ASCR Update

August 11, 2009

Michael Strayer

Associate Director, Advanced Scientific Computing Research

Staffing
Research Division

Walt Polansky, Acting Division Director

Applied Mathematics Team
Base Math, Multi scale Math, and SciDAC Math Institutes and Centers

Sandy Landsberg, Karen Pao
Steven Lee (Detailee),
Bill Spotz (IPA)

Computer Science Team
Base Computer Science, Data and Visualization, and SciDAC Computer Science Centers and Institutes

Dan Hitchcock, Lucy Nowell
Osni Marques (Detailee)

Computational Partnerships Team
Partnerships with other SC offices

Lali Chatterjee, Bill Spotz
Christine Chalk, Osni Marques (Detailee)

Next Generation Networking Team
Network Research and Collaboratories

Thomas Ndousse-Fetter
Susan Turnbull (Detailee from GSA)

Education Program Team

Barb Helland, Christine Chalk, George Seweryniak

Staffing
Facilities Division

Vince Dattoria, Acting Division Director

Facilities Team

Responsible for NERSC, Leadership Computing Facilities and ESnet; project management

Yukiko Sekine (NERSC)
Dan Hitchcock (OLCF)
Barbara Helland (ALCF)
Vince Dattoria (ESnet)
Robert Lindsay

Staffing
Small Business Division

SBIR Team

Responsible for administering Small Business Innovative Research (SBIR) program for DOE

Larry James
Carl Hebron
Chris O'Gwin
Dave Goodwin (on Detail from ASCR)

New Positions

to be posted

- Research Program Managers
  - Computer Science
  - Computer Science
  - Physical Scientist/SciDAC – SC programs
  - Physical Scientist/SciDAC – Applied programs

- Facilities Program Manager
  - Leadership Computing

ASCR Budget Details

	FY 2009 Appropriation	FY 2010 Request	Change from FY09 to FY 10
Advanced Scientific Computing Research			
Applied Mathematics	40,164	44,850	4,686
Computer Science	33,618	46,800	13,182
Computational Partnerships (includes SciDAC)	52,064	53,235	1,171
Next Generation Networking for Science	14,321	14,321	0
SBIR/STTR	4,038	4,586	548
Total, Mathematical, Computational, and Computer Sciences Research	***144,205***	***163,792***	***+19,587***
High Performance Production Computing (NERSC)	54,790	55,000	210
Leadership Computing Facilities	115,000	130,000	15,000
Research and Evaluation Prototypes	23,900	23,900	0
High Performance Network Facilities and Testbeds (ESnet)	25,000	29,862	4,862
SBIR/STTR	5,925	6,446	521
High Performance Computing and Network Facilities	***224,615***	***245,208***	***+20,593***
Total, Advanced Scientific Computing Research	**368,820**	**409,000**	**+40,180**

President's FY2010 Budget Request
Highlights

- Applied Math
  - Cyber Security research moved from Next Generation Networking
  - Proposed new fellowship program in Applied Math and High performance computer science
- Computer Science
  - New effort in Advanced Computer Architecture design for science
  - Bridges efforts in advanced computer architecture design with ongoing efforts in computer science and applied mathematics to address needs of DOE science applications
- Computational Partnerships
  - Support for interdisciplinary teams focused on transforming critical DOE applications for extreme scale computing
- Facilities
  - Increases support lease payments and site preparation at ANL for proposed upgrade
  - ESnet will begin to deliver 100-400 Gbps to SC laboratories

ADVANCED SCIENTIFIC COMPUTING RESEARCH

The Committee recommendation is $409,000,000, the same as the request and $40,180,000 above the fiscal year 2009 appropriation excluding emergency appropriations, for Advanced Scientific Computing Research.

Senate Energy and Water Development Appropriations Report

Advanced Scientific Computing Research

The Committee recommends $399,000,000 for Advanced Scientific Computing Research. The Committee expects the Office of Science to continue to support joint research with the NNSA laboratories through the Institute for Advanced Architecture and Advanced Algorithms. Within available funds, $5,000,000 shall be provided to collaborate in a joint program to enhance the production of unconventional fossil energy using advanced simulation and visualization

Solicitations Just Closed:
Base Math Programs

- Mathematics for Analysis of Petascale Data: $4M/year
  - 81 proposals from universities & national labs, closed May 29
  - Mathematical challenges in extracting insights from “petascale” datasets
  - Topic areas include anomaly detection, machine learning, streaming data, dimensionality reduction, visualization
  - Proposals described wide variety of university, lab projects and collaborations
  - 11 awards made: 50% funds to labs, 50% funds to universities
- Mathematics for Complex, Distributed, Interconnected Systems: $3.5M/year
  - 38 proposals, all DOE national lab-led projects, closed June 12
  - Emphasis on interconnected systems operating within purview of DOE: computer networks, electric power grid, critical infrastructures
  - Lab-based projects: foundation for engaging university researchers in 2010
  - Anticipate 5-7 awards: 100% funds to labs (w/ some university subcontracts)

Solicitations Just Closed:
Joint Math/CS Institute

- Solicitation
  - Sought "*applications for research under a unified management structure to address key challenges where collaborative research in applied mathematics and computer science efforts are required to bridge the gap between large complex scientific applications software and next-generation hardware*"
  - Closed June 5, 2009
- $4M/year available
- 29 applications received
  - 25 were reviewed in a combination of panel and mail reviews;
  - 4 were deemed out of scope.
- Three awards have been made so far
  - Two laboratory-led
  - One university-led

Solicitations Just Closed:
Ice Sheet Modeling

- Joint ASCAC-BERAC Report in March 2008 identified the need to
  - include fully dynamic ice sheet models and ocean/ice shelf interactions
  - assess the rate and magnitude of sea level rise due to rapid ice sheet melting as a high priority for climate models.
- Solicitation
  - Sought "*computational science/applied mathematics/computer science research to accelerate scientific and computational breakthroughs to improve Ice Sheet Modeling*
  - Complements DOE SC SciDAC, ASCR and BER funded research
  - Closed May 26, 2009
- $3M/year available for three years
- Eight proposals received & reviewed
- Six Projects awarded late June, 2009
  - Two University -led
  - Four Laboratory-led

Awards
R&D 100s

Three ASCR funded projects win R&D 100s

PETSc, a suite of data structures and routines for solving PDEs.
Funded by TOPS SciDAC project and ASCR Base Math

ROSE, a compiler infrastructure.
Funded by ASCR Computer Science program.

Catamount N-Way (CNW) lightweight kernel, operating system.
Supported by ASCR built on work funded by NNSA-ASC program.

Awards

PECASE winners

Cecilia Aragon, staff scientist at LBNL, received the PECASE for her groundbreaking research in data-intensive scientific workflow management, and pioneering development of innovative methods for visualization, analysis, and organization of massive scientific data sets. She is funded by ASCR.

Alexandre Tartakovsky, computational mathematician at PNNL, received the PECASE for his research on subsurface flow that addresses past and future energy needs: cleaning up buried nuclear or toxic contaminants and storing carbon dioxide from fossil fuels underground. He is also supported by the BER program.

Oliver Fringer, assistant professor of civil and environmental engineering at Stanford University, received a PECASE. Dr. Fringer was a fellow in the ASCR Computational Science Graduate Fellowship (CSGF) program from 1997-2001.

SIAM Fellows

A Cadre of Game Changers

Of the 191 SIAM Fellows in Class of 2009:

- Over 40 have been or are currently funded by ASCR

Currently Funded SIAM Fellows

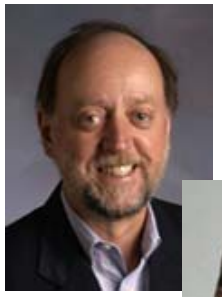
John B. Bell	LBNL
Marsha J. Berger	Courant
Russel E. Caflisch	UCLA
Alexandre J. Chorin	UC Berkeley
Phillip Colella	LBNL
Howard C. Elman	U. MD College Park
James W. Demmel	UC Berkeley
Jack J. Dongarra	UT Knoxville
C. William Gear	NEC Research
James G. Glimm	SUNY Stony Brook
Leslie F. Greengard	Courant
John Guckenheimer	Cornell
James M. Hyman	LANL
Thomas Yizhao Hou	Caltech
Christopher R. Johnson	U Utah
Sven Leyffer	ANL
Thomas A. Manteuffel	CU Boulder
Jorge J. More	ANL
J. Tinsley Oden	UT Austin
Dianne P. O'Leary	U MD College Park
Michael L. Overton	Courant
Linda R Petzold	UCSB
James A. Sethian	UC Berkeley
Michael J. Shelley	Courant
Chi-Wang Shu	Brown
Margaret H. Wright	Courant
Mary F. Wheeler	UT Austin

Some of ASCR SIAM Fellows and Their Citations

For contributions to scientific computing and visualization.

For contributions to finite difference methods, numerical methods, adaptive mesh refinement, and interface tracking.

For contributions to numerical ordinary differential equations and differential-algebraic equations and computational science.

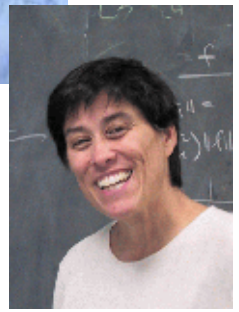


For contributions to numerical linear algebra, including EISPACK, LINPACK, and LAPACK, and high-performance computing.

For contributions to iterative methods for linear systems and numerical methods for partial differential equations.

For contributions to conservation laws, scattering theory, integrable systems, and numerical analysis.

For contributions to the numerical solution of partial differential equations and modeling of biological systems.



For the development of adaptive algorithms and software for partial differential equations

For contributions to computational fluid dynamics

For contributions to the numerical solution of partial differential equations, especially level set methods.

For contributions to numerical optimization and service to the profession.

For advances in algorithms and software for continuous optimization.

ASCR Accomplishments Review
Applied Mathematics

Chair: David Keyes	Columbia
David L. Brown	LLNL
Phillip Colella	LBNL
Donald Estep	Colorado State
Paul Fischer	ANL
Omar Ghattas	U. Of Texas
Leslie Greengard	Courant Institute
Bruce Hendrickson	SNL
Michael Holst	U. of California, San Diego
Sallie Keller-McNulty	Rice
Randall Leveque	U. of Washington
Tom Manteuffel	U. of Colorado
Dianne O'Leary	U. of Maryland
Linda Petzold	U. of California Santa Barbara
James Sethian	U. of California, Berkeley
Margaret Wright	Courant Institute

ASCR Accomplishments Review
Computer Science

Chair: Kathy Yelick,	LBNL and U. California, Berkeley
Arie Shoshani	LBNL,
Barton Miller	U. of Wisconsin
Garth Gibson	Carnegie Mellon University
Ian Foster	ANL and U. of Chicago
Jack Dongarra	ORNL and U. of Tennessee
Jeffrey Vetter	ORNL and Georgia Tech
Leonid Oliker	LBNL
Mary Hall	U. of Utah
Michael Heroux	SNL
Pete Beckman	ANL
Rusty Lusk,	ANL
Wes Bethel	LBNL
Rob Ross	ANL
Brian Tierney	LBNL

ASCR Accomplishments Review
Computational Science

	Area of Expertise
Chair: Tony Mezzacappa, ORNL	Astrophysics
Jackie Chen, SNL	Combustion, Energy Science
Giulia Galli, U. of California Davis	Materials Science
Jim Hack, ORNL	Climate Science
Doug Kothe, ORNL	CFD
Paul Messina, ANL	Applied Mathematics, Computer Science
Juan Meza, LBL	Applied Mathematics
Chris Mundy, PNL	Chemistry
Claudio Rebbi, Boston University	Nuclear Physics
Nagiza Samatova, North Carolina State	Biology
Panagiotis Spentzouris, Fermilab	Accelerators
Bill Tang, PPPL	Fusion

Facilities Update

- NERSC
  - Quad core upgrade to Franklin accepted June 17, 2009
  - NERSC-6 contract awarded to Cray for at least 1 petaflop Cray XT5
- LCFs Next Generation
  - Mission needed approved January, 2009: "
    - "The upgrade of the Leadership Computing Facilities to tens of petaflops by the 2011-2013 timeframe is vital to the U.S. playing a leading role in several important international programs including: climate science (International Panel on Climate Change), fusion energy research (ITER) and the Nuclear Energy Advanced Modeling and Simulation (NEAMS) program"
  - Follow-on Lehman Reviews held
    - OLCF -- July 7-8, 2009
    - ALCF -- July 28-29, 2009
- OLCF Operational Assessment Review
  - August 25, 2009
  - Vicky White, Chair

American Recovery and Reinvestment Act (Recovery Act)

- Recovery Act ground rules
  - Shovel ready,
  - Enhancing research infrastructure and supporting high-priority R&D, and
  - No out year mortgages
- Recovery Act Process within DOE
  - ASCR identified several potential projects
  - SC reviewed SC-Programs list and developed SC-wide list.
  - SC priority list reviewed by Secretary Chu to develop Department of Energy proposal to OMB
- ASCR's Recovery Act Projects
  - Advanced Networking Initiative
  - Leadership Computing Facility Upgrades
  - Advanced Computer Architectures
  - Magellan
  - SciDAC-e

Workshop calendar
Exascale

- Previous workshops
  - BER/Climate Workshop: Challenges in Climate Change Science and the Role of Computing at the Extreme Scale, 11/08
  - HEP/High Energy Physics Workshop: Scientific Challenges for Understanding the Quantum Universe and the Role of Computing at the Extreme Scale, 12/08
  - NP/Nuclear Physics Workshop: Forefront Questions in Nuclear Science and the Role of High Performance Computing, 2/09
  - FES/Fusion Workshop: Extreme Scale Computing Challenges in Fusion Science, 3/09
  - NE/Nuclear Energy Workshop: Extreme Scale Computing Challenges in Nuclear Energy, 5/09
- Upcoming workshops
  - BES/Materials Workshop: Extreme Scale Computing Challenges in Materials Science, August 12-14, 2009 in Washington DC
  - BER/Biology Workshop: Extreme Scale Computing Challenges in Biology, August 17-19, 2009 in Chicago
  - NNSA/ASCR Workshop: Science Grand Challenges, October, 6-7, 2009, in Washington DC

NNSA-ASCR Exascale Partnership

- Executive Oversight Committee
  - ASCR: Michael Strayer, Barbara Helland (POC), Dan Hitchcock, Paul Messina (Consultant)
  - NNSA: Bob Meisner, Thuc Hoang, Atinuke Ogunde (POC), Sander Lee, Fred Johnson (Consultant)

- Steering Committee
  - ANL: Rick Stevens (co-Chair), Pete Beckman
  - LANL: Andy White (co-Chair), John Morrison
  - LBNL: Horst Simon, Kathy Yelick
  - LLNL: Michel McCoy, Mark Seeger
  - ORNL: Thomas Zacharia, Jeff Nichols
  - SNL: James Peery, Sudip Dosanjh
  - BNL: James Davenport
  - PNNL: Steve Ashby
  - Ex officio: Paul Messina, Fred Johnson

U.S. DEPARTMENT OF ENERGY

Steering Committee
Initial Tasks

- Develop the science case for the Exascale Initiative. The science case should focus on the Department's energy, environmental, security and societal grand challenges that will require exascale computing to solve and whenever possible, address the need for early starts or the consequences/risks of delays.

  Deliverables for task 1:

  a) High-level slide presentation by August 28, 2009

  b) Report with initial analysis of representative Science applications by November, 2009

- Develop a high level roadmap for the Exascale Initiative. Each entry in the roadmap should identify start dates, approximate duration and high level dependencies. In addition characterize each task as either: going to happen by itself; needs engineering or development effort; or needs new insight or knowledge.

  Deliverables for task 2:

  a) High-level slide presentation by September 25, 2009

  b) Final roadmap with full characterizations by December 4, 2009