Office of Science
Notice DE-FG01-05ER05-17

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-FG01-05ER05-17; 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. The purpose of this program is to support research in applied mathematics, computer science, and high-performance networks performed by exceptionally talented scientists and engineers early in their careers. The full text of Program Notice DE-FG01-05ER05-17, is available via the Internet using the following web site address: http://www.science.doe.gov/grants/.

DATES: To permit timely consideration for award in Fiscal Year 2005, completed applications in response to this notice must be received by 8:00 P.M., Eastern Time, March 15, 2005, to be accepted for merit review and funding in Fiscal Year 2005.

ADDRESSES: Formal applications referencing Program Notice DE-FG01-05ER05-17, must be sent electronically by an authorized institutional business official through DOE's Industry Interactive Procurement System (IIPS) at: http://e-center.doe.gov/. 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. **IIPS offers the option of using multiple files, please limit submissions to one volume and one file if possible, with a maximum of no more than four PDF files.** 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. 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 grant application as 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 an 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 instructions on how to submit printed applications.

FOR FURTHER INFORMATION CONTACT: Dr. Thomas D. Ndousse, Office of Advanced Scientific Computing Research, SC-31/Germantown Building, U.S. Department of Energy, 1000 Independence Avenue, SW, Washington, DC 20585-1290, Telephone: (301) 903- 5800, E-mail: tndousse@er.doe.gov

SUPPLEMENTARY INFORMATION:

Program Mission

The mission of the Advanced Scientific Computing Research Program is to deliver forefront computational and networking capabilities to scientists nationwide that enable them to extend the frontiers of science, answering critical questions that range from the function of living cells to the power of fusion energy.

In order to accomplish this mission, this program fosters and supports fundamental research in advanced computing research (applied mathematics, computer science and networking), and operates supercomputer, networking, and related facilities to enable the analysis, modeling, simulation, and prediction of complex phenomena important to DOE.

The following long-term goals will be indicators of ASCR's success in meeting its mission:

1) Develop mathematics, algorithms, and software that enable effective models of complex systems, including highly nonlinear or uncertain phenomena, or processes that interact on vastly different scales or contain both discrete and continuous elements.

2) Develop, through the Genomes to Life partnership with the DOE Office of Biological and Environmental Research, the computational science capability to model a complete microbe and a simple microbial community.

The primary mission of the ASCR program is carried out by the Mathematical, Information, and Computational Sciences (MICS) Division. This Division is responsible for discovering, developing, and deploying advanced scientific computing and communications tools and operating the high performance computing and network facilities that researchers need to analyze, model, simulate, and - most importantly - predict the behavior of complex natural and engineered systems of importance to SC and to DOE.

The computing, networking middleware required to meet SC needs exceed the state-of-the-art by a wide margin. Furthermore, the algorithms, the software tools, the software libraries, and the

distributed software environments needed to accelerate scientific discovery through modeling and simulation are beyond the realm of commercial interest. 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:

Applied Mathematics Research

The objective of the applied mathematics component of the MICS research portfolio is to support the advancement of the science missions of the Office of Science's applications program offices. 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.

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 petabyte-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.

High-Performance Networks Research

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. The current focus of network research activities is on end-to-end ultra high-speed network technologies not currently commercially available. 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 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 an experimental ultra high-speed network called Ultra-Science Net available to researchers. Applicants are encouraged to proposed research activities that make extensive use of Ultra-Science Net. More information on the Ultra-Science Net can be found at http://www.csm.ornl.gov/ultranet.

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 tenure-track-equivalent position) as an assistant professor (or equivalent title) 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. All applicants who began their first tenure track appointment after June 2002 are eligible to apply.

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 30% of their allocated research time) to their ECPI project.

Applications should be submitted through an institution in the US, 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.

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 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 2005, 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.

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, and they will not normally be renewed after the project period has been completed. 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 2005.

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 base research programs in Applied Mathematics, Research, Computer Science, and Network Research.

It is expected that the application will include involvement of graduate and/or undergraduate students in the proposed work.

Applicants are 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 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 high-performance computing and network resources at several National Laboratories. Such resources include, but are not limited to:

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

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

the DOE experimental network (Ultra-Science Net): http://www.csm.ornl.gov/ultranet;

the Energy Sciences Network: http://www.science.doe.gov/ascr/mics/esnet/index.html;

and the High-Performance Networking Research effort at the Oak Ridge National Laboratory; http://www.csm.ornl.gov/net.

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 four following components of the MICS research portfolio the application is focused: Applied Mathematical Sciences Research, Computer Science Research, or High-Performance Networks Research.

The Project Description should be 20 pages or less, exclusive of the bibliography and other 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, and a short curriculum vita for the applicant. Applicants must also complete and submit with their application a supplementary information form available at: http://www.science.doe.gov/ascr/mics/hpn/ECPI-%20Applicant%20Information.doc.

To provide a consistent format for the submission, review, and solicitation of grant applications 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.

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Grants and Contracts Division
Office of Science

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