

Office of Science
Notice DE-FG01-04ER04-05

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

Department of Energy

Office of Science Financial Assistance Program Notice DE-FG01-04ER04-05; Early Career Principal Investigator Program in Applied Mathematics, Collaboratory Research, 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 applications for grant applications in support of its Early Career Principal Investigator Program. The purpose of this program is to support research in applied mathematics, collaboratory research, computer science, and networks performed by exceptionally talented scientists and engineers early in their careers. The full text of Program Notice DE-FG01-04ER04-05, is available via the Internet using the following web site address:
<http://www.science.doe.gov/production/grants/grants.html>.

DATES: To permit timely consideration for award in Fiscal Year 2004, completed applications in response to this notice must be received by February 10, 2004, to be accepted for merit review and funding in Fiscal Year 2004.

ADDRESSES: Formal applications referencing Program Notice DE-FG01-04ER04-05 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.sc.doe.gov/production/grants/grants.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. Samuel J. Barish, 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: sam.barish@science.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:

- 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.
- 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 Mathematical Sciences Research

The objective of the applied mathematics component of the MICS research portfolio is to support 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 such as fluids, materials, magnetized plasmas, or protein molecules. This includes, 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, and developing techniques for reliably estimating the errors in simulations of complex physical phenomena.

In addition to the existing research topics described, MICS plans to invest in new areas of applied mathematics research to support DOE's mission. Such investments may include research in multiscale algorithms, the mathematics of feature identification in large datasets, asymptotically optimal algorithms for solving PDEs, fast multipole and related hybrid methods, and algorithms for handling complex systems with constraints. The MICS research portfolio in Applied Mathematics emphasizes investment in long-term research that will result in the next generation of computational tools for scientific discovery.

Collaboratory Research

Collaboratories link geographically dispersed researchers, data, and tools via high performance networks to enable remote access to facilities, access to large datasets, shared environments, and ease of collaboration. The objective of the collaboratory component of the MICS portfolio is to support research for developing the software infrastructure that will enable universal, ubiquitous, easy access to remote resources or that will contribute to the ease with which distributed teams work together. Enabling high performance for distributed scientific applications is an important consideration. The middleware component for collaboratories encompasses activities in:

- Building the application frameworks that allow discipline scientists to express and manage the simulation, analysis, and data management aspects of overall problem solving.
- Supporting construction, management, and use of widely distributed application systems.
- Facilitating human collaboration through common security services, and resource and data sharing.
- Providing remote access to, and operation of, scientific and engineering instrumentation systems.
- Managing and securing the computing and data infrastructure as a persistent service.

This announcement also calls for grant applications to address the fundamental issues involved in providing uniform software services that manage and provide access to heterogeneous, distributed resources, that is, high-performance middleware services that support DOE's science mission. The emphasis is on investment in long-term research that will result in the next generation of high-performance software infrastructure for scientific discovery.

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:

- 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.
- 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.
- 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.
- Problem Solving Environments - Unified systems focused on the needs of specific scientific applications, which enable radically improved ease-of-use of complex systems software and tools by domain application scientists.

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

In the next few years, complex science experiments in DOE are expected to generate several petabytes of data that will be transferred to geographically distributed terascale computing facilities for analysis and visualization by thousands of scientists across the world. In addition, many emerging energy research problems require coordinated access to distributed resources – people, data, computers, and facilities. This emerging, distributed terascale-science environment calls for ultra-high-speed networks – networks that can deliver multi-gigabits/sec throughput to scientific applications securely. Grant applications in network research must therefore address the issues of ultra high-speed networks by focusing on:

- Ultra high-speed network protocols – innovative, new approaches to transport protocols and dynamic provisioning technologies for ultra-high-speed networks that will enable large-scale distributed science applications to efficiently harness the abundant bandwidth made possible by Dense Wave Division Multiplexing (DWDM) optical technologies. For ultra-high-speed transport protocols, this may include, but is not limited to, significant modifications to existing transport protocols, such as UDP, TCP, TCP variants, and TCP alternatives that can deliver multi-gigabit throughput to high-end scientific applications. For dynamic provisioning, the focus is on advanced network technologies for agile DWDM networking that offer bandwidth on-demand, scheduled end-to-end bandwidth, differentiated DWDM services, and DWDM traffic engineering. Respondents must address the theoretical foundations of the proposed work with rigorous mathematical and algorithm principles.
- Performance evaluation of cyber security systems – formal techniques for modeling and evaluating the performance and effectiveness of cyber security systems and policies. This may include techniques for formal specification of cyber security requirements and implementation.
- Ultra-high-speed network services – advanced network-aware services that enable the efficient, effective, and secure utilization of ultra-high-speed networks for data transfers over long distances.
- Optimization techniques for complex networks – advanced stochastic optimization techniques that can be used to characterize complex traffic processes in large-scale networks. This may include, but is not limited to, computational intelligence, chaos theory, large-scale simulations, and multi-scale theory.

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.

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, collaboratory researchers, 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) Be employed in a tenure-track position (or tenure-track-equivalent position) as an assistant professor (or equivalent title).

(2) Are conducting research in applied mathematics, collaboratories, computer science, or high-performance networks.

Applications should be submitted through a U.S. academic institution. Applicants should request support under this notice for normal research project costs as required to conduct 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. 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 2004, 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 2004.

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, Collaboratory 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.sc.doe.gov/ascr/mics/nersc/index.html>; the Advanced Computing Research Testbeds: <http://www.sc.doe.gov/ascr/mics/acrt/index.html>; the Energy Sciences Network: <http://www.sc.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, Collaboratory 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.

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.sc.doe.gov/production/grants/grants.html>. 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.

John Rodney Clark
Associate Director of Science
for Resource Management

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