

**Program Announcement  
To DOE National Laboratories  
LAB 08-13**

***Multiscale Mathematics and Optimization for Complex  
Systems***

**SUMMARY:** 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 proposals 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](mailto:complexsystems@ascr.doe.gov). Please use "Letter of Intent for Announcement LAB 08-13" in the subject line. A copy to your Laboratory's ASCR Point of Contact (POC) is also encouraged.

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 LAB 08-13; 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 and content 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 full proposals will be communicated to the applicants by March 17, 2008. **Formal proposals will be accepted only from those encouraged to submit.**

**DATES:** Full proposals submitted in response to this Announcement must be submitted using the **Office of Science Field Work Proposal Instructions** provided in the Notice to Users section on the ePMA home page: <http://epma.energy.gov>, and must be received no later than 8:00 p.m., Eastern Time, April 28, 2008, to be accepted for merit review and to permit timely consideration for award in Fiscal Year 2008.

Please see the "Addresses" section below for further instructions on the methods of submission for the full proposal.

**ADDRESSES:** A complete formal FWP in a single Portable Document Format (PDF) document that has 'formatted text and graphics' (also known as "native" PDF) must be submitted using the **Office of Science Field Work Proposal Instructions** provided in the Notice to Users section on the ePMA home page: <http://epma.energy.gov>. (This submission process includes sending the FWP via CD, with 2 hard copies, using Federal Express).

**Please send the CD and 2 hard copies via Federal Express to:**

Complex Systems  
c/o Dr. Homer Walker  
Applied Mathematics Program, SC-21.1  
Office of Advanced Scientific Computing Research  
Office of Science  
19901 Germantown Road  
Germantown, MD 20874-1290  
ATTN: Program Announcement LAB 08-13

In addition to following the submission instructions on the <http://epma.energy.gov> web site, please submit, via email, a single PDF file of the entire LAB proposal and FWP. This will assist in expediting the review process. Please send the email to: [complexsystems@ascr.doe.gov](mailto:complexsystems@ascr.doe.gov). Please include, "Program Announcement LAB 08-13" in the subject line of the email.

**FOR FURTHER INFORMATION/GENERAL INQUIRIES, CONTACT:**

Dr. Homer Walker  
Applied Mathematics Program  
Telephone: (301) 903-1465  
Email: [walker@ascr.doe.gov](mailto: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 Announcement solicits innovative basic research proposals in multiscale mathematics and optimization for complex natural and engineered systems. Particularly innovative proposals 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 proposals 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.
- 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 nonsmooth and/or nontraditional 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. Further information on preparation of collaborative proposals 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 will be available for new projects starting in Fiscal Year 2008. All awards are subject to the availability of appropriated funds and programmatic needs. Proposers may request project support for up to three years.

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 proposals submitted.

The instructions and format described below should be followed. You must reference Program Announcement LAB 08-13 on all submissions and inquiries about this program.

**OFFICE OF SCIENCE**  
**GUIDE FOR PREPARATION OF SCIENTIFIC/TECHNICAL PROPOSALS**  
**TO BE SUBMITTED BY NATIONAL LABORATORIES**

Proposals from National Laboratories submitted to the Office of Science (SC) as a result of this program announcement will follow the Department of Energy Field Work Proposal process with additional information requested to allow for scientific/technical merit review. The following guidelines for content and format are intended to facilitate an understanding of the requirements necessary for SC to conduct a merit review of a proposal. Please follow the guidelines carefully, as deviations could be cause for declination of a proposal without merit review.

### **1. Evaluation Criteria**

Proposals will be subjected to formal merit review (peer review) and will be evaluated against the following criteria which are listed in descending order of importance:

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 announcement and the agencies' programmatic needs.

### **2. Summary of Proposal Contents**

- Field Work Proposal (FWP) Format (Reference DOE Order 412.1A) (DOE ONLY)
- Proposal Cover Page
- Table of Contents
- Budget (DOE Form 4620.1) and Budget Explanation
- Abstract (one page)
- Narrative (main technical portion of the proposal, including background/introduction, proposed research and methods, timetable of activities, and responsibilities of key project personnel)
- Literature Cited
- Biographical Sketch(es)
- Description of Facilities and Resources
- Other Support of Investigator(s)
- Appendix (optional)

#### **2.1 Number of Copies to Submit**

A complete formal FWP in a single Portable Document Format (PDF) document that has 'formatted text and graphics' (also known as "native" PDF) must be submitted using the **Office of**

**Science Field Work Proposal Instructions** provided in the Notice to Users section on the ePMA home page: <http://epma.energy.gov>. (This submission process includes sending the FWP via CD, with 2 hard copies, using Federal Express).

**Please send the CD and 2 hard copies via Federal Express to:**

Complex Systems  
c/o Dr. Homer Walker  
Applied Mathematics Program, SC-21.1  
Office of Advanced Scientific Computing Research  
Office of Science  
19901 Germantown Road  
Germantown, MD 20874-1290  
ATTN: Program Announcement LAB 08-13

In addition to following the submission instructions on the <http://epma.energy.gov> web site, please submit, via email, a single PDF file of the entire LAB proposal and FWP. This will assist in expediting the review process. Please send the email to: [complexsystems@ascr.doe.gov](mailto:complexsystems@ascr.doe.gov). Please include, "Program Announcement LAB 08-13" in the subject line of the email.

### **3. Detailed Contents of the Proposal**

Adherence to type size and line spacing requirements is necessary for several reasons. No researcher should have the advantage, or by using small type, of providing more text in their proposals. Small type may also make it difficult for reviewers to read the proposal. Proposals must have 1-inch margins at the top, bottom, and on each side. Type sizes must be 11 point. Line spacing is at the discretion of the researcher but there must be no more than 6 lines per vertical inch of text. Pages should be standard 8 1/2" x 11" (or metric A4, i.e., 210 mm x 297 mm).

#### **3.1 Field Work Proposal Format (Reference DOE Order 412.1A)**

The Field Work Proposal (FWP) is to be prepared and submitted consistent with policies of the investigator's laboratory and the local DOE Operations Office. Additional information is also requested to allow for scientific/technical merit review. Laboratories may submit proposals directly to the SC Program office listed above. A copy should also be provided to the appropriate DOE operations office.

#### **3.2 Proposal Cover Page**

The following proposal cover page information may be placed on plain paper. No form is required.

Title of proposed project  
SC Program announcement title  
Name of laboratory  
Name of principal investigator (PI)

Position title of PI  
Mailing address of PI  
Telephone of PI  
Fax number of PI  
Electronic mail address of PI  
Name of official signing for laboratory\*  
Title of official  
Fax number of official  
Telephone of official  
Electronic mail address of official  
Requested funding for each year; total request

Use of human subjects in proposed project:

If activities involving human subjects are not planned at any time during the proposed project period, state "No"; otherwise state "Yes", provide the IRB Approval date and Assurance of Compliance Number and include all necessary information with the proposal should human subjects be involved.

Use of vertebrate animals in proposed project:

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

Signature of PI, date of signature

Signature of official, date of signature\*

\*The signature certifies that personnel and facilities are available as stated in the proposal, if the project is funded.

### **3.3 Table of Contents**

Provide the initial page number for each of the sections of the proposal. Number pages consecutively at the bottom of each page throughout the proposal. Start each major section at the top of a new page. Do not use unnumbered pages and do not use suffices, such as 5a, 5b.

### **3.4 Budget and Budget Explanation**

A detailed budget is required for each fiscal year. It is preferred that DOE's budget page, Form 4620.1 be used for providing budget information\*. Modifications of categories are permissible to comply with institutional practices, for example with regard to overhead costs.

A written justification of each budget item is to follow the budget pages. For personnel this should take the form of a one-sentence statement of the role of the person in the project. Provide a detailed justification of the need for each item of permanent equipment. Explain each of the other direct costs in sufficient detail for reviewers to be able to judge the appropriateness of the amount requested.

Further instructions regarding the budget are given in section 4 of this guide.

\* Form 4620.1 is available at web site: <http://www.science.doe.gov/grants/budgetform.pdf>

### **3.5 Abstract**

Provide an abstract of less than 400 words. Give the project objectives (in broad scientific terms), the approach to be used, and what the research is intended to accomplish. State the hypotheses to be tested (if any). At the top of the abstract give the project title, names of all the investigators and their institutions, and contact information for the principal investigator, including e-mail address.

**3.6 Narrative** (main technical portion of the proposal, including background/introduction, proposed research and methods, timetable of activities, and responsibilities of key project personnel).

The narrative comprises the research plan for the project and is **limited to 15 pages** (maximum). It should contain enough background material in the Introduction, including review of the relevant literature, to demonstrate sufficient knowledge of the state of the science. The major part of the narrative should be devoted to a description and justification of the proposed project, including details of the methods to be used. It should also include a timeline for the major activities of the proposed project, and should indicate which project personnel will be responsible for which activities.

If any portion of the project is to be done in collaboration with another institution (or institutions), provide information on the institution(s) and what part of the project it will carry out. Further information on any such arrangements is to be given in the sections "Budget and Budget Explanation," "Biographical Sketches," and "Description of Facilities and Resources."

### **3.7 Biographical Sketches**

This information is required for senior personnel at the institution submitting the proposal and at all subcontracting institutions (if any). The biographical sketch is limited to a maximum of **two pages** for each investigator.

To assist in the identification of potential conflicts of interest or bias in the selection of reviewers, the following information **must be provided in each biographical sketch**.

**Collaborators and Co-editors:** A list of all persons in alphabetical order (including their current organizational affiliations) who are currently, or who have been, collaborators or co-authors with the investigator on a research project, book or book article, report, abstract, or paper during the 48 months preceding the submission of the proposal. Also include those individuals who are currently or have been co-editors of a special issue of a journal, compendium, or conference proceedings during the 24 months preceding the submission of the proposal. If there are no collaborators or co-editors to report, this should be so indicated.

**Graduate and Postdoctoral Advisors and Advisees:** A list of the names of the individual's own graduate advisor(s) and principal postdoctoral sponsor(s), and their current organizational affiliations. A list of the names of the individual's graduate students and postdoctoral associates during the past five years, and their current organizational affiliations.

### **3.8 Description of Facilities and Resources**

Facilities to be used for the conduct of the proposed research should be briefly described. Indicate the pertinent capabilities of the institution, including support facilities (such as machine shops), that will be used during the project. List the most important equipment items already available for the project and their pertinent capabilities. Include this information for each subcontracting institution (if any).

### **3.9 Statement of all Current and Pending Support**

Other support is defined as all financial resources, whether Federal, non-Federal, commercial, or institutional, available in direct support of an individual's research endeavors. Information on active and pending other support is required for all senior personnel, including investigators at collaborating institutions to be funded by a subcontract. For each item of other support, give the organization or agency, inclusive dates of the project or proposed project, annual funding, and level of effort (months per year or percentage of the year) devoted to the project.

### **3.10 Appendix (optional)**

Information not easily accessible to a reviewer may be included in an appendix. Reviewers are not required to consider information in an appendix, and reviewers may not have time to read extensive appendix materials with the same care they would use with the proposal proper. The appendix may contain the following items: up to five publications, manuscripts accepted for publication, abstracts, patents, or other printed materials directly relevant to this project, but not generally available to the scientific community; and letters from investigators at other institutions stating their agreement to participate in the project (do not include letters of endorsement of the project).

## **4. Detailed Instructions for the Budget**

(DOE Form 4620.1 "Budget Page" may be used).

### **4.1 Salaries and Wages**

List the names of the principal investigator and other key personnel and the estimated number of person-months for which DOE funding is requested. Proposers should list the number of postdoctoral associates and other professional positions included in the proposal and indicate the number of full-time-equivalent (FTE) person-months and rate of pay (hourly, monthly or annually). For graduate and undergraduate students and all other personnel categories such as secretarial, clerical, technical, etc., show the total number of people needed in each job title and total salaries needed. Salaries requested must be consistent with the institution's regular

practices. The budget explanation should define concisely the role of each position in the overall project.

## **4.2 Equipment**

DOE defines equipment as "an item of tangible personal property that has a useful life of more than two years and an acquisition cost of \$25,000 or more." Special purpose equipment means equipment which is used only for research, scientific or other technical activities. Items of needed equipment should be individually listed by description and estimated cost, including tax, and adequately justified. Allowable items ordinarily will be limited to scientific equipment that is not already available for the conduct of the work. General purpose office equipment normally will not be considered eligible for support.

## **4.3 Domestic Travel**

The type and extent of travel and its relation to the research should be specified. Funds may be requested for attendance at meetings and conferences, other travel associated with the work and subsistence. In order to qualify for support, attendance at meetings or conferences must enhance the investigator's capability to perform the research, plan extensions of it, or disseminate its results. Consultant's travel costs also may be requested.

## **4.4 Foreign Travel**

Foreign travel is any travel outside Canada and the United States and its territories and possessions. Foreign travel may be approved only if it is directly related to project objectives.

## **4.5 Other Direct Costs**

The budget should itemize other anticipated direct costs not included under the headings above, including materials and supplies, publication costs, computer services, and consultant services (which are discussed below). Other examples are: aircraft rental, space rental at research establishments away from the institution, minor building alterations, service charges, and fabrication of equipment or systems not available off-the-shelf. Reference books and periodicals may be charged to the project only if they are specifically related to the research.

### **a. Materials and Supplies**

The budget should indicate in general terms the type of required expendable materials and supplies with their estimated costs. The breakdown should be more detailed when the cost is substantial.

### **b. Publication Costs/Page Charges**

The budget may request funds for the costs of preparing and publishing the results of research, including costs of reports, reprints page charges, or other journal costs (except costs for prior or early publication), and necessary illustrations.

### **c. Consultant Services**

Anticipated consultant services should be justified and information furnished on each individual's expertise, primary organizational affiliation, daily compensation rate and number of days expected service. Consultant's travel costs should be listed separately under travel in the budget.

### **d. Computer Services**

The cost of computer services, including computer-based retrieval of scientific and technical information, may be requested. A justification based on the established computer service rates should be included.

### **e. Subcontracts**

Subcontracts should be listed so that they can be properly evaluated. There should be an anticipated cost and an explanation of that cost for each subcontract. The total amount of each subcontract should also appear as a budget item.

## **4.6 Indirect Costs**

Explain the basis for each overhead and indirect cost. Include the current rates.