# Office of Science Financial Assistance Funding Opportunity Announcement DE-PS02-07ER07-20

# Scientific Discovery through Advanced Computing: Computational Magnetohydrodynamics

The Office of Fusion Energy Sciences (OFES) of the Office of Science (SC), U.S. Department of Energy (DOE), hereby announces its interest in receiving applications for the development and application of high performance scientific simulation codes on topical areas that are important to burning plasma physics experiments, such as ITER, and which will contribute to establishing the scientific foundation for an integrated fusion simulation in the future. The goal is the creation of codes that achieve high performance on a single node, scale to thousands of nodes and tens-of-thousands of processors, and have the potential to be ported to future generations of high performance computers.

A companion Program Announcement to DOE Laboratories (LAB 07-20) will be posted on the Office of Science Grants and Contracts web site at: <a href="http://www.science.doe.gov/grants/LAB07\_20.html">http://www.science.doe.gov/grants/LAB07\_20.html</a>.

# **LETTER OF INTENT DUE DATE:** April 10, 2007

A Letter of Intent (LOI) to submit an application is **REQUIRED** and should be submitted by April 10, 2007. **Failure to submit a Letter of Intent by an applicant may preclude the full application from due consideration.** The Letter of Intent should be submitted electronically by E-mail to: John.Sauter@science.doe.gov and Rostom.Dagazian@science.doe.gov. Please include "Letter of Intent for Announcement DE-PS02-07ER07-20" in the subject line.

The purpose of the Letter of Intent (LOI) is to facilitate the OFES in planning the peer review and the selection of potential reviewers for the proposal. For this purpose, the LOI must include a one-page abstract of the proposed research and list the names and institutional affiliations of Principal Investigators, any Co-Principal Investigators, key investigators, collaborators or consultants, so as to identify any potential conflict of interest in the selection of qualified reviewers for the application.

**APPLICATION DUE DATE:** May 22, 2007, 8 PM Eastern Time

Applications must be submitted using <u>Grants.gov</u>, the Funding Opportunity Announcement can be found using the CFDA Number, 81.049 or the Funding Opportunity Announcement Number, DE-PS02-07ER07-20. Applicants must follow the instructions and use the forms provided on Grants.gov.

#### FOR FURTHER INFORMATION CONTACT:

**PROGRAM MANAGER:** Dr. Rostom Dagazian, Office of Fusion Energy Sciences, SC-24.2

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E-MAIL: Rostom.Dagazian@science.doe.gov

### SUPPLEMENTARY INFORMATION:

Applications for development of codes to model macro-scale dynamics in fusion-grade tokamak plasmas should address relevant physics issues in 3-dimensional extended magnetohydrodynamics (MHD), such as 1) full nonlinear sawtooth oscillation modeling in fusion-grade plasmas, 2) tearing mode and neoclassical tearing mode excitation and control in high-beta plasmas, 3) nonlinear evolution and control of resistive wall modes, including toroidal flows, 4) effects of fast ions, such as fusion-produced alpha particles, on MHD phenomena in tokamak plasmas, 5) edge MHD-type instabilities and their non-linear evolution, 6) two-fluid and kinetic effects on MHD modes, 7) the onset and evolution of major disruptions, 8) differences in modeling resulting from the employment of different closures, 9) differences in scalability to teraflop and petaflop computing scales resulting from differences in numerical treatments and finally 10) Validation and Verification of nonlinear results. Strong team effort focusing on a single (integrated) code will be given preference.

In addition to descriptions of the physical models in the codes, applications should include information on the proposed mathematical algorithms, computer science methods, and data management and visualization techniques. Applicants should include information on the readiness of their codes to run on today's terascale computing facilities supported by the Office of Science-including results from realistic scaling studies, if available-and should discuss their plans for taking advantage of the emerging availability of petascale resources. In particular, applicants should address the question of how access to increasingly powerful computational resources will make a difference in achieving their targeted research goals and how it will enhance the overall physics fidelity of their simulation models.

A strong verification and validation (V&V) component is essential for this effort and therefore applicants should discuss their V&V plans in sufficient detail. In addition, since crossbenchmarking of different codes is an indispensable and often-used verification tool for large-scale simulation codes, successful applicants are expected to share data and other supporting information in a timely fashion with other researchers. Applicants are expected to follow the OFES data sharing guidelines for large-scale computational projects which can be found at: <a href="http://www.ofes.fusion.doe.gov/FusionDocuments/OFES\_DataSharingGuidelines.pdf">http://www.ofes.fusion.doe.gov/FusionDocuments/OFES\_DataSharingGuidelines.pdf</a>.

Applicants should also discuss their plans for forming substantive partnerships that integrate applied mathematics and computer science enabling technologies with their proposed efforts, as well as their plans for collaboration and interaction with the other SciDAC projects in the OFES portfolio, including the Fusion Simulation Project (FSP) prototype centers.

Applications should include a timeline for the major activities of the proposed project and should indicate which project personnel will be responsible for which activities. Tables of quarterly milestones should also be provided by each of the collaborating institutions for each year of proposed work.

## **Scientific Discovery through Advanced Computing**

Beyond the scientific computing and computational science research embedded in the Office of Science (SC) core research programs, SC invests in a portfolio of coordinated research efforts directed at exploiting the emerging capabilities of terascale and petascale computing under the collective title of Scientific Discovery through Advanced Computing (SciDAC). The research projects in the SciDAC portfolio respond to the extraordinary difficulties of realizing sustained peak performance for scientific applications, such as simulating combustion, making multicentury climate predictions, understanding and controlling a burning plasma, and designing new particle accelerators that require terascale and petascale capabilities to accomplish their research goals. In recognition of these difficulties, the SciDAC research projects are collaborative efforts involving teams of physical scientists, mathematicians, computer scientists, and computational scientists working on major software and algorithm development for problems in the core research programs of the Office of Science. Research funded in the SciDAC portfolio is enabling teams of laboratory and university researchers to solve some of the most challenging scientific problems in the core programs of the Office of Science at a level of accuracy and detail never before achieved. A complete description of the SciDAC program can be found at: http://www.scidac.gov/

#### **Background: Advanced Simulation of Fusion Plasmas**

U.S. participation in the international ITER Project-a Presidential Initiative-is an important next step in fusion research. ITER is designed to produce, control, and sustain a burning plasma and research on ITER is expected to provide sufficient information on the complex science of burning plasmas to make a definitive assessment of the scientific feasibility of fusion power. The U.S. and the other ITER partners signed a 35-year agreement on November 21, 2006, to construct, operate, and decommission the ITER facility.

Following the signing of the ITER agreement, the Office of Fusion Energy Sciences decided to focus its part of the SciDAC program on burning plasma physics needs. Accordingly, the new and renewal applications for the fusion SciDAC program will concentrate on developing reliable computational modeling capabilities for dealing with burning plasma physics issues relevant to ITER, and on establishing the scientific groundwork for an integrated fusion simulation project. Such a project is needed to develop the predictive capability necessary to improve experimental planning for ITER and enhance scientific understanding gained from the operation of ITER.

The scope and complexity of these projects will require close collaboration among researchers from the computational and theoretical plasma physics, computer science, and applied mathematics disciplines. Thus, this solicitation calls for the creation of topical centers as the organizational basis for a successful application. A topical center is a multi-institutional, multi-disciplinary team that will:

- Create scientific simulation codes that take full advantage of terascale computers
- Work closely with other SciDAC teams to ensure that the best available mathematical algorithms and computer science methods are employed, and
- Manage the work of the Center in a way that will foster good communication and decision making.

#### Collaboration

Collaborative research projects with other institutions, such as universities, industry, non-profit organizations, and Federally Funded Research and Development Centers (FFRDCs), including the DOE National Laboratories, are encouraged under this Announcement. Applications submitted from different institutions, which are directed at a single research activity, should clearly indicate they are part of a proposed collaboration and contain a brief description of the overall research project. However, each application must have a distinct scope of work and a qualified principal investigator who is responsible for the research effort being performed at his or her institution. Further information on preparation of collaborative applications may be accessed via the Internet at: http://www.science.doe.gov/grants/Colab.html.

Posted on the Office of Science Grants and Contracts Web Site March 6, 2007.