated to be 2.9% for FY2006, 3.2% for FY2007 and 3.5% for FY20081% each year.

**Cover Page**

**Title of Proposed Project:**

Performance Engineering for the Next Generation  
Community Climate System Model  
FWP # 57648

**Office of Science Program Announcement Title/#:**

Lab 06-04  
Scientific Discovery through Advanced Computing

**Name of Laboratory:**

Argonne National Laboratory

**Principal Investigator(s):**

Raymond M. Loy, Senior Software Developer  
Argonne National Laboratory  
Mathematics and Computer Science Division  
9700 So. Cass Avenue - Bld.221  
Argonne, IL 60439  
(T) 630-252-7205 (Fax) 630-252-6104  
[rloy@mcs.anl.gov](mailto:rloy@mcs.anl.gov)

**Official signing for Laboratory:**

Rick L. Stevens, Associate Laboratory Director-PBCS  
Argonne National Laboratory  
Mathematics and Computer Science Division  
9700 So. Cass Avenue - Bld.221  
Argonne, IL 60439  
(T) 630-252-3378, ( Fax) 630-252-6333  
[stevens@mcs.anl.gov](mailto:stevens@mcs.anl.gov)

**Requested funding for Argonne National Laboratory  
for Proposed Project:**

Year 1	\$	224,000
Year 2	\$	224,000
Year 3	\$	224,000
Total:	\$	<u>672,000</u>

**Duration of Entire Project Period:**

07/01/2006 to 06/30/2009

**Use of human subjects in proposed project:**

No

**Use of vertebrate animals in proposed project:**

No

**Signature of PI, Date of Signature:**

PI's electronic signature on file

March 6, 2006

**Signature of Official, Date of Signature:**



March 6, 2006

**U.S. Department of Energy**  
**Budget Page**  
(See reverse for Instructions)

ORGANIZATION <b>The University of Chicago, Operator of Argonne National Laboratory</b>				Budget Page No: <u>pg 1 of 4</u> Yr 1 of 3		
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Raymond M. Loy</b>				Requested Duration: <u>12</u> (Months) FWP # 57648		
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)		DOE Funded Person-mos.		Funds Requested	Funds Granted	
		CAL	ACAD	SUMR		
					by Applicant	by DOE
1.	Raymond M. Loy, PI	9.00			\$159,119	
2.						
3.						
4.						
5.						
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7.	( 1 ) TOTAL SENIOR PERSONNEL (1-6)	9.00			\$159,119	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)						
1.	( ) POST DOCTORAL ASSOCIATES					
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3.	( ) GRADUATE STUDENTS					
4.	( ) UNDERGRADUATE STUDENTS					
5.	( ) SECRETARIAL - CLERICAL					
6.	( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)					\$159,119	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)						
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$159,119	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)						
TOTAL PERMANENT EQUIPMENT						
E. TRAVEL		1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)			\$2,800	
		2. FOREIGN				
TOTAL TRAVEL					\$2,800	
F. TRAINEE/PARTICIPANT COSTS						
1. STIPENDS (Itemize levels, types + totals on budget justification page)						
2. TUITION & FEES						
3. TRAINEE TRAVEL						
4. OTHER (fully explain on justification page)						
TOTAL PARTICIPANTS ( ) TOTAL COST						
G. OTHER DIRECT COSTS						
1. MATERIALS AND SUPPLIES					\$2,981	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION						
3. CONSULTANT SERVICES						
4. COMPUTER (ADPE) SERVICES						
5. SUBCONTRACTS						
6. OTHER						
TOTAL OTHER DIRECT COSTS					\$2,981	
H. TOTAL DIRECT COSTS (A THROUGH G)					\$164,900	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)						
Section H. Direct cost X Aggregate rate of: 35.840%						
TOTAL INDIRECT COSTS					\$59,100	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$224,000	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES						
L. TOTAL COST OF PROJECT (J+K)					\$224,000	

**U.S. Department of Energy**  
**Budget Page**  
(See reverse for Instructions)

ORGANIZATION <b>The University of Chicago, Operator of Argonne National Laboratory</b>				Budget Page No: <u>2 of 4</u> Yr. 2 of 3	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Raymond M. Loy</b>				Requested Duration: <u>12</u> (Months) FWP # 57648	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested
			CAL	ACAD	SUMR
					by Applicant
					by DOE
1. Raymond M. Loy, PI			8.80		
2.					
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. ( 1 ) TOTAL SENIOR PERSONNEL (1-6)			8.80		\$164,322
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)					\$164,322
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$164,322
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL			1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)		
			2. FOREIGN		
TOTAL TRAVEL					
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					\$578
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS					\$578
H. TOTAL DIRECT COSTS (A THROUGH G)					\$164,900
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
Section H. Direct cost X Aggregate rate of: 35.840%					
TOTAL INDIRECT COSTS					\$59,100
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$224,000
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					\$224,000

**U.S. Department of Energy**  
**Budget Page**  
(See reverse for Instructions)

ORGANIZATION <b>The University of Chicago, Operator of Argonne National Laboratory</b>				Budget Page No: <u>3 of 4</u> Yr 3 of 3	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Raymond M. Loy</b>				Requested Duration: <u>12</u> (Months) FWP # 57648	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested
			CAL	ACAD	SUMR
					by Applicant
					by DOE
1. Raymond M. Loy, PI			8.50		
2.					
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. ( 1 ) TOTAL SENIOR PERSONNEL (1-6)			8.50		\$164,530
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)					\$164,530
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$164,530
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL			1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)		
			2. FOREIGN		
TOTAL TRAVEL					
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					\$370
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS					\$370
H. TOTAL DIRECT COSTS (A THROUGH G)					\$164,900
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
Section H. Direct cost X Aggregate rate of: 35.840%					
TOTAL INDIRECT COSTS					\$59,100
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$224,000
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					\$224,000



## U.S. Department of Energy

## Budget Page

(See reverse for Instructions)

ORGANIZATION The University of Chicago, Operator of Argonne National Laboratory				Budget Page No: <u>4 of 4</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Raymond M. Loy				3-Yr. ANL Total Project Requested Duration: <u>36</u> (Months) FWP # 57648	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)			DOE Funded Person-mos.		Funds Requested
			CAL	ACAD	SUMR
					by Applicant
					by DOE
1. Raymond M. Loy, PI			26.30		
2.					
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. ( 1 ) TOTAL SENIOR PERSONNEL (1-6)			26.30		\$487,971
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)					\$487,971
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					\$487,971
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL			1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)		\$2,800
			2. FOREIGN		
TOTAL TRAVEL					\$2,800
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					\$3,928
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS					\$3,928
H. TOTAL DIRECT COSTS (A THROUGH G)					\$494,700
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS					\$177,300
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)					\$672,000
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)					\$672,000

**Lab 06-04: Scientific Discovery through Advanced Computing**  
**Performance Engineering for the Next Generation**  
**Community Climate System Model**

**Raymond M. Loy, PI**

**FWP # 57648**

**Budget Explanation**

**A-C Salaries and Fringe Benefits**

Argonne National Laboratory is a government-owned facility operated by the University of Chicago. As a contractor for the Department of Energy, Argonne National Laboratory must comply with DOE general policies and procedures on budgeting and accounting. The Laboratory's costing procedures are based on the assumption that all costs incurred will be recovered. The costing procedures use standard rates, which are used throughout the Laboratory on a consistent basis and uniformly applied to all work supported by the Department of Energy and other federal agencies.

Standard rates are established at the beginning of the fiscal year for each research division, and are monitored and revised as necessary. All labor costs are distributed using standard rates which are developed by the laboratory's budget office for each major payroll classification within the lab. The division-wide rates are based on pay bands ( salary ranges ) and fringe benefits (35.2% for a regular staff and clerical, and 11% for post/pre doctoral appointees), plus a factor for divisional overhead and for paid absences. Graduate and undergraduate students costs include housing allowance and fringe benefits( 7.65%). Effort is escalated each year by a rate provided by the Argonne Budget Department.

The principal investigator for this proposal is:

Raymond M. Loy

The PI's effort charged per year to this proposal is :

9.00 man-months

**E Travel**

Domestic: \$1.4 K per trip/escalate 4.5% per yr.

Foreign: \$2.6 K per trip/escalate 4.5% per yr.

**G Other Direct Costs**

1. Materials and Supplies:

Hardware/software maintenance, software, low-end computers (<\$5k), computer and misc.supplies.

2. Publication Costs:

Books/literature, subscriptions, publishing costs related to research.

**I Indirect Costs**

Standard rates are also developed for Laboratory General and Administrative (G&A) expense. The procedures for distributing Laboratory G&A and program expense is applied on the basis of the total cost of the work performed. The following indirect rates are provisional and have been estimated for each fiscal year budget period:

PBCS Program Expenses @ 3.7%

Laboratory G&A:

Common Support @ 27.3%

Service Centers @ 21.3%

Equipment/Subcontracts@ 8.1%

G&A Burden @ 2.9%

Argonne' s indirect rates are continuously reviewed and audited by

Cognizant Federal Agency:

Martin Straka

630-252-7724

Department of Energy-Chicago Operations Office



# Face Page

**TITLE OF PROPOSED RESEARCH:**

Performance Engineering for the Next Generation Community Climate System Model

**1. CATALOG OF FEDERAL DOMESTIC ASSISTANCE #**

81.049

**2. CONGRESSIONAL DISTRICT:**

Applicant Organization's District: 10th

Project Site's District: 10th

**3A. I.R.S. ENTITY IDENTIFICATION OR SSN:**

95-6031193

**3B. DUNS Number:**

**4. AREA OF RESEARCH OR ANNOUNCEMENT TITLE/#:**

SciDAC 2 Lab 06 04

**5. HAS THIS RESEARCH PROPOSAL BEEN SUBMITTED TO ANY OTHER FEDERAL AGENCY?**

YES  NO

PLEASE LIST \_\_\_\_\_

**6. DOE/OER PROGRAM STAFF CONTACT (if known):**

Anil Deane (301) 903-1465

**7. TYPE OF APPLICATION:**

- New  Renewal  
 Continuation  Revision  
 Supplement

**8. ORGANIZATION TYPE:**

- Local Govt.  State Govt.  
 Non-Profit  Hospital  
 Indian Tribal Govt.  Individual  
 Other  Inst. of Higher Educ.  
 For-Profit  Disadvan. Business  
 Small Business  Women-Owned  8(a)

**9. CURRENT DOE AWARD # (IF APPLICABLE):**

**10. WILL THIS RESEARCH INVOLVE:**

- 10A. Human Subjects  No  If yes  
Exemption No. \_\_\_\_\_ or  
IRB Approval Date \_\_\_\_\_  
Assurance of Compliance No: \_\_\_\_\_  
10B. Vertebrate Animals  No  If yes  
IACUC Approval Date \_\_\_\_\_ or  
Animal Welfare Assurance No: \_\_\_\_\_

**11. AMOUNT REQUESTED FROM DOE FOR ENTIRE PROJECT PERIOD \$** 504,000.00

**12. DURATION OF ENTIRE PROJECT PERIOD:**

07/01/06 to 06/30/09  
MM/DD/YY MM/DD/YY

**13. REQUESTED AWARD START DATE**

07/01/06  
MM/DD/YY

**14. IS APPLICANT DELINQUENT ON ANY FEDERAL DEBT?**

Yes (attach an explanation)  No

**15. PRINCIPAL INVESTIGATOR/PROGRAM DIRECTOR**

NAME Arthur Mirin

TITLE Principal Investigator

ADDRESS 7000 East Avenue, L-561  
Livermore, CA 94550

PHONE NUMBER (925) 422-4020

**SIGNATURE OF PRINCIPAL INVESTIGATOR/ PROGRAM DIRECTOR**

(please type in full name if electronically submitted)

Date \_\_\_\_\_

PI/PD ASSURANCE: I agree to accept responsibility for the scientific conduct of the project and to provide the required progress reports if an award is made as a result of this submission. Willful provision of false information is a criminal offense. (U.S. Code, Title 18, Section 1001).

**16. ORGANIZATION'S NAME** Regents of the University of California

ADDRESS Lawrence Livermore National Laboratory  
7000 East Avenue  
Livermore, CA 94550

**CERTIFYING REPRESENTATIVE'S**

NAME Dona L. Crawford

TITLE Computation, Associate Director

PHONE NUMBER (925) 422-1985

**SIGNATURE OF ORGANIZATION'S CERTIFYING REPRESENTATIVE**  
(please type in full name if electronically submitted)

Date \_\_\_\_\_

CERTIFICATION and ACCEPTANCE: I certify that the statements herein are true and complete to the best of my knowledge, and accept the obligation to comply with DOE terms and conditions if an award is made as the result of this submission. A willfully false certification is a criminal offense. (U.S. Code, Title 18, Section 1001).

**NOTICE FOR HANDLING PROPOSALS**

This submission is to be used only for DOE evaluation purposes and this notice shall be affixed to any reproduction or abstract thereof. All Government and non-Government personnel handling this submission shall exercise extreme care to ensure that the information contained herein is not duplicated, used, or disclosed in whole or in part for any purpose other than evaluation without written permission except that if an award is made based on this submission, the terms of the award shall control disclosure and use. This notice does not limit the Government's right to use information contained in the submission if it is obtainable from another source without restriction. This is a Government notice, and shall not itself be construed to impose any liability upon the Government or Government personnel for any disclosure or use of data contained in this submission.

**PRIVACY ACT STATEMENT**

If applicable, you are requested, in accordance with 5 U.S.C., Sec. 562A, to voluntarily provide your Social Security Number (SSN). However, you will not be denied any right, benefit, or privilege provided by law because of a refusal to disclose your SSN. We request your SSN to aid in accurate identification, referral and review of applications for research/training support for efficient management of Office of Science grant/contract programs.

DOE F 4620.1

(04-93)

All Other Editions Are Obsolete

U.S. Department of Energy
Budget Page
(See reverse for Instructions)

OMB Control No.

1910-1400

OMB Burden Disclosure
Statement on Reverse

Year 1

Table with columns for Organization (Lawrence Livermore National Laboratory), Principal Investigator (Art Mirin), and various budget categories (A-L) including Personnel, Salaries, Fringe Benefits, Travel, and Direct Costs. Includes sub-columns for DOE Funded (CAL, ACAD, SUMR) and Funds Requested/Granted.

DOE F 4620.1

(04-93)

All Other Editions Are Obsolete

**U.S. Department of Energy  
Budget Page**  
(See reverse for Instructions)

OMB Control No.

1910-1400

OMB Burden Disclosure  
Statement on Reverse

Year 2

ORGANIZATION <b>Lawrence Livermore National Laboratory</b>				Budget Page No: <u>2</u>	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR <b>Art Mirin</b>				Requested Duration: <u>12</u> (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)				Year 2	
	DOE Funded Person-mos.			Funds Requested	Funds Granted
	CAL	ACAD	SUMR	by Applicant	by DOE
1.	4.32			\$53,324	
2.					
3.					
4.					
5.					
6.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE) TSM 110-119				
7.	4.32			\$53,324	
B. ( ) OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1.	( ) POST DOCTORAL ASSOCIATES				
2.	( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( ) GRADUATE STUDENTS				
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL - CLERICAL				
6.	( ) OTHER				
TOTAL SALARIES AND WAGES (A+B)				\$53,324	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				\$22,663	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				\$75,987	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL				\$1,500	
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL				\$1,500	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				\$500	
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES				\$900	
5. SUBCONTRACTS					
6. OTHER				\$7,342	
TOTAL OTHER DIRECT COSTS				\$8,742	
H. TOTAL DIRECT COSTS (A THROUGH G)				\$86,229	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS				\$81,787	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				\$168,016	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				\$168,016	

DOE F 4620.1

(04-93)

All Other Editions Are Obsolete

U.S. Department of Energy
Budget Page
(See reverse for Instructions)

OMB Control No.

1910-1400

OMB Burden Disclosure
Statement on Reverse

Year 3

Table with columns for Organization (Lawrence Livermore National Laboratory), Principal Investigator (Art Mirin), and various budget categories (A-L) including Personnel, Fringe Benefits, Travel, and Direct/Indirect Costs. Includes sub-tables for DOE Funded Person-mos. and Funds Requested/Granted.

DOE F 4620.1

(04-93)

All Other Editions Are Obsolete

U.S. Department of Energy
Budget Page
(See reverse for Instructions)

OMB Control No.

1910-1400

OMB Burden Disclosure
Statement on Reverse

Years 1 - 3

Table with columns for Organization (Lawrence Livermore National Laboratory), Principal Investigator (Art Mirin), and various budget categories (A-L) including Personnel, Salaries, Fringe Benefits, Travel, and Direct/Indirect Costs. Total project cost is \$504,006.

**Performance Engineering for the Next Generation Community  
Climate System Model  
Budget Justification**

**A. Senior Personnel**

The PI, Arthur A. Mirin, will analyze and optimize performance of the next generation Community Climate System Model. The work will include performance modeling using both analytic and artificial neural network approaches, scaling to thousands of processors, and extending to the chemistry-dominated regime, alternative meshes, and high resolution.

**B. Other Personnel**

Bronis deSupinski will act as a PERC liaison at no cost, particularly vis-a-vis the artificial neural network approach.

**C. Fringe Benefits**

The Laboratory's Payroll Burden Rate is 42.5% and is applied to the non-leave standard salary of all Laboratory employees, including overtime. PostDocs are charged a 35% Payroll Burden, and students are charged 9.5%.

**D. Equipment**

None planned.

**E. Travel**

The anticipated travel is 1-2 trips per year for one person to interact with other researchers doing related work. Travel cost is estimated at \$4,500.

**F. Trainee/Participant Costs**

N/A.

**G. Other Costs**

- 2.) Publication costs for technical review and release of publishing project results is anticipated at \$1,500.
- 4) Computer services, as needed on the project, are estimated at \$2,700.
- 6.) Office space is estimated at \$22,056.

**H. Total Direct Costs**

\$258,685

**I. Indirect Costs**

Total Indirect Costs are estimated at \$245,321. LLNL rate amounts and their definitions are explained in Attachment A. Note that rates are applied in a specified order and not all taxes apply to each direct cost.



## Attachment A

### Lawrence Livermore National Laboratory Current FY2006 Rates

Indirect Cost Pool	Rate (%)	Allocation Base/Rate Determination
<u>Organization Personnel Charge (OPC):</u> Computation - Associate Director's Office	19.09%	Distribution of specific Organization's personnel management costs to users of the Organization Personnel Charge accounts. The rates vary by the Organization providing the service.
<u>Program Management Charge (PMC):</u> Computation - Associate Director's Office	4.50%	A distribution of costs associated with managing and administering direct funded Programs within a Directorate. PMC is allocated on a value-added cost input base to Direct Operating, LDRD, Capital Equipment,
Computation - Program	8.10%	
<u>General &amp; Administrative (G&amp;A):</u>	31.50%	G&A is allocated on a value-added base, which is total operating costs less direct materials, subcontracts, and the Electricity Recharge. Supplemental Labor is included included in the base. G&A is applied to Direct Operating, Capital Equipment and Construction accounts.
<u>Strategic Mission Support (SMS):</u>	7.00%	SMS costs include institutional strategic planning, institutional capabilities, outreach, and special employees. Applied to direct operating, WFO, and capital equipment accounts using a value-added base.
<u>Institutional General Purpose Equipment (IGPE):</u>	0.80%	The IGPE allocation is for capital equipment of a general use or institutional nature that benefits multiple cost objectives and is required for general-purpose site-wide needs. It is allocated on a total-cost base, and is not applied to DOE major items of equipment, general plant projects, line item construction or Work for Others - DOE.
<u>Institutional General Plant Projects</u>	0.65%	The IGPP allocation is for new construction projects that cost less than \$5M and are of a general institutional nature benefiting multiple cost objectives and required for general-purpose site-wide needs.
<u>Laboratory Directed Research &amp; Development (LDRD):</u> Operating Calculation - An assessment applied to Laboratory operating costs to support exploratory research and development.	6.38%	Rate is applied against total capital equipment (excluding line items) and operating costs, excluding Federal Administrative Charge.



## Earth System Grid

February 27, 2006

To: John Drake and Philip Jones

From: Dean N. Williams  
Mail Stop: L-103  
Lawrence Livermore National Laboratory  
7000 East Ave., P.O. Box 808  
Livermore, CA 94550

Re: Intent of the Scaling the Earth System Grid to Petascale Data Center for Enabling Technologies to collaborate with A Scalable and Extensible Earth System Model for Climate Change Science

---

Dear John and Philip:

I am writing to confirm that my project, entitled “Scaling the Earth System Grid to Petascale Data” intends to collaborate with the proposed SciDAC project “A Scalable and Extensible Earth System Model for Climate Change Science”.

As you know, our project is focused on establishing a Center for Enabling Technologies that will enable broad community access to, and deep analysis of, simulated and experimental data from a distributed network on a petabyte scale. We believe that the technology developed in our project will play an important role in the success of your project. In particular, we are interested in supplying your project with the needed coverage of petabyte-scale synchronized federated metadata and data access, integration of a full-suite of server-side analysis, model/observation integration, embedded desktop productivity tools, and user support and life cycle maintenance. We feel these components and others not listed above will help you reach your scientific application goal “to determine the range of possible climate changes of the 21<sup>st</sup> century and beyond through simulations ...”. We also feel that the technology developed under our CET will greatly benefit other DOE SciDAC applications areas as well.

I look forward to a productive collaboration, with you as the primary point of contact.

Sincerely,

Dean N. Williams  
Principal Investigator for Scaling the Earth System Grid to Petascale Data  
Software Project Leader, Program for Climate Model Diagnosis and Intercomparison



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**Sandia Corporation**

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**Patricia Crossno**  
**Senior Member of the Technical Staff**  
**Data Analysis and Visualization**

February 27, 2006

John B. Drake, Group Leader  
Climate Dynamics  
Computer Science and Mathematics  
Oak Ridge National Laboratory  
Oak Ridge, Tennessee

John:

I wish to confirm that our project, "Abstract Visual Metaphors for Science" intends to partner with the proposed SciDAC Science Application: A Scalable and Extensible Earth System Model for Climate Change Science.

Our project focuses on the development of informational visualization techniques which will provide new ways to address the challenge of comparing data from multiple simulations. We believe that partnering with the Earth System Model for Climate Change Science will be of significant benefit to our project. We are particularly interested in developing new visual techniques for climate researchers for the analysis of differences, similarities and more abstract statistical relationships between multiple simulations and observations.

Sincerely,

Patricia Crossno

# ARGONNE NATIONAL LABORATORY

Mathematics and Computer Science Division

9700 South Cass Avenue, Argonne, Illinois 60439



Telephone: 630-252-6018

Fax: 630-252-5986

E-mail: [fischer@mcs.anl.gov](mailto:fischer@mcs.anl.gov)

John B. Drake, Group Leader  
Climate Dynamics  
Computer Science and Mathematics  
Oak Ridge National Laboratory  
Oak Ridge, Tennessee

February 27, 2006

Dear John,

I wish to confirm that our project, A High-Order Library of Methods for Engineering and Science (HOLMES), intends to partner with the proposed SciDAC Science Application: A Scalable and Extensible Earth System Model for Climate Change Science.

HOLMES will build libraries and conduct algorithm research for high order element based methods. NCAR's HOMME model will be one of our core applications. Our partnership with the Earth System Model for Climate Change Science will ensure our work on locally conservative high order methods and tracer advection schemes is directly beneficial to your work on atmospheric dynamical cores.

Sincerely,

A handwritten signature in black ink that reads 'Paul F. Fischer'.

Paul F. Fischer

# ARGONNE NATIONAL LABORATORY

MATHEMATICS AND COMPUTER SCIENCE DIVISION  
9700 SOUTH CASS AVENUE, ARGONNE, ILLINOIS 60439-4844

TELEPHONE 630-252-1556  
FAX: 630-252-5986  
EMAIL: PAPKA@MCS.ANL.GOV

March 2, 2006

John B. Drake  
Oak Ridge National Laboratory  
One Bethel Valley Rd.  
POB 2008, MS 6016  
Oak Ridge, TN 37831-6016

Dear John:

As the lead PI of the proposed SciDAC *Center for Enabling Technology for Distance and Collaborative Visualization* I am writing to express our project's intent to collaborate with the proposed SciDAC Science Application on *A Scalable and Extensible Earth System Model for Climate Change Science*.

Our Center proposes to improve SC simulation and experimental science by providing the ability to visualize and analyze datasets located at distant sites. We also plan to improve SC large application team collaboration by supporting group interaction on the most important part of the scientific workflow; understand the results. We know that for your project, scientists, simulation and observational results are located at Los Alamos, Lawrence Livermore, Lawrence Berkeley, Oak Ridge, Pacific Northwest and Argonne National Labs as well as the National Center for Atmospheric Research. We look forward to a productive collaboration with your project including receiving input on your distance and collaborative visualization requirements and your evaluation of our software as you use it for your work.

Sincerely,



Michael E. Papka  
Research Manager Futures Laboratory  
Argonne National Laboratory



**ICLUT**

February 24, 2006

**Jack Dongarra**

**University Distinguished Professor  
Innovative Computing Laboratory**  
Computer Science Department  
The University of Tennessee  
dongarra@cs.utk.edu

Dr. John Drake  
Oak Ridge National Laboratory  
P.O. Box 2008  
Oak Ridge, TN 37831

Dear John,

After reviewing the outline for your SciDAC proposal on A scalable and extensible earth system model for climate change science, and comparing your ambitious plan with the goals and strategies of the "Institute for the Support of the SciDAC Software Ecosystems" (ISSSE) that we are proposing, it is clear to me that the efforts are complimentary and that we should work together when these efforts are funded. The large software infrastructure for SciDAC with which your work must engage involves a complex web of interdependent software elements, which is changing more or less constantly in response to the demands of the people, organizations, and new technologies that animate it. We believe that, through the work of ISSSE, we can help facilitate the development, dissemination, maintenance, and overall stewardship of the critical software of this SciDAC computing "ecosystem," and thereby accelerate progress and enable sustainable gains in research productivity for you and your community. At the same time, the feedback and creative ideas generated by collaborating with your project on the difficult software lifecycle issues that ISSSE will address will help deepen our understanding and substantially improve the support that ISSSE can offer to the entire SciDAC community. In addition we can participate and each others outreach and workshop efforts.

Consequently, we strongly endorse your effort. We are convinced that our two projects will reinforce one another in ways that are not only mutually beneficial, but which also have a powerful impact on SciDAC research program wide.

Best wishes,

Jack Dongarra  
University Distinguished Professor



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(512) 471-3312 • FAX (512) 471-8694

February 28, 2006

Dr. John Drake  
Oak Ridge National Laboratory  
One Bethel Valley Rd.  
POB 2008, MS 6016  
Oak Ridge, TN 37831-6016

Dear John,

I am very pleased to offer this letter of intent to collaborate with the *Scalable and Extensible Earth System Model for Climate Change Science project* that you are leading. Modeling climate change is a problem of great complexity but also of great importance. Uncertainties arise in the parameterizations used in the various physical submodels, and optimization offers the prospect of reducing the uncertainties by estimating values of these parameters that are most consistent with observations. However, optimization of large, complex, multiphysics, multiscale problems such as coupled atmosphere-land-sea-ice models is a challenge of the highest order, and requires advances in optimization algorithms and software.

As you know, our proposed *SciDAC Institute for Optimization of Petascale Simulations (SciOPS)* aims to catalyze a transformation from simulation to simulation-based optimization. This entails the creation of a suite of optimization methods and associated software components that are tailored to the structure of terascale and petascale simulations. Our focus is on optimization of complex nonlinear multiphysics simulations in the context of design, control, and inverse problems.

I foresee a fruitful and exciting collaboration that will not only make progress on a challenging scientific problem, but also serve as a blueprint for parameter estimation and data assimilation projects in other areas. Moreover, the complexities of climate modeling will help to drive and stress research in optimization algorithms and software. Rob Jacob's expertise in both climate modeling as well as parameter estimation will help serve as a natural bridge between the two centers.

In conclusion, SciOPS enthusiastically supports the efforts of the SEESMCCS and looks forward to close cooperation and collaboration over the coming years.

Sincerely,

A handwritten signature in black ink, appearing to read "Omar Ghattas", written over a horizontal line.

Omar Ghattas

John A. and Katherine G. Jackson Chair in Computational Geosciences  
Director, Center for Computational Geosciences and Optimization  
Institute for Computational Engineering and Sciences  
Prof. of Geological Sciences, Mechanical Engineering, Biomedical Engineering, and Computer Sciences  
Research Professor, Institute for Geophysics