Office of Science
Notice DE-FG01-05ER05-16

Multiscale Mathematics Research and Education

Department of Energy

Office of Science Financial Assistance Program Notice DE-FG01-05ER05-16: Multiscale Mathematics Research and Education

AGENCY: U.S. Department of Energy

ACTION: Notice inviting grant applications.

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 grants 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 applicants should observe that:

1) Applications 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 applications 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 applicants 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 applications 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: Formal applications in response to Program Notice DE-FG01-05ER05-16, must be electronically submitted by an authorized institutional business official through DOE's Industry Interactive Procurement System (IIPS) at: http://e-center.doe.gov/ (see also http://www.science.doe.gov/grants/). IIPS provides for the posting of solicitations and receipt of applications in a paperless environment via the Internet. In order to submit applications through IIPS your business official will need to register at the IIPS website. It is suggested that this registration be completed several days prior to the date on which you plan to submit the formal application. The Office of Science will include attachments as part of this notice that provide the appropriate forms in PDF fillable format that are to be submitted through IIPS. IIPS offers the option of submitting multiple files-please limit submissions to only one volume and one file if possible, with a maximum of no more than four files. Color images should be submitted in IIPS as a separate file in PDF format and identified as such. These images should be kept to a minimum due to the limitations of reproducing them. They should be numbered and referred to in the body of the technical scientific application Color image 1, Color image 2, etc. Questions regarding the operation of IIPS may be e-mailed to the IIPS Help Desk at: helpdesk@pr.doe.gov or you may call the help desk at: (800) 683- 0751. Further information on the use of IIPS by the Office of Science is available at: http://www.science.doe.gov/grants/IIPS-Instructions.html.

If you are unable to submit the application through IIPS, please contact the Grants and Contracts Division, Office of Science at: (301) 903-5212 or (301) 903-3604, in order to gain assistance for submission through IIPS or to receive special approval and instruction on how to submit printed applications.

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: garyj@er.doe.gov. The full text of Program Notice DE-FG01-05ER05-16 is available via the Internet using the following web site address: http://www.science.doe.gov/grants/.

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

> *"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 applications. 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 applications 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 applications 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, applicants should craft applications 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 applications problems of importance to the SC's mission. For those applicants 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 applications problems. Any and all applications considered under this solicitation 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 applications areas as possible. Illustrative examples should be drawn from applications 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

Applicants 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 Application 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 will be available in Fiscal Year 2005, contingent upon availability of appropriated funds. Applications for individual research are welcome, as are larger applications, 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 applicants may request periods of performance ranging up to three years.

Merit Review

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,
4) 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 Applicant'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 an application constitutes agreement that this is acceptable to the investigator(s) and the submitting institution.

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 applicant, mailing address, phone, Fax and E-mail listed. The application must include letters of intent from collaborators (briefly describing the intended contribution of each to the research), and short curriculum vitaes for the principal investigator and all co- investigators.

Applicants must disclose all information on their current and pending grants. To provide a consistent format for the submission, review and solicitation of grant applications submitted under this notice, the preparation and submission of grant applications must follow the guidelines given in the Application Guide for the Office of Science Financial Assistance Program, 10 CFR Part 605. Access to SC's Financial Assistance Application Guide is possible via the World Wide Web at: http://www.science.doe.gov/grants/. DOE is under no obligation to pay for any costs associated with the preparation or submission of applications if an award is not made.

The Catalog of Federal Domestic Assistance number for this program is 81.049, and the solicitation control number is ERFAP 10 CFR Part 605.

Martin Rubinstein
Grants and Contracts Division
Office of Science

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