Office of Science
Financial Assistance
Funding Opportunity Announcement
DE-PS02-06ER06-26

Accelerating Delivery of Petascale Computing Environment At the DOE Leadership Computing Facility At the Oak Ridge National Laboratory

The Office of Science (SC), U.S. Department of Energy (DOE), hereby announces interest in receiving applications for projects in the Advanced Scientific Computing Research program to accelerate delivery of a petascale computing environment to meet scientific computational needs. Many challenges of multi-scale, multi-disciplinary problems now facing science programs in DOE require advanced modeling and simulation capabilities of petascale computers. This Notice is seeking applications that contribute to the creation of Computational End Stations or the development of Computational Environments.

Computational End Stations: The creation of Computational End Stations will provide the scientific applications software and world-class computational specialists needed for researchers in science and/or engineering to take full advantage of the extraordinary capabilities provided by the Leadership Computing Facility (LCF) at Oak Ridge National Laboratory (ORNL) (see supplementary information). This concept is described in the report produced by the High-End Computing Revitalization Task Force Workshop, which notes that "establishing Computational End Stations is one integrated solution to the needs of developers and users.... Application codes and their associated analysis tools are the instruments of computational science."

Each Science/Engineering End Station team will be responsible for:

- Creating, maintaining, evolving, and supporting the suite of capability computational codes needed to advance the scientific research program proposed for this End Station and the represented research field.
- Executing the scientific research program laid out in their Computational End Station application.
- Providing outreach to their research community through workshops, web portals, and other mechanisms.

Computational Environment: A comprehensive, scientific computing software infrastructure that fully integrates applied mathematics, computer science, and computational science in the physical, biological, and environmental sciences for scientific discovery is required at the petascale level.

Applications are sought that:

- Create or adapt existing scientific simulation codes to achieve high single node performance; scale to thousands of nodes and tens-of-thousands of processors; and be readily portable to other computer architectures.
- Integrate computational science focused on the petascale with discipline-driven applications through teaming and partnerships with computer scientists and applied mathematicians through mechanisms and innovative approaches that include:

    Algorithms, methods and libraries fully scalable to many thousands of processors with full performance portability.

    Component-based, fully integrated, terascale and petascale program development and tools, which scale effectively and provide maximum utility and ease-of-use to developers and scientific end users.

    Systems software that scale to hundreds-of-thousands of processors, support high performance application-level communication, I/O, performance analysis and optimization, and provide the highest levels of fault tolerance, reliability, manageability, and ease of use for end users, tool developers and system administrators.

    Scalable, intuitive systems fully supportive of SciDAC see: (http://www.scidac.org) application requirements for moving, storing, analyzing, querying, manipulating and visualizing multi-petabytes of scientific data and objects.

It is expected that applications submitted in response to this Notice will be:

- For scientific simulation teams involving more than one university, industry or non- profit organization. (Note- Federal Laboratories (FL) and Federally Funded Research and Development Centers (FFRDCs) are not eligible for award under this Notice.)
- Focused on the goals of either the Computational End Stations or Computational Environments

Applications must describe the computational approach for interacting with the Leadership Computing Facility at Oak Ridge National Laboratory. At a minimum, this description should include:

- Programming languages, libraries, and other software used.
- Description of the underlying mathematical formulation (e.g., ODE, PDE).
- Algorithms and numerical techniques employed (e.g., finite element, iterative solver).
- Parallel programming system used (e.g., MPI, OpenMP, "embarrassingly" parallel).
- Evidence that the principal computational codes to be used in this project will make effective use of the LCF at ORNL.
- For data-intensive applications, describe the data storage and transfer requirements.

APPLICATION DUE DATE: October 11, 2006, 8 PM Eastern Time

Applications must be submitted using Grants.gov, the Funding Opportunity Announcement can be found using the CFDA Number, 81.049 or the Funding Opportunity Announcement number,

DE-PS02-06ER06-26. Applicants must follow the instructions and use the forms provided on Grants.gov.

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SUPPLEMENTARY INFORMATION:

Background: Leadership Computing at ORNL
The Leadership Computing Facility at Oak Ridge National Laboratory has become a unique world-class scientific resource that provides the scientific community with orders of magnitude more computing capability (performance, memory, etc.) than is now available. While establishing this new level of scientific capability for the Nation, the LCF proactively engages the scientific and engineering communities and issues calls for applications to realize the breakthroughs promised by its extraordinary capabilities. Currently, LCF at ORNL houses two different systems purpose-built for science - an 18.5TF Cray X1E scalable vector system and a 25TF Cray XT3 super scalar system. It is planned that the Cray XT3 will be upgraded to 250+ TF in 2007 and a new 1000TF Cray Baker system will be deployed in 2008.

LCF continues to leverage the substantial number of core system and applications software packages and kernels currently being developed and optimized for the XT3 and Red Storm systems under DOE-SC and DOE-NNSA sponsorship, as well as the growing base of application from other Cray XT3 customers.

The allocation of computing resources available to individual projects will not be part of this solicitation but will be contingent on review and award through the process as described at: http://hpc.science.doe.gov/. Within the available computational resources, every effort will be made to ensure that successful applications will have the resources needed to support their efforts.

Posted on the Office of Science Grants and Contracts Web Site
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