FISCAL YEAR 2005 MULTISCALE MATHEMATICS RESEARCH AWARDS
DEPARTMENT OF ENERGY OFFICE OF SCIENCE
ADVANCED SCIENTIFIC COMPUTING RESEARCH PROGRAM

SOME MULTISCALE MATHEMATICS FUNDING STATISTICS

Numbers

Number of Projects Funded	13
Number of Institutions Funded	28
Number of Universities Funded	17
Number of Labs Funded	11
Total Three-Year Funding	$20,607,242
Number of Senior Researchers Supported	65
Number of Post Docs Supported	11
Number of Grad Students Supported	33
Number of Undergraduates Supported	5

Universities Funded

Colorado State University	Fort Collins, CO
Columbia University	New York City, NY
Florida Atlantic University	Boca Raton, FL
Florida State University	Tallahassee, FL
George Mason University	Fairfax, VA
Georgia Institute of Technology	Atlanta, GA
Oregon State University	Corvallis, OR
Rensselaer Polytechnic Institute	Troy, NY
University of California, Los Angeles	Los Angeles, CA
University of California, San Diego	San Diego, CA
University of California, Santa Barbara	Santa Barbara, CA
University of Delaware	Newark, DE
University of Minnesota	Minneapolis, MN
University of New Mexico	Albuquerque, NM
University of Texas at Austin	Austin, TX
University of Wisconsin	Madison, WI
Washington State University	Pullman, WA

Labs Funded	Awards
• Ames Laboratory	1
• Argonne National Laboratory	1
• Sandia National Laboratories	2
• Lawrence Livermore National Laboratory	1
• Los Alamos National Laboratory	2
• Oak Ridge National Laboratory	1
• Pacific Northwest National Laboratory	2
• Princeton Plasma Physics Laboratory	1

Award to Team led by:
Georgia Institute of Technology
Konstantin Mischaikow, Principal Investigator
With Research Partners:
George Mason University
Thomas Wanner, Principal Investigator
Florida Atlantic University
William Kalies, Principal Investigator
$1.13 million over 3 years
Multiscale Analysis of Nonlinear Systems Using Computational Topology

Complicated patterns that change subtly or dramatically with time can be found throughout the applied sciences. Because of the high dimensionality associated with these patterns, quantitatively capturing the essential geometric structures is a difficult task. This project will use computational homology as a tool for the quantification, identification, analysis, and classification of complicated time-dependent geometric patterns.

Award to:
Oregon State University
Ralph Showalter, Principal Investigator
$647 thousand over 3 years
Modeling, Analysis and Simulation of Multiscale Preferential Flow

Preferential flow occurs in natural porous media such as soils and aquifers due to the presence of unusually large connected pores or fast flow channels in which fluids flow at velocities much larger than the filtration velocities in the surrounding porous material. For some time it has been standard to use a two-scale approach to relate lab scale numerical models to field scale numerical models. This project will develop methods to blend scale separations so as to describe flow processes at intermediate scales and address the consequences of preferential flow patterns. This research will be of benefit to many DOE groundwater remediation programs.

Award to Team led by:
University of California, Los Angeles
Russel Caflisch, Principal Investigator
With Research Partner:
Lawrence Livermore National Laboratory
Andris Dimits, Principal Investigator
$1.8 million over 3 years
Multiscale Mathematics for Plasma Kinetics

Plasmas, sometimes referred to as the 4^{th} state of matter, are ubiquitous in nature. This research will provide a major step forward in enabling the solution of a class of multiple timescale kinetic plasma calculations that will directly impact physics problems of great interest in many plasma physics research areas. Researchers in the Department of Energy's ongoing research efforts in magnetic and inertial fusion will be particularly interested because multiple time- and space-scale, collisional kinetic plasma phenomena are important research challenges

Award to:
University of Delaware
Dionisios Vlachos, Principal Investigator
Multiscale Modeling of Spatially Distributed Biological Systems
$1.1 million over 3 years

Most biological systems exhibit a vast disparity of length and time scales. Biological systems are different from most traditional chemical systems due to the large spatial heterogeneity. Even at the single living cell level inherently complex regulatory reaction networks are needed to describe fundamental processes. These issues point to the fact that multiscale, stochastic, spatially distributed type simulation is a necessity for understanding and predicting the behavior of biological systems. One goal of this project is to develop hybrid multiscale methods to allow simulations ranging from intracellular processes to entire populations of cells. Included is a comprehensive, multi-institutional educational and training program.

Award to Team led by:
University of Minnesota
Mitchell Luskin, Principal Investigator
With Research Partners:
University of California, San Diego
Michael Holst, Principal Investigator
Pacific Northwest National Laboratory
Eric Bylaska, Principal Investigator
Multiscale Design of Advanced Materials based on Hybrid Ab-Initio and Quasicontinuum Methods
$2.3 million over 3 years

This project unites experts from mathematics, chemistry, computer science, and engineering for the development of new multiscale methods for the design of materials. The project focuses on three families of materials that are of central interest to the mission of the DOE: (1) interfacial catalysts, (2) metal organic framework (MOF) materials for hydrogen storage and (3) fusion materials. Two unifying themes of this highly interdisciplinary project are: (1) utilize modern mathematical ideas about change-of-scale and state-of-the-art numerical analysis to develop computational methods and codes to solve real multiscale problems of DOE interest and (2) acknowledge the need for quantum mechanics-based atomistic forces. This approach leads to a very forward-looking integration of chemistry and numerical analysis in the area of multiscale methods.

Award to
University of Texas, Austin
J. Tinsley Oden, Principal Investigator
Adaptive Multi-Scale Modeling Based on Goal Oriented Error Estimation and Control
$1.2 million over 3 years

The goal of this project is to develop methodologies applicable to very broad classes of multi-scale phenomena. To focus the work it will primarily be concerned with applications in the design of materials, or nano-fabrication, particularly the quantum/molecular dynamics/continuum interfaces in the study of both crystalline structures in metals and in polymerized materials such as those in use in semi-conductors– chip fabrication, lithography, and areas related to nano-scale manufacturing. The project will develop adaptive modeling algorithms to control error in multi-scale models.

Award to Team led by:
Washington State University
Alexander Panchenko, Principal Investigator
With Research Partner:
Pacific Northwest National Laboratory
Rogene Eichler West, Principal Investigator
Northwest Consortium for Multiscale Mathematics and Applications Educational Strategies and Critical Problems in Thermo-mechanics of Materials
$2.6 million over 3 years

Traditional mathematical education of engineers is focused on practical, one-scale models of engineering problems. These are usually continuum models: solid mechanics, fluid mechanics and heat transfer. Such models served the applied mathematics community well for decades. However, as the industrial focus shifted from traditional engineering problems – first to micro-scale problems and, recently to nano-technology, the inadequacy of the traditional continuum models and analysis tools is brought to light. The goal of this project is to bring the full power of multiscale mathematics into engineering and scientific research and graduate education, using a combination of curriculum reform and well-targeted research activities.

Award to:
Argonne National Laboratory
Hans Kaper, Principal Investigator
A Multiscale Approach to Self-Organization of Microtubules
$1.0 million over 3 years

How do random mixtures of molecular components organize themselves into large-scale cellular structures? Can we model this process mathematically, can we simulate it computationally, and what can we learn about the process of self-organization? This project addresses these questions by studying a system of microtubules and molecular motors. The project is motivated by a central problem of science—the emergence of large-scale coherent structures. It has significant computational complexity, and the proposed approach is fundamental for a broad range of problems relevant to the mission of the Office of Science.

Award to Team led by:
Los Alamos National Laboratory
Alan Graham, Principal Investigator

With Research Partners:
University of California, Santa Barbara
L. Gary Leal, Principal Investigator
University of New Mexico
Marc Ingber, Principal Investigator
Sandia National Laboratories
Lisa Mondy, Principal Investigator
Localized Scale Coupling and New Educational Paradigms in Multiscale Mathematics and Science
$2.4 million over 3 years

The main objective of the proposed research is to develop a robust numerical simulation capability for suspension flows that incorporates effects spanning diverse time and length scales. Linking recent progress in molecular and nanoscale science to progress in the ability to accurately model suspension flows at the macroscale is an important challenge for several energy-related technologies. The numerical investigation will be based on a novel multiscale approach that seamlessly couples micro/nanoscale and mesoscale simulations using an "equivalent force" approach and couples mesoscale and macroscale simulations using a sub structuring approach.

Award to Team led by:
Los Alamos National Laboratory
Susan Kurien, Principal Investigator
With Research Partner:
University of Wisconsin, Madison
Zhengyu Liu, Principal Investigator
Multi-Scale Coupling in Ocean and Climate Modeling
$846 thousand over 3 years

High-resolution simulations of planetary-scale, rotating flows using the Primitive Equations can now resolve the Rossby deformation radius, the scale at which the baroclinic instability converts available potential energy to kinetic energy, thereby creating eddies. As it becomes possible to increase resolution beyond the Rossby deformation radius, more intermediate-scale and small-scale dynamics will contribute to mathematical simulations. This project addresses mathematical modeling issues that are fundamental for atmosphere and ocean modeling, and ultimately for climate modeling as well. Specifically, it addresses interscale coupling between fast, small-scale inertial-gravity waves and slow, large-scale coherent motions such as the jet stream and large-scale cyclones. The project provides a unique opportunity for PhD students to acquire mathematical and practical knowledge necessary to develop the next generation of ocean and climate models.

Award to Team led by:
Oak Ridge National Laboratory
Sreekanth Pannala, Principal Investigator
With Research Partner:
Ames Laboratory
Rodney Fox, Principal Investigator

Micro-Mesoscopic Modeling of Heterogeneous Chemically Reacting Flows (MMM-HCRF) Over Catalytic/Solid Surfaces
$1.6 million over 3 years

The goal of this project is to develop a multiscale framework for coupling two methods that will enable accurate modeling of heterogeneous reacting flows over catalytic surfaces. The methods to be coupled are the mesoscale Lattice Boltzmann Method, which is suitable for modeling multiphase reacting flows with low Mach numbers, and the microscale Kinetic Monte Carlo method for modeling of chemical reactions on the catalytic surfaces. This multiscale framework will be demonstrated for a heterogeneous chemically reacting flow over a flat plate, a basic building-block for many reacting systems which is of utmost interest to various applications in combustion, catalysis, biology, material production, emissions control.

Award to Team led by:
Princeton Plasma Physics Laboratory
Wei-li Lee, Principal Investigator
With Research Partner:
Columbia University
Mark Adams, Principal Investigator
Multiscale Gyrokinetic Particle Simulation of Magnetized Plasmas
$1.7 million over 3 years

A suite of multi-resolution numerical algorithms for particle-in-cell (PIC) codes will be developed to solve the gyrokinetic equations for studying magnetized plasmas. These multi-spatio-temporal algorithms will be able to handle high frequency short wavelength oscillations of ion cyclotron waves and the low frequency large-scale MHD modes as well as all range of mesoscale physics with intermediate frequencies. It will have wide applications in fusion, space and astronomical physics and will provide training for graduate students and postdocs who are interested in computational plasma physics.

Award to Team led by:
Sandia National Laboratories
Richard Lehoucq, Principal Investigator
With Research Partners:
Colorado State University
Donald Estep, Principal Investigator
Florida State University
Max Gunzburger, Principal Investigator
Rensselaer Polytechnic Institute
Jacob Fish, Principal Investigator
A Mathematical Analysis of Atomistic-to-Continuum (AtC) Multiscale Coupling Methods
$2.3 million over 3 years

Atomistic-to-Continuum (AtC) coupling has emerged as a critical component in computational materials science and other applications of interest to the DOE Office of Science. Past research in AtC model and algorithm development has been primarily driven by applications and has paid off in the formulation of effective procedures that address specific applications. This previous research has also begun to lead to some degree of generalization. . However, much less effort has been directed at the mathematical theory of AtC methods. This project will develop an operator based mathematical formalism that addresses and quantifies critical formulation issues such as well-posedness, stability, error estimation and the inherent uncertainty of the AtC coupling process.