Office of Science Financial Assistance Funding Opportunity Announcement DE-PS02-09ER09-22

Joint Mathematics/Computer Science Institute

The Office of Advanced Scientific Computing Research (ASCR) of the Office of Science (SC), U.S. Department of Energy (DOE), hereby invites applications for research under a unified management structure to address key challenges where collaborative research in applied mathematics and computer science efforts are required to bridge the gap between large complex scientific applications software and next-generation hardware.

The strategic vision for the Advanced Scientific Computing Research (ASCR) program in the Department of Energy's Office of Science includes a portfolio of high performance computing resources to enable DOE and the Nation's world leadership in areas of science important to the Department's mission. ASCR plans to address these challenges through a balanced program that provides DOE's and the Nation's scientists with high performance production and leadership-class computing resources while fostering the architectural development of the next generation of high end computer hardware and supporting software. One key assumption that underpins the success of the "petascale to extreme scale" plan is that the scientific software application-computer hardware gaps expected to appear can be successfully addressed.

General-purpose, extreme scale computing systems are likely to be technologically feasible within the next 10-15 years. These systems could contain between 10 million and 100 million processing elements or cores. There is widespread agreement that these systems will push the envelope of a number of important technologies, including processor architecture, scale of multicore integration (perhaps into the range of 1000 cores per chip or beyond), power management, and packaging. Incremental or evolutionary advances of current programming paradigms and strategies have little chance of providing the functionality and utility needed to harness extreme scale computing for scientific discovery and advances. Transformational breakthroughs in programming models, system software, and algorithms will be necessary to enable scientific discovery through simulation on these leadership computers.

This Funding Opportunity Announcement calls for innovative approaches that integrate applied mathematics and computer science to develop the insights and tools that are required for computers at extreme scales to be effective tools for scientific discovery through simulation. The activities supported by this Announcement may be a combination of basic research, creation of algorithms for advanced architectures, and demonstration of new mathematical, computer science and algorithmic concepts. Conferences, "summer schools", or other similar activities that explore, in a collaborative setting, the research and utilization of the combination of applied mathematics and computer science to enable high-performance computing at the extreme scale may be considered. Partnerships among universities, National Laboratories, and industry are strongly encouraged.

More information on this solicitation is provided in the Supplementary Information below.

APPLICATION DUE DATE: June 5, 2009, 8:00 p.m., Eastern Time

<u>Formal applications</u> submitted in response to this Announcement must be received by June 5, 2009, 8:00 p.m. Eastern time, to permit timely consideration of awards. You are encouraged to transmit your application well before the deadline. APPLICATIONS RECEIVED AFTER THE DEADLINE WILL NOT BE REVIEWED OR CONSIDERED FOR AWARD.

ATTENTION - CHANGE IN SUBMISSION REQUIREMENT EFFECTIVE March 12, 2009

The Office of Science is now requiring all financial assistance applications be submitted through the Department of Energy e-Center (IIPS) <u>http://doe-iips.pr.doe.gov/</u>. Applicants will still need to visit the Grants.gov website <u>http://www.grants.gov/</u> to download the required Application Package (forms), by clicking on "Apply for Grants" and searching for the Funding Opportunity Announcement.

For Instructions on the Use of IIPS visit this web page, IIPS Instructions. <u>http://www.sc.doe.gov/grants/iips-Instructions.html</u>

Registration Requirements: There are several one-time actions you must complete in order to submit an application (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 Grants.gov). See http://www.grants.gov/GetStarted. Use the Grants.gov Organization Registration Checklist at

<u>http://www.grants.gov/assets/OrganizationRegCheck.doc</u> 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 least 21 days to complete these requirements. It is suggested that the process be started as soon as possible.

FOR FURTHER INFORMATION CONTACT: Karen Pao, karen.pao@science.doe.gov, (301) 903-5384; and Osni Marques, oamarques@ascr.doe.gov, (301) 903-9925.

SUPPLEMENTARY INFORMATION:

The complexity of extreme-scale systems represent a major challenge to large application codes: how can the scientific applications efficiently use these systems?

With the hardware breakthroughs required to reach extreme scales, application software can no longer ignore the radical increases in node and processor core counts, multi-mode parallelism, reduced memory per core, heterogeneous nodes, and fault tolerance. This unprecedented level of complexity will require significant new levels of scalability and functionality - as well as reliability and ease of use - in application software.

A wide variety of topics may be appropriate for this research effort. Examples may include, but not limited to:

- Synchronization barrier: Algorithms for science and engineering applications require synchronization. These barriers may be implemented in the application codes either explicitly or by using parallel language directives, in the communication libraries, in systems calls, or a combination of all of the above. Are there opportunities for distributing barriers and achieving greater performance?
- Fault tolerance for optimizing systems performance: For large-scale science and engineering applications, it is imperative that the entire system can handle faults and failures gracefully. Are there new tools that will inform the application teams as to how to optimally divide fault tolerance amongst the numerical algorithms for an application, the simulation software, and the systems software and hardware?
- Efficient implementation and optimization of scientific software: Algorithms for science and engineering applications often follow certain computation and communication patterns. Are there novel methods for the analysis of these patterns that may lead to compiler optimization, performance tuning, automated tuning of application codes, and the efficient implementation of these algorithms on current and future architecture?
- Architecture-aware programming models and algorithms: Whether the architecture is manycore, multicore, or anything else, scalability of the applications is the key to fully utilizing the available compute power. Can we develop portable programming models that achieve scalability of the application codes on a class or multiple classes of architecture? Can numerical algorithms for applications be developed so that they are aware of the architecture and automatically perform a variety of tasks to optimize performance?

For more information, please see the following workshop and conference reports:

- Workshop on Computer Science/Applied Math Institutes and High Risk / High Payoff Technologies for Applications, October 7-9, 2008. http://www.sc.doe.gov/ascr/ProgramDocuments/Docs/MathCSWorkshopReport.pdf
- Scientific Impacts and Opportunities in Computing, January 9-12, 2008. http://www.sc.doe.gov/ascr/ProgramDocuments/Docs/ScientificImpacts&Oppor.pdf
- Software Development Tools for Petascale Computing, August 1-2, 2007. http://www.sc.doe.gov/ascr/WorkshopsConferences/Docs/sdtpc_workshop_report.pdf
- Modeling and Simulation at the Exascale for Energy and the Environment Town Hall Meetings, April 17-18, 2007, May 17-18, 2007, and May 31-June 1, 2007. http://www.sc.doe.gov/ascr/ProgramDocuments/Docs/TownHall.pdf

Management Plan

The application must contain a management plan that establishes and maintains the appropriate balance between research activities in applied mathematics and computer science. The Principal Investigator will be identified in the application as the individual responsible for managing the overall project. The management plan will be evaluated for feasibility and compatibility with the proposed technical goals.

Community Building

An important goal of this notice is to establish the foundation for expanding the traditional boundaries of both mathematics and computer science to continuously advance both fields, and to build a community of versatile researchers who are committed to the common goal of high-performance computing for scientific discovery. The application will need to include plans for the dissemination of research results, such as:

- Publications, conferences, and other educational activities: what mechanisms will the project employ to present its work to a broader community to ensure sustained activities in the research area?
- Code release: how will the codes be released to allow other researchers to continue building and expanding on the knowledge gained?
- Testing at scale: will the project perform software testing at scale? If so, what are the requirements for this testing (for example, hardware, specific architecture, specific testbed, etc)?

Collaboration and Communication

The application should identify potential collaborations or other interactions that will facilitate the exchange of ideas and dissemination of information among research centers in industry, universities, and/or laboratories. Synergistic collaborations with researchers in Federally Funded Research and Development Centers (FFRDCs), including the DOE National Laboratories, are also encouraged, though no funds will be provided to these organizations under this Announcement. Further information on preparation of collaborative applications may be accessed via the internet at: <u>http://www.sc.doe.gov/grants/Colab.html</u>

Program Funding

It is anticipated that up to a total of \$4 million annually will be available for multiple awards for this program. Awards are planned to be made in Fiscal Year 2009, and applications may request project support for up to three years. All awards are contingent on the availability of funds and programmatic needs. DOE is under no obligation to pay for any costs associated with the preparation or submission of an application. DOE reserves the right to fund, in whole or part, any, all, or none of the applications submitted in response to this Notice.

Merit Review Criteria

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 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; and
- 4. Reasonableness and Appropriateness of the Proposed Budget.

The evaluation process will include program policy factors, such as the relevance of the proposed research in terms of the solicitation and the agencies' programmatic needs. Note that external peer reviewers are selected with regard to both their scientific expertise and the absence of conflict-of-interest issues. Both Federal and non-Federal reviewers may be used, and submission of an application constitutes agreement that this is acceptable to the investigator(s) and the submitting institution.

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

Posted on the Office of Science Grants and Contracts Web Site May 6, 2009.