Office of Science
Financial Assistance
Funding Opportunity Announcement
DE-PS02-08ER08-13

Multiscale Mathematics and Optimization for Complex Systems

The Office of Advanced Scientific Computing Research (ASCR) of the Office of Science (SC), U.S. Department of Energy (DOE), hereby announces its interest in receiving grant applications for research addressing multiscale mathematics and optimization for complex natural and engineered systems. Awards for this solicitation will be made in two categories:

1) Multiscale Mathematics for Complex Systems, and

2) Optimization of Complex Systems.

Areas of focus within these categories include the development of:

- Mathematical tools needed for the modeling, analysis, and simulation of multiscale phenomena, including those associated with complex multiphysics systems or hybrid discrete-continuum models.
- Techniques for formulating, analyzing and solving challenging optimization problems arising in complex natural and engineered systems.

Additional areas of interest in both categories include sensitivity analysis, risk analysis, and the quantification and mitigation of uncertainty.

More information on this solicitation is provided in the Supplementary Information below.

LETTER OF INTENT DUE DATE: March 3, 2008, 4:30 p.m., Eastern Time

A one-page Letter of Intent (LOI) to submit an application is **REQUIRED** and must be received by **March 3, 2008, 4:30 p.m., Eastern Time.** The Letter of Intent should be submitted by e-mail as a PDF file attachment to: complexsystems@ascr.doe.gov. Please use "Letter of Intent for Announcement DE-PS02-08ER08-13" in the subject line.

The purpose of the Letter of Intent (LOI) is to facilitate the planning of the peer review process and the selection of reviewers, including identifying any potential conflicts of interest. The one-page LOI must include the following information: the announcement number DE-PS02-08ER08-13; the category being addressed (Multiscale Mathematics or Optimization); name, institutional affiliation, and contact information for the Principal Investigator (PI); names and institutional affiliations of other PIs and senior personnel; projected funding request (if possible); title of the

proposed effort; and an abstract of the proposed research. For collaborations involving multiple institutions, a single Letter of Intent should be submitted by the PI of the lead institution. An example of the format for the one-page Letter of Intent can be viewed at: http://www.science.doe.gov/ascr/Research/08AMSolicit.html.

A response to the Letters of Intent encouraging or discouraging formal applications will be communicated to the applicants by March 17, 2008. **Formal applications will be accepted only from those encouraged to submit. No other formal applications will be considered.**

APPLICATION DUE DATE: April 28, 2008, 8 PM Eastern Time

Applications must be submitted using Grants.gov, the Funding Opportunity Announcement can be found using the CFDA Number, 81.049 or the Funding Opportunity Announcement number, DE-PS02-08ER08-13. Applicants must follow the instructions and use the forms provided on Grants.gov.

FOR FURTHER INFORMATION, CONTACT: Dr. Homer Walker, Applied Mathematics Program, Telephone: (301) 903-1465, Fax: (301) 903-7774, E-mail: walker@ascr.doe.gov.

SUPPLEMENTARY INFORMATION: In order to meet the needs of scientific discovery over the coming decades, the scientific and technical issues that DOE must address will require new, rigorously justified mathematical developments in predictive modeling, simulation, analysis and understanding of complex natural and engineered systems. The Applied Mathematics Program within the Office of Advanced Scientific Computing Research supports basic research on the mathematical methods and numerical algorithms that support these long-term needs.

This Notice solicits innovative basic research applications in multiscale mathematics and optimization for complex natural and engineered systems. Particularly innovative applications addressing other approaches for promoting multiscale mathematics or optimization research, including but not limited to workshops and conferences, will also be considered under this solicitation.

Prospective researchers should observe that:

- Collaborative applications involving multiple institutions, which may include universities, laboratories, and/or private institutions, are encouraged but not required.
- Proposed research activities should be relevant to the mission of the Department of Energy and, in particular, to the long-term goals of its research programs.
- No funds will be provided to Federal Laboratories and Federally Funded Research and Development Centers (FFRDCs), including the DOE National Laboratories, under this Notice. Laboratories should respond to the LAB 08-13 Announcement posted at: http://www.science.doe.gov/grants/grants.html.
- Researchers may request a period of performance of up to three (3) years.

For the purposes of this solicitation, a complex system is defined to be a natural or engineered system that is difficult to understand and analyze because of one or more of the following properties:

- The system may involve interactions among many phenomena over a wide range of scales.
- The system may have multiple components or subsystems with mathematically dissimilar structures.
- The system components may be connected in a variety of different ways, often nonlinearly. Furthermore, local and system-wide phenomena may depend on each other in complicated ways.
- The behavior of the overall system can be difficult to predict from the behavior of individual components. Moreover, the overall system behavior may evolve along qualitatively different pathways that may display great sensitivity to small perturbations at any stage.

Such systems are often described as "multicomponent systems," or as "multiphysics systems" if the components are based on physical, chemical and/or biological processes. The adjective "multiscale" is often used if the components involve multiple spatial or temporal scales.

Illustrative examples of complex systems for which new mathematical analysis, methodologies, and computational algorithms are needed include:

- Problems that involve a single physical system, which becomes complex when modeled using a multiscale approach. An example occurs in the composite design of materials when a hybrid discrete-continuum model is used to describe atomistic-macroscopic phenomena.
- Problems that involve the coupling of multiple physical processes described with different models. An example occurs in the modeling of carbon sequestration, where a quantitative study may require the simulation of multiple fluids, a solid phase, and a complex set of biogeochemical reactions over a wide range of scales.
- Problems that describe complex engineered systems. An example is the electric power grid, where models may involve inequality and other types of constraints, severe nonlinearities and discontinuities, a mixture of continuous and integer variables, a large number of variables, a huge range of scales, and non-unique solutions that may make it difficult to characterize the most physically reasonable result.

There are many other examples of complex systems of importance to DOE. For more information on multiscale mathematics and optimization research challenges for complex systems, see the four (4) reports from the DOE Workshops on Multiscale Mathematics and on Mathematical Research Challenges in Optimization of Complex Systems. These reports can be downloaded from: http://www.sc.doe.gov/ascr/Research/AM/ConferencesWorkshops.html.

The following topics exemplify but do not exhaustively list areas where advances in fundamental understanding are required:

1. Multiscale Mathematics for Complex Systems

Analytical and computational approaches are needed to understand and model the multiscale behavior of complex multiphysics and multicomponent phenomena. Also needed are theory and tools for the sensitivity analysis of complex multiscale, multicomponent models and for the quantification of uncertainty in model predictions.

Areas of interest include:

- Algorithmic techniques for simulating multiphysics and multiscale processes with quantifiable fidelity.
- Methodologies for representing fine-scale behavior in models for the system at larger scales and for the corresponding analytical tools and computational approaches needed to quantify the variability of the large-scale dynamics with respect to the fidelity of the finer-scale models.
- Analytical and computational tools for decomposing complex, multiphysics systems into their component processes and for elucidating the couplings among these component processes.
- The development and analysis of numerical methods for hybrid models that couple discrete and continuum processes.
- New mathematical tools and algorithmic approaches for modeling and simulating large stochastic systems, particularly spatially dependent systems, and efficient strategies for estimating the probabilities of rare events.
- Mathematical and computational frameworks and tools for sensitivity analysis, inverse sensitivity analysis, risk analysis, and model calibration for complex multiscale, multicomponent systems, including approaches that address high- dimensional parameter and data spaces or combine statistical and deterministic methodologies.
- Mathematical, statistical and hybrid approaches for treating uncertainty and error from multiple sources having multiple representations and for analyzing and quantifying the effects of uncertainty and error on model predictions, model calibration and data assimilation analysis.

2. Optimization of Complex Systems

Techniques are needed for formulating, analyzing and solving challenging optimization problems arising in complex natural and engineered systems.

Areas of interest include:

- Analysis and algorithms for optimization problems with mixed variable types, including continuous, discrete and categorical variables, and with non-smooth and/or non-traditional objective and constraint functions.
- Theory and algorithms for very large, structured optimization problems and for solving formulations of multilevel and multi-objective optimization problems that exhibit special structure.

- Analysis and algorithms for stochastic optimization, with emphasis on expanding the field to address nonlinearities, special structures, and nontraditional probability distributions.
- Statistical approaches, especially those that use a limited number of observed data for validating and improving mathematical models.
- Techniques for integrating models with data to support decision-making and adaptive control.
- Related methods for sensitivity analysis, risk analysis, and uncertainty assessment in complex systems.

Collaboration and Communication

The application should identify potential collaborations or other interactions that will facilitate the exchange of ideas and dissemination of information among research centers in industry, universities, and/or laboratories. Synergistic collaborations with researchers in Federally Funded Research and Development Centers (FFRDCs), including the DOE National Laboratories, are also encouraged, though no funds will be provided to these organizations under this Notice. Further information on preparation of collaborative applications may be accessed via the Internet at: http://www.science.doe.gov/grants/Colab.html.

Program Funding

It is anticipated that up to $5 million total will be available for multiple awards for this solicitation in Fiscal Year 2008. Proposers may request project support for up to three years. All awards are contingent on the availability of funds and programmatic needs. DOE is under no obligation to pay for any costs associated with the preparation or submission of a proposal. DOE reserves the right to fund, in whole or in part, any, all, or none of the applications submitted in response to this Notice.

Merit Review Criteria

Applications will be subjected to scientific merit review (peer review) and will be evaluated against the following evaluation criteria which are listed in descending order of importance codified at 10 CFR 605.10(d):

1. Scientific and/or Technical Merit of the Project;
2. Appropriateness of the Proposed Method or Approach;
3. Competency of Applicant's Personnel and Adequacy of Proposed Resources; and
4. Reasonableness and Appropriateness of the Proposed Budget.

The evaluation process will include program policy factors, such as the relevance of the proposed research to the terms of the soliciation and the agencies' programmatic needs. Note that external peer reviewers are selected with regard to both their scientific expertise and the absence of conflict-of-interest issues. Both Federal and non-Federal reviewers may be used, and submission of an application constitutes agreement that this is acceptable to the investigator(s) and the submitting institution.

Posted on the Office of Science Grants and Contracts Web Site
February 19, 2008.