Office of Science
Financial Assistance
Funding Opportunity Announcement
DE-PS02-07ER07-09

Scientific Discovery Through Advanced Computing: Accelerator Science and Simulation

The Offices of Advanced Scientific Computing Research (ASCR), High Energy Physics (HEP), Nuclear Physics (NP), and Basic Energy Sciences (BES), U.S. Department of Energy (DOE), hereby announce their interest in receiving applications for basic Research and Development (R&D) projects relevant to the development of advanced simulations of particle accelerators and associated technologies. This research should provide the capability for comprehensive 3-dimensional, end-to-end modeling of existing and proposed particle accelerators, and advanced acceleration concepts, particularly aimed at HEP and NP applications, to optimize operations of current facilities and the design of future facilities. Subject to appropriations, funds are anticipated to be available within the SciDAC programs of ASCR, HEP, and NP to support this research.

A companion Program Announcement to DOE Laboratories (LAB 07-09) will be posted on the Office of Science Grants and Contracts Web Site at: http://www.science.doe.gov/grants/.

APPLICATION DUE DATE: January 17, 2007, 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-PS02-07ER07-09. Applicants must follow the instructions and use the forms provided on Grants.gov.

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SUPPLEMENTARY INFORMATION:

Background: Scientific Discovery Through Advanced Computing Program (SciDAC)

The Scientific Discovery through Advanced Computing (SciDAC) program was initiated in 2001 as a partnership involving all SC program offices - Advanced Scientific Computing Research, Basic Energy Sciences, Biological and Environmental Research, Fusion Energy Sciences, High-Energy Physics and Nuclear Physics - to fully realize the potential of emerging high performance computers at that time for advancing scientific discovery. Researchers have achieved key scientific insights in a number of areas of National importance, yet many challenges of multi-scale, multi-disciplinary problems now facing science programs in DOE require advanced modeling and simulation capabilities on petascale computers. SciDAC projects should:

- **Address obtaining significant insight into, or actually solve, a challenging problem of National scientific or engineering significance clearly related to DOE missions through computational science,**
- **Create open source scientific simulation codes that: achieve high single node performance; scale to thousands of nodes and tens-of-thousands of processors; and can be readily ported to other computer architectures,**
- **Develop applied mathematics and computer science methodology focused on computational science at the petascale and work with application scientists to apply innovations,**
- **Integrate computational science with discipline-driven applications through teaming and partnerships with computer scientists and applied mathematicians,**
- **Engage experimental and observational data-intensive science, and/or**
- **Empower new scientific communities to achieve scientific discovery through computational science.**

Grant Application

Accelerator Science and Simulation: A comprehensive, coherent petascale simulation capability for the U.S. accelerator community is critical for the near and long-term priorities of DOE's Office of Science. We desire grant applications that can deliver a wide range of simulation capabilities in accelerator physics, and in particular those that broadly address the needs and priorities of the High Energy Physics and Nuclear Physics communities, and can integrate electrodynamic modeling of accelerator structures with end-to-end beam dynamics and propagation. Applications that are limited to only particular phenomena or narrow aspects of accelerator physics will receive lower priority for funding.

High Energy Physics priorities in accelerator simulation are driven by optimization needs of existing HEP accelerators, such as the B-Factory and Tevatron; design of possible future accelerators, such as International Linear Collider (ILC) and other next-generation facilities including the neutrino factory / muon collider concept; and maintaining a vital DOE accelerator R&D program. Nuclear Physics priorities are the development of a design for a US rare isotope beam capabilities and maintaining an accelerator R&D development plan which includes the needs of the Continuous Electron Beam Accelerator Facility (CEBAF) Upgrade, electron cooling required for the luminosity upgrade of the Relativistic Heavy Ion Collider and, in the future, addresses the exploration of an electron-ion collider that would allow the gluon saturation of nuclear matter to be seen.

Basic Energy Sciences priorities include the optimization and upgrade of the accelerator-based BES light sources and neutron scattering facilities. In the design and commissioning of new Free Electron Lasers (FELS) such as the Linac Coherent Light Source (LCLS) simulations of the creation and transport of high brightness electron beams are another BES priority.

Topic areas for advanced modeling include, but are not limited to: high-accuracy computation of modes for superconducting RF cavities; realistic simulation of wakefield effects; parallelization of Radio Frequency Quadrupole simulations; self-consistent 3D calculations of Coherent Synchrotron Radiation, forces and their effects on the beam; electron cooling of beams; heavy ion transport: optimization of Particle-In-Cell codes; and adaptive mesh techniques for intense beams. Accelerator simulation codes which run on a variety of platforms; scale to petaflops and many thousands of processors; which are robust, documented, and can be easily used by the community of accelerator researchers; and are well integrated with visualization capacities will have the greatest impact on the field. Applications should address how they will meet these criteria.

In addition, grant applications must describe the computational approach for interacting with the SciDAC Institutes and Centers for Enabling Technologies. 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).**
- **Or data-intensive applications, describe the data storage and transfer requirements.**

Synergistic collaborations with researchers in Federal Laboratories and Federally Funded Research and Development Centers (FFRDCs), including the DOE National Laboratories are expected, though no funds will be provided to these organizations under this Notice. Laboratories should respond to the LAB 07-09 Announcement posted at: http://www.science.doe.gov/grants/. Partnerships among multiple institutions, that may include universities, laboratories, and/or private institutions, are anticipated for the scientific selection teams of the submissions. Additional information on collaboration is available in the Application Guide for the Office of Science Financial Assistance Program that is available via the Internet at the web address: http://www.science.doe.gov/grants/Colab.html. In view of the wide applicability of the simulation codes called for in this request, and a potentially large group of users with different needs and requirements, we expect that successful applications will incorporate a clear management structure, as well as deliver the tools needed by the scientific applications in a timely fashion. The scientific teams should propose a program of work that achieves their goals consistent with this management structure, and aligned with the priorities of the High Energy Physics and Nuclear Physics programs as outlined above.

Applications that do not include a formal collaboration with one, or more, SciDAC Centers for Enabling Technology will not be considered for award. The Centers for Enabling Technology are authorized to enter into such collaborations within their existing scope and budget. No funds are to be requested under this Notice for sub-contracts, or task orders, to a Center for Enabling Technology for participation in a proposed collaboration.

Applicants must include a separate budget and statement for each proposed funding source. Successful applicants are not required to request funding from all three participating Office of Science programs; however, proposed funding sources should align with the specific nature of the work being performed, as documented in the application, and reflect the collaborative nature of the SciDAC program.

Posted on the Office of Science Grants and Contracts Web Site
December 1, 2006.