

**Program Announcement  
To DOE National Laboratories  
LAB 05-16**

***Multiscale Mathematics Research  
and Education***

**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 research proposals for multiscale mathematics research and education, in support of the ASCR program, the ASCR-SciDAC (Scientific Discovery through Advanced Computing) partnership, and the broader SC research programs. Prospective researchers should observe that:

- 1) Proposals serving two complementary objectives - the advancement of multiscale mathematics research, both as an intellectual pursuit and a computational science enabler; and innovative approaches to educating computational scientists in the effective use of multiscale mathematics - are sought;
- 2) Proposed research and educational activities should be relevant to the mission of the Office of Science and, in particular to the long term goals of its proposals research programs;
- 3) In order to maximize the dissemination of information, promote and support technology commercialization, and avoid unnecessary duplication of effort; collaboration and communication amongst industry, laboratories, research centers and universities is encouraged;
- 4) Multiple year funding is not guaranteed, although researchers may request periods of performance ranging up to three years;

More specific information on this solicitation is outlined in the Supplementary Information section below.

**DATES:** The deadline for receipt of formal proposals is 4:30 P.M., Eastern Time, March 28, 2005, in order to be accepted for merit review and to permit timely consideration for award in Fiscal Year 2005.

**ADDRESSES:** A completed formal FWP in a single Portable Document Format (PDF) file referencing Program Announcement LAB 05-16 must be submitted via email to Dr. Gary M. Johnson at: [appliedmath@mics.doe.gov](mailto:appliedmath@mics.doe.gov). Please use "Program Announcement LAB 05-16" in the subject line of the email.

**FOR FURTHER INFORMATION CONTACT:** Dr. Gary Johnson, Mathematical, Information, and Computational Sciences Program, SC-31/Germantown Building, Office of

Advanced Scientific Computing Research, Office of Science, U.S. Department of Energy, 1000 Independence Avenue, SW, Washington, D.C. 20585-1290, Telephone: (301) 903-5800, Fax: (301)-903-7774, E-mail: appliedmath@mics.doe.gov.

**SUPPLEMENTARY INFORMATION:** In order to accomplish its mission, the DOE Office of Science is faced with the need for multiscale mathematics capabilities that far exceed what is currently available. In particular, the SC's requirements for advances in multiscale mathematics (a.k.a. Atomic to Macroscopic Mathematics) are documented in the President's Fiscal Year 2005 budget request to Congress:

#### **Atomic to Macroscopic Mathematics**

*The Fiscal Year 2005 budget also includes \$8,500,000 for the new "Atomic to Macroscopic Mathematics" (AMM) research effort to provide the research support in applied mathematics needed to break through the current barriers in our understanding of complex physical processes that occur on a wide range of interacting length- and time-scales. The current state-of-the-art in the theory and modeling of complex physical systems generally requires that the physical phenomena being modeled either occur at a single scale, or widely separated scales with little or no interaction. Complex physical systems frequently involve highly nonlinear interactions among many phenomena at many different scales. Increases in computational power over the last decade have enabled scientists to begin the process of creating sophisticated models with fewer simplifying assumptions. These new models cannot succeed without a deeper understanding of the mathematics of phenomena at multiple scales and how they interact, from the atomic scale through the mesoscopic to the macroscopic. Achieving this basic mathematical understanding will provide enabling technology to virtually every challenging computational problem faced by SC.*

*Progress in AMM will best be achieved through a combination of investments, including: (1) funds for innovative approaches to multiscale mathematics at universities throughout the country; (2) investments in partnerships between university researchers and investigators at the National laboratories; and (3) additional investments in multidisciplinary teams at the National laboratories. Category (1) represents investment in relatively high-risk/high-payoff approaches. Categories (2) and (3) follow the SciDAC model of building teams that involve National laboratory researchers in various critical proposals. AMM research will support the development of new high-fidelity simulations that are crucial to our improved understanding of important problems across the Office of Science, including fuel cell design, understanding of microbial cells and communities, accelerator design and optimization, combustion processes including clean and efficient engine design, fusion reactor design and optimization, design of materials atom-by-atom, and many more.*

This Notice announces ASCR's interest in receiving proposals for activities to advance multiscale mathematics research and education, serving two complementary objectives:

- **Multiscale Mathematics Research:** Develop and apply new multiscale mathematics algorithms and analysis to support the Office of Science's proposals research missions; and
- **Multiscale Mathematics Education:** Develop, implement, and publicly share programs to educate computational scientists in the use of multiscale mathematics as a tool for computational research and discovery

As integrated activities are sought, researchers should craft proposals that respond to both of these objectives, rather than selecting just one.

With regard to the multiscale mathematics research objective, the entire spectrum of activities is available for consideration - from individual research projects through multiscale mathematics institutes that provide an intellectual home for one or more scientific communities carrying out research enabling the solution of cutting-edge proposals problems of importance to the SC's mission. For those researchers who choose to propose group activities, such activities should be designed to support interdisciplinary and inter-institutional collaborations. These collaborations should focus on the development of novel multiscale mathematics and on harnessing its power for the solution of science proposals problems. Any and all proposals considered under this Announcement may include researchers drawn from the physical and life sciences, mathematics, computer science, or any other discipline essential to the successful completion of the proposed research.

With regard to the multiscale mathematics education objective, the proposed activity should develop, implement, publicly share and disseminate materials for the education of computational scientists in the techniques of multiscale mathematics. The education program should be tested through actual prototyping and use. Any courseware developed should cover as broad a spectrum of both data-intensive and computation-intensive proposals areas as possible. Illustrative examples should be drawn from proposals of interest to the Office of Science, to the extent possible.

The proposed activities should include a plan for playing an active role in maintaining a dialogue with industry, universities, and other laboratories and centers in order to maximize the dissemination of information, promote and support technology commercialization, and avoid unnecessary duplication of effort.

### **Collaboration**

Researchers are encouraged to collaborate with researchers in other institutions, such as: universities, industry, non-profit organizations, federal laboratories and Federally Funded Research and Development Centers (FFRDCs), including the DOE National Laboratories, where appropriate, and to include cost sharing wherever feasible. Additional information on collaboration is available in the Proposal Guide for the Office of Science Financial Assistance Program that is available via the Internet at: <http://www.science.doe.gov/grants/Colab.html>.

### **Program Funding**

It is anticipated that up to \$5.8 million in this Announcement will be available in Fiscal Year 2005, contingent upon availability of appropriated funds. Proposals for individual research are welcome, as are larger proposals, including those involving group and inter-institutional collaborations and including multiscale mathematics institutes. The number and character of the awards made will depend strongly on the nature and quality of the activities proposed. Multiple year funding is not guaranteed, although researchers may request periods of performance ranging up to three years.

### **Submission Information**

The Project Description must be 20 pages or less, exclusive of attachments. It must contain an abstract or project summary on a separate page with the name of the researcher, mailing address, phone, Fax and E-mail listed. The proposal must include letters of intent from collaborators (briefly describing the intended contribution of each to the research), and short curriculum vitae for the principal investigator and all co-investigators.

Researchers must disclose all information on their current and pending awards. DOE is under no obligation to pay for any costs associated with the preparation or submission of proposals if an award is not made.

The instructions and format described below should be followed. Reference Program Announcement LAB 05-16 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:

Scientific and/or technical merit of the project

Appropriateness of the proposed method or approach

Competency of the personnel and adequacy of the proposed resources

Reasonableness and appropriateness of the proposed budget

The evaluation under item 1, Scientific and/or Technical Merit of the Project, will also consider the following elements:

- a) The relevance of the proposed program of multiscale mathematics research and education to the mission of the Office of Science.
- b) The potential of the proposed project to make a significant impact on multiscale mathematics research and education.
- c) The potential of the proposed project to identify and advance the development of new research and educational techniques intended to accelerate the adoption of multiscale mathematics as an enabler for computational science research.

The evaluation under item 2, Appropriateness of the Proposed Method or Approach, will also consider the following elements:

- a) The degree to which the project adheres to the management philosophy of integrating both research and education into the project execution.
- b) The extent to which the proposed activities are new and crafted specifically as a response to this call for participation.
- c) The extent to which the project incorporates broad community (industry/academia/other federal programs) interaction and outreach.
- d) Quality and clarity of proposed work schedule and deliverables.
- e) Extent to which materials developed under this project will be available to the public (e.g. as "open source").

The evaluation under item 3, Competency of Researcher's Personnel and Adequacy of Proposed Resources, will also consider the following elements:

- a) Quality of the intellectual environment for both research and educational activities in multiscale mathematics.
- b) Quality of the physical resources, (e.g. computing capabilities; networking infrastructure; educational infrastructure...) for both research and educational activities in multiscale mathematics.

The evaluation will include program policy factors, such as the relevance of the proposed research to the terms of the announcement and the agency's programmatic needs. External peer reviewers are selected with regard to both their scientific expertise and the absence of conflict-of-interest issues. Non-federal reviewers will often be used, and submission of a proposal constitutes agreement that this is acceptable to the investigator(s) and the submitting institution.

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

Field Work Proposal (FWP) Format (Reference DOE Order 5700.7C) (DOE ONLY)  
Proposal Cover Page  
Table of Contents  
Abstract  
Narrative  
Literature Cited  
Budget and Budget Explanation  
Other support of investigators  
Biographical Sketches  
Description of facilities and resources  
Appendix

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

A completed formal FWP in a single Portable Document Format (PDF) file referencing Program Announcement LAB 05-16 must be submitted via email to Dr. Gary M. Johnson at: [appliedmath@mics.doe.gov](mailto:appliedmath@mics.doe.gov). Please use "Program Announcement LAB 05-16" in the subject line of the email.

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

Proposals must be readily legible, when photocopied, and must conform to the following three requirements: the height of the letters must be no smaller than 10 point with at least 2 points of spacing between lines (leading); the type density must average no more than 17 characters per inch; the margins must be at least one-half inch on all sides. Figures, charts, tables, figure legends, etc., may include type smaller than these requirements so long as they are still fully legible.

#### **3.1 Field Work Proposal Format (Reference DOE Order 5700.7C) (DOE ONLY)**

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 Abstract**

Provide an abstract of no more than 250 words. Give the broad, long-term objectives and what the specific research proposed is intended to accomplish. State the hypotheses to be tested. Indicate how the proposed research addresses the SC scientific/technical area specifically described in this announcement.

### **3.5 Narrative**

The narrative comprises the research plan for the project and is limited to 5 pages per task. It should contain the following subsections:

**Background and Significance:** Briefly sketch the background leading to the present proposal, critically evaluate existing knowledge, and specifically identify the gaps which the project is

intended to fill. State concisely the importance of the research described in the proposal. Explain the relevance of the project to the research needs identified by the Office of Science. Include references to relevant published literature, both to work of the investigators and to work done by other researchers.

**Preliminary Studies:** Use this section to provide an account of any preliminary studies that may be pertinent to the proposal. Include any other information that will help to establish the experience and competence of the investigators to pursue the proposed project. References to appropriate publications and manuscripts submitted or accepted for publication may be included.

**Research Design and Methods:** Describe the research design and the procedures to be used to accomplish the specific aims of the project. Describe new techniques and methodologies and explain the advantages over existing techniques and methodologies. As part of this section, provide a tentative sequence or timetable for the project.

**Subcontract or Consortium Arrangements:** If any portion of the project described under "Research Design and Methods" is to be done in collaboration with another institution, provide information on the institution and why it is to do the specific component of the project. 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".

### **3.6 Literature Cited**

List all references cited in the narrative. Limit citations to current literature relevant to the proposed research. Information about each reference should be sufficient for it to be located by a reviewer of the proposal.

### **3.7 Budget and Budget Explanation**

A detailed budget is required for the entire project period, which normally will be three years, and 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.sc.doe.gov/production/grants/Forms-E.html>

### **3.8 Other Support of Investigators**

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 devoted to the project.

### **3.9 Biographical Sketches**

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

### **3.10 Description of Facilities and Resources**

Describe briefly the facilities to be used for the conduct of the proposed research. Indicate the performance sites and describe pertinent capabilities, 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.

### **3.11 Appendix**

Include collated sets of all appendix materials with each copy of the proposal. Do not use the appendix to circumvent the page limitations of the proposal. Information should be included that may not be easily accessible to a reviewer.

Reviewers are not required to consider information in the Appendix, only that in the body of the proposal. Reviewers may not have time to read extensive appendix materials with the same care as they will read 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.