Office of Science Notice DE-FG01-05ER05-25

Early Career Principal Investigator Program in Applied Mathematics, Computer Science, and High-Performance Networks

Department of Energy

Office of Science Financial Assistance Program Notice DE-FG01-05ER05-25; Early Career Principal Investigator Program in Applied Mathematics, Computer Science, and High-Performance Networks

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 grant applications in support of its Early Career Principal Investigator Program (ECPI). The overall objective the ECPI program is to stimulate academic research in scientific areas of interest to ASCR programs, especially among faculty in the early stages of their academic profession. The specific research areas of interest to ASCR include: applied mathematics, computer science, and high-performance networks. The full text of Program Notice DE-FG01-05ER05-25; is available via the Internet using the following web site address: http://www.science.doe.gov/grants/grants.html.

DATES: A Letter-of-Intent (LOI) to submit an application is REQUIRED and should be submitted by October 31, 2005. Failure to submit the LOI by the due date may preclude the full application from due consideration for award. Formal applications will be accepted only from applicants whose LOI is determined to be responsive to the announcement.

Formal applications submitted in response to this notice must be received by DOE no later than 8:00 p.m., Eastern Time, January 31, 2006, to be accepted for merit review and to permit timely consideration for award in Fiscal Year 2006. Awardees are expected to be selected and announced by March 31, 2006. Electronic submission of formal applications in PDF format is REQUIRED.

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

ADDRESSES: Letters-of-Intent should be submitted electronically by email to Dr. Thomas D. Ndousse-Fetter at ecpi@mics.doe.gov citing "Letter-of-Intent for Notice DE-FG01-05ER05-25 ECPI-2006" in the subject line of the email. The purpose of the LOI is to expedite the planning of the review of the applications. For this purpose, the LOI should contain a one-page abstract of the proposed research, together with a list of potential collaborators and their institutional affiliations, to enable potential conflict of interest issues to be determined in relation to the review.

Formal Applications

Applications submitted to the Office of Science must be submitted electronically through Grants.Gov to be considered for award. The Funding Opportunity Number is: DE-FG01-05ER05-25 and the CFDA Number for the Office of Science is: 81.049. Instructions and forms are available on the <u>Grants.Gov</u> website. Please see the information below and also refer to the "Funding Opportunity Announcement", Part IV - Application and Submission Information; H. Other Submission and Registration Requirements for more specific guidance on "Where to Submit" and "Registration Requirements." If you experience problems when submitting your application to Grants.gov, please visit their customer support website: http://www.grants.gov/CustomerSupport; email: support@grants.gov; or call 1-800-518-4726.

Registration Requirements: There are several one-time actions you must complete in order to submit an application through Grants.gov (e.g., obtain a Dun and Bradstreet Data Universal Numbering System (DUNS) number, register with the Central Contract Registry (CCR), register with the credential provider and register with <u>Grants.Gov</u>). See http://www.grants.gov/GetStarted. Use the Grants.gov Organization Registration Checklist to guide you through the process. Designating an E-Business Point of Contact (EBiz POC) and obtaining a special password called an MPIN are important steps in the CCR registration process. Applicants, who are not registered with CCR and Grants.gov, should allow at <u>least 14</u> <u>days</u> to complete these requirements. It is suggested that the process be started as soon as possible.

VERY IMPORTANT - Download PureEdge Viewer: In order to download the application package, you will need to install PureEdge Viewer. This small, free program will allow you to access, complete, and submit applications electronically and securely. For a free version of the software, visit the following Web site: <u>http://www.grants.gov/DownloadViewer</u>.

FOR FURTHER INFORMATION, CONTACT: Dr. Thomas D. Ndousse, Office of Advanced Scientific Computing Research, SC-21.1/Germantown Building, U.S. Department of Energy, 1000 Independence Avenue, SW, Washington, DC 20585-1290, Telephone: (301) 903-5800, E-mail: ecpi@mics.doe.gov

SUPPLEMENTARY INFORMATION: In selecting experimental applications for funding, the Mathematical, Informational, and Computational Sciences (MICS) division will give priority to applications that have the potential of establishing new research directions in the areas of interest to DOE computational sciences and networks priorities outlined in this announcement.

To facilitate the review process, all applications should be limited to a maximum of twenty-five (25) pages (including text and figures) of technical information. Applications exceeding these page limits may be rejected without review. The PDF file may also include a few selected publications in an Appendix as background information. In addition, in the electronic submission, please limit biographical and publication information for the principal investigator and key personnel to no more than two pages each. Each principal investigator should provide an e-mail address. The page count of 25 does not include the face page, budget pages, title page, the biographical material and publication information, or any appendices. However, it is important that the 25 page technical information section provide a complete description of the proposed work, since reviewers are not obliged to read the appendices.

Application

The application should be prepared and each file attached within the Grants.gov application package according to the instructions provided. Please follow the additional guidance below, and include in the appropriate places, all the following items when preparing the attachments:

1. Executive Summary - summarize in no more than a page. It must be contain PI's contact information and date of the first tenure tract appointment at the top.

2. Abstract - One paragraph summary of the planned work in no more than one page.

3. Background and recent accomplishments relevant to the proposed research.

3.1 Background**3.2** Recent accomplishments relevant to the proposed work by the PI

4. Proposed research.

- **4.1** Detailed plan (scope)
- **4.2** Project schedules and milestones
- **4.3** Statement of work and deliverables

5. Textual summary of budget (in addition to the formal budget pages) - in particular, showing how the budget relates to the research and task plans.

6. Management plan - if appropriate (for projects of large size and complexity.)

7. Description of facilities, resources, and personnel.

8. Other current and pending support. Indicate the time commitment to each current and pending project in calendar months.

General information about development and submission of applications, eligibility, limitations, evaluations and selection processes, and other policies and procedures may be found in the Application Guide for the Office of Science Financial Assistance Program and 10 CFR Part 605.

Electronic access to SC's Financial Assistance Guide is possible via the Internet using the following website address: <u>http://www.science.doe.gov/grants/grants.html</u>. Any specific instructions included in this notice supersede those in the general information referred to above. DOE is under no obligation to pay for any costs associated with the preparation or submission of an application if an award is not made.

Program Mission

The mission of ASCR, carried out by the MICS division, is to deliver forefront computational and networking capabilities to scientists nationwide that enable them to extend the frontiers of science, answer critical questions that range from the function of living cells to the power of fusion energy. The MICS division is responsible for discovering, developing, and deploying computational sciences tools, terascale computing facilities, and high-performance networking facilities that researchers need to analyze, model, simulate, and - most importantly - predict the behavior of complex natural and engineered systems of importance to DOE science mission.

ASCR programs achieve the mission objective by fostering and supporting fundamental research activities in advanced scientific research the execution of the following research and development strategies: Build leading research programs in focused disciplines of applied mathematics and computer science that enable scientific simulation and modeling codes to take full advantage of the extraordinary capabilities of terascale computers.

Create advanced networking technologies and distributed software infrastructure to spur revolutionary advances in the use of high performance computers and networks, which enable geographically-separated scientists to effectively work together as a team, as well as provide electronic access to both facilities and data.

To establish and maintain DOE's modeling and simulation leadership in scientific areas that are important to its mission, the MICS program employs a broad, but integrated, research strategy. The basic research portfolio in applied mathematics and computer science provides the foundation for enabling research activities, which includes efforts to advance high-performance networking, to develop software tools, software libraries, and software environments. Results from enabling research supported by the MICS program are used by computational scientists supported by other SC and other DOE programs.

Further descriptions of the base research portion of the MICS portfolio, which is the scope of this Notice, are provided below:

Topic I: Applied Mathematics Research

Research on the underlying mathematical understanding as well as the numerical algorithms needed to enable effective description and prediction of physical, chemical, and biological systems of importance to the Office of Science - such as fluids, materials, magnetized plasmas, or protein molecules (to cite just a few examples) - is sought. This may include, but is not limited to, methods for solving large systems of partial differential equations (PDEs) on parallel computers: techniques for choosing optimal values for parameters in large systems with

hundreds to hundreds of thousands of parameters; improving our understanding of fluid turbulence; research in multiscale algorithms; the mathematics of feature identification in large datasets; asymptotically optimal algorithms for solving PDEs; fast multipole and related hybrid methods; algorithms for handling complex systems with constraints; and developing techniques for reliably estimating the errors in simulations of complex physical phenomena. In addition to the research topics mentioned above, MICS is open to investment in new areas of applied mathematics research to support the Office of Science's mission.

Grant applications targeting this topic must emphasize applied mathematics over the underlying science problems. The proposed mathematic research activities must be clearly identified in grant applications and must be designated as "Applied Math" in the subtitle. Grant applications which concentrate on solving specific science problems with complex mathematical formulation will be considered non-responsive.

Topic II: Computer Science Research

The objective of the computer science component of the MICS research portfolio is to support research that results in a comprehensive, scalable, and robust high performance software infrastructure that translates the promise and potential of high peak performance to real performance improvements in DOE scientific applications. This software infrastructure must address needs for: portability and interoperability of complex high performance scientific software packages; operating systems tools and support for the effective management of terascale and beyond systems; and effective tools for feature identification, data management, and visualization of petabytes-scale scientific data sets. The computer science component encompasses a multi-discipline approach with activities in:

1) Program development environments and tools - Component-based, fully integrated, terascale program development and runtime tools, which scale effectively and provide maximum performance, functionality, and ease-of-use to developers and scientific end users.

2) Operating system software and tools - Systems software that scales to tens of thousands of processors, supports high performance application-level communication, and provides the highest levels of performance, fault tolerance, reliability, manageability, and ease of use for system administrators, tool developers, and end users.

3) Visualization and data management systems - Scalable, intuitive systems fully supportive of DOE application requirements for moving, storing, analyzing, querying, manipulating, and visualizing multi-petabytes of scientific data and objects.

4) Performance Measurement and Analysis -- Tools and methodology to enable improved understanding of end-to-end application performance, identify performance bottlenecks, and support rapid testing of code performance enhancements.

The MICS research portfolio in computer science emphasizes investment in long-term research that will result in the next generation of high performance tools for scientific discovery. Grant applications targeting this topic must be designated as "Computer Science" in the subtitle.

Topic III: High-Performance Networks and Middleware

The goal of the network research program in the MICS division is to conduct basic and applied research on high-capacity network technologies needed to interconnect science facilities and to provide unfettered access to terascale computing resources data repositories. The current focus of network research activities is on advanced ultra high-speed and high-capacity network technologies. This may include but are not limited to the following:

1) Ultra high-speed network protocols - Innovative, new approaches to transport protocols to harness the abundant bandwidth made possible by Dense Wave Division Multiplexing (DWDM) optical technologies.

2) Agile system-level optical networks - Advanced switching network technologies to enable end-to-end dynamic provisioning services such on-demand circuits, guaranteed bandwidth, control and signaling plane technologies, and advanced optical network services.

3) Cyber security systems - Formal techniques for modeling and evaluating the performance of cyber security systems. This may include techniques for formal specification of cyber security requirements and implementation.

4) High-performance middleware - Advanced network services that enable the coupling of scientific applications to the underlying high-speed networks.

5) Optimization techniques for complex networks - Advanced techniques for modeling complex traffic processes in ultra high-speed networks.

Grant applications addressing the above problems must go beyond the development of tools and emphasize mathematical analysis, formal specification, and rigorous techniques for validating the performance of their proposed solutions. The MICS division operates a production high-speed network called ESnet (<u>http://www.es.net</u>) and an experimental ultra high-speed network called Ultra-Science Net (<u>http://www.csm.ornl.gov/ultranet</u>) available to researchers. Applicants are encouraged to proposed research activities that make extensive use of these networks, especially Ultra-Science Net testbed. Grant applications targeting high performance network research subtopic must be designated as "High-Performance Networks" in the subtitle.

Background: Early Career Principal Investigator Program

This is the third year of the Early Career Principal Investigator Program. A principal goal of this program is to identify exceptionally talented applied mathematicians, computer scientists, and high-performance networks researchers early in their careers and assist and facilitate the development of their research programs. Eligibility for awards under this notice is restricted to applicants who meet all of the following criteria:

1) Hold a PhD or equivalent degree and be employed in a full-time tenure-track position or equivalent position as an assistant professor at an institution in the U.S., its territories or possessions, or the Commonwealth of Puerto Rico.

2) Be within the first or second year of their first tenure track appointment at the date of submitting this grant application. The date of the applicant's first tenure track appointment must be clearly marked in CV and in the abstract of the proposal.

3) Hold no active or pending awards at the date of this submission that will prevent the applicant from devoting a substantial time (at least summer month) to their ECPI project.

Applications should be submitted through an institution in the U.S., its territories, or the Commonwealth of Puerto Rico that awards advanced degree in a field mathematical, network, and computing sciences supported by the MICS division at DOE. Applicants should request support under this notice for normal research project costs as required conducting their proposed research activities, such as part of the PI's salary, graduate and/or undergraduate students, post-doctoral researchers, equipment and facilities, and travel. However, no salary support will be provided for other faculty members or senior personnel. Travel budget should not be more than 6% of the budget of the award and should not include foreign travel.

Applicants who have submitted or will be submitting similar grant applications to other programs are eligible for this notice, as long as the details of the other submission are contained in the grant application to DOE. Applicants who have an NSF CAREER award, or are applying for such an award, are eligible for this notice. However, applicants will be required to disclose information on all their current and pending awards. Applicants do not have to be U.S. citizens, and may be non-permanent resident aliens or have an H1b visa.

Program Funding

It is anticipated that up to \$2 million will be available for up to twenty (20) awards for exceptional applications in Fiscal Year 2006, to meet the needs of the program, contingent upon the availability of appropriated funds. The maximum support that can be requested under this notice is \$100,000 per year for three years. Grant applications requesting more that \$100,000/per year will not reviewed.

Multiple-year funding of grant awards is expected, with funding provided on an annual basis subject to the availability of funds, progress of the research, and programmatic needs. The typical duration of these grants is three years, <u>and they will not normally be renewed after the project period has been completed</u>. It is anticipated that at the end of the grant period, grantees will submit new grant applications to continue their research to DOE or other Federal funding agencies. We expect that the awards will be announced and the projects will begin in early summer 2006.

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 as 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 of applications under item 1, Scientific and Technical Merit, will pay attention to the responsiveness of the proposed research to the challenges of the MICS research priorities outlined in the announcement. It is expected that the application will include involvement of graduate and/or undergraduate students in the proposed work.

Applicants are strongly encouraged to collaborate with DOE National Laboratory researchers. The collaborations may include one, or more, extended visits to the laboratory by the applicant each year. Such an arrangement, if proposed, must be budgeted for and clearly explained in the grant application. Furthermore, a letter of support from the DOE National Laboratory collaborator(s) should be included with the application. A list of the DOE National Laboratories can be found at:

http://www.science.doe.gov/Sub/Organization/Map/national_labs_and_userfacilities.htm.

Grantees under the Early Career Principal Investigator Program may apply for access to highperformance computing and network resources at several National Laboratories. Such resources include but are not limited to following:

The National Energy Research Scientific Computing (NERSC) Center: <u>http://www.science.doe.gov/ascr/mics/nersc/index.html</u>;

The Advanced Computing Research Testbeds: http://www.science.doe.gov/ascr/mics/acrt/index.html;

DOE Experimental Network (Ultra-Science Net): <u>http://www.csm.ornl.gov/ultranet;</u>

The evaluation under item 2, Appropriateness of the Proposed Method or Approach, will consider the quality of the proposed plan, if any, for interacting with a DOE National Laboratory. Please note that external peer reviewers are selected with regard to both their scientific expertise in the subject area of the grant application 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 and the submitting institution.

Submission Information

Each grant application submitted should clearly indicate on which of the three following research components of the MICS research portfolio the application is focused: Applied Mathematical Sciences Research, Computer Science Research, or High-Performance Networks Research. Grants with no designated research components will not be reviewed.

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 Director Science Programs Support Division Office of Science

Posted on the Office of Science Grants and Contracts Web Site September 9, 2005.