

**Office of Science
Notice 03-11**

***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 03-11: 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 grants 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 03-11 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 2003, completed applications in response to this notice must be received by February 20, 2003, to be accepted for merit review and funding in Fiscal Year 2003.

ADDRESSES: Formal applications in response to this solicitation are to be electronically submitted 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. 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 Office of the Director, Grants and Contracts Division, Office of Science, DOE at: (301) 903-5212 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 primary mission of the Office of Advanced Scientific Computing Research, which is carried out by the Mathematical, Information, and Computational Sciences (MICS) Division, is to discover, develop, and deploy the computational and networking tools that enable researchers in the scientific disciplines to analyze, model, simulate, and predict complex physical, chemical, and biological phenomena important to DOE. To accomplish this mission, the MICS Division fosters and supports fundamental research in advanced scientific computing-applied mathematics, collaborative research, computer science, and networking-and operates supercomputers, a high performance network, and related facilities. Further descriptions of the base research portion of the MICS portfolio, which is the scope of this Notice, is 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 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-radical new approaches to ultra high-speed transport protocols that will outperform existing Transmission Control Protocol (TCP) and User Designed Datagram (UDP) to efficiently harness the abundant bandwidth made possible by Dense Wave Division Multiplexing (DWDM) optical technologies. This may include transport mechanisms such as Remote Direct Memory Access (RDMA) over Lambda and OS-bypass over Lambda, that are capable of delivering and sustaining multi-Gigabits/sec (Gbs) throughput to high-end scientific applications.
- Intelligent high-speed network interfaces-to significantly improve the end-to-end performance by addressing host system congestion issues, such as dynamically programmed transport protocol off-loading, OS bypass, electro-optical middleware, and high-speed I/O.
- High-speed cyber security systems-that operate efficiently at ultra high-speed (2.5 Gbs and 10 Gbs). Such systems should be based on a sound theoretical foundation and formal techniques, and in addition could exploit Artificial Intelligence (AI) techniques, such as fuzzy logic, neural networks, and genetic algorithms to improve their effectiveness.
- Network modeling and traffic engineering-new techniques for modeling and characterization of chaotic behaviors in complex traffic patterns, dynamic behavior of protocols, cyber security systems, and congestion control mechanisms.

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 second year of the Early Career Principal Investigator Program. A principal goal of this program is to identify exceptionally talented applied mathematicians, collaborative 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) Hold a tenure-track regular academic faculty position.
- (2) Have earned a Ph.D. degree or equivalent after July 1, 1998.
- (3) Are conducting research in applied mathematics, laboratories, 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 FY 2003 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 2003.

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.sc.doe.gov/sub/lab_map/index.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.science.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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