

**Office of Science**  
**Notice DE-FG01-04ER04-09**

*Scientific Discovery  
through Advanced Computing -  
Advanced Simulation of Fusion Plasmas*

**Department of Energy**

**Office of Science Financial Assistance Program Notice DE-FG01-04ER04-09: Scientific Discovery through Advanced Computing - Advanced Simulation of Fusion Plasmas**

**AGENCY:** U.S. Department of Energy

**ACTION:** Notice inviting grant applications.

**SUMMARY:** 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 grant applications for the development of scientific simulation codes needed to address complex problems in fusion energy sciences. The goal is the creation of codes that achieve high performance on a single node, scale to hundreds of nodes and thousands of processors, and have the potential to be ported to future generations of high performance computers. This announcement is focused on topical areas that are important to a burning plasma physics experiment, such as ITER, and will contribute to establishing the scientific foundation for an integrated fusion simulation in the future. Specific areas of interest include:

- turbulence and transport in order to understand energy and particle confinement in burning plasmas,
- macroscopic equilibrium and stability to predict stability limits in magnetically confined plasmas,
- boundary layer effects in plasmas in order to understand the transport of heat and particles in the edge region of a fusion device, and
- electromagnetic wave/particle interactions to be able to predict heating and current drive in burning plasmas.

The full text of Program Notice DE-FG01-04ER04-09 is available via the Internet at the following web site address: <http://www.science.doe.gov/production/grants/grants.html>.

**DATES:** Applicants are requested to submit a Letter-of-Intent by February 16, 2004. This letter should include the name of the applicant, the title of the project, the name of the Principal Investigator(s)/project director, the amount of funds requested, and a one-page abstract. Letters-of-Intent will be used to organize and expedite the merit review process. Failure to submit such letters will not negatively affect a responsive application submitted in a timely fashion. The

Letter-of-Intent should be sent by E-mail to [john.sauter@science.doe.gov](mailto:john.sauter@science.doe.gov), and the subject line should state: Letter-of-Intent regarding Program Notice DE-FG01-04ER04-09.

Formal applications submitted in response to this notice must be received by DOE no later than 4:30 p.m., March 23, 2004. Electronic submission of formal applications in PDF format is required.

**ADDRESSES:** Letters-of-Intent should be sent by E-mail to [john.sauter@science.doe.gov](mailto:john.sauter@science.doe.gov), and the subject line should state: Letter-of-Intent regarding Program Notice DE-FG01-04ER04-09. Full applications in response to this solicitation Number DE-FG01-04ER04-09 must be submitted electronically 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. It is suggested that this registration be completed several days prior to the date on which you plan to submit the formal application. 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. **IIPS offers the option of submitting multiple files—please limit submissions to only one file within the volume if possible, with a maximum of no more than four files.** 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](mailto:helpdesk@pr.doe.gov), or you may call the help desk at: 800-683-0751; residents of Canada call: 202-287-1491. Further information on the use of IIPS by the Office of Science is available at: <http://www.sc.doe.gov/production/grants/grants.html>.

[The following was omitted from the Federal Register version: If you are unable to submit an application through IIPS, please contact the Grants and Contracts Division, Office of Science at: (301) 903-5212 or (301) 903-3604, 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. Stephen Eckstrand or Dr. Arnold Kritz, Office of Fusion Energy Sciences, SC-55/Germantown Building, U.S. Department of Energy, 1000 Independence Ave. SW, Washington, DC 20585-1290. Telephone numbers and e-mail addresses are listed below:

Stephen Eckstrand: telephone 301-903-5546, e-mail [steve.eckstrand@science.doe.gov](mailto:steve.eckstrand@science.doe.gov)  
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## **SUPPLEMENTARY INFORMATION:**

### **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 multi-century 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.osti.gov/scidac/>.

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

In January 2003, the President announced that the United States would seek to join ITER negotiations, and the United States has subsequently done so. ITER is an ambitious international research project to harness the promise of fusion energy. Following this announcement, 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 (see section on Collaboration and Coordination below).

Partnerships among universities, national laboratories, and industry are encouraged. Collaborations between computational plasma physicists, applied mathematicians and computer scientists are also encouraged. Applicants may request additional funding for associated applied mathematics or computer science work that is needed to support the development of the scientific applications codes as part of Scientific Application Partnership Program.

Applications are being sought in the following four topical areas:

### **1. Macroscopic Equilibrium and Stability:**

Applications for development of codes to model macroscale 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 nonlinear evolution, 6) two-fluid and kinetic effects on MHD modes, and 7) the onset and evolution of major disruptions.

### **2. Turbulence and Transport:**

Applications for studies of microturbulence and transport of energy, particles and momentum need to address key scientific problems, such as 1) Bohm versus gyro-Bohm scaling and the transition between the two regimes, 2) transport barrier formation and dynamics including the different transport channels, 3) statistics of mesoscale intermittency in transport (e.g., avalanches), 4) the dynamics of transport perturbation events such as heat pulse propagation, and 5) electromagnetic turbulence and electron heat transport due to magnetic perturbations.

### **3. Boundary Layer/Edge Plasma Modeling:**

Applications related to edge modeling should address scientific issues such as 1) evolution of the edge transport barrier including the mechanism for L-H mode transition, transport within the edge barrier, the trigger mechanism for ELM crashes, the frequency of ELM crashes, and the plasma energy, density and current lost during each ELM crash, 2) effects associated with the scrape-off layer, divertor and plasma wall interaction including plasma convective transport to the wall, neutral recycling, wall erosion, and inward impurity transport from the wall.

### **4. Electromagnetic Wave/Plasma Interaction:**

Applications related to the role of radio frequency waves in burning plasmas need to address topics such as 1) wave-plasma interactions in plasmas with a large energetic alpha particle population and in plasmas with a radio frequency driven high velocity tail population, 2) the role of non-inductive currents and energetic particle populations on MHD equilibrium and instabilities in burning plasmas, such as the effects of localized radio frequency currents or heating on island formation in neoclassical tearing modes, sawtooth oscillations and disruptions, 3) the effect of radio frequency on the control of turbulence and transport barrier formation due to localized heating, current drive, or radio frequency driven plasma flows, and 4) the effect of the plasma edge on the antenna and the ability to launch radio frequency waves in burning plasma experiments.

## **Collaboration and Coordination**

It is expected that all applications submitted in response to this notice will be for collaborative centers involving more than one institution. Each institution involved in a proposed collaborative research project must submit a separate application, identifying the co-PI who has responsibility for the project research carried out at that institution. Also, each institution must include a separate Face Page (DOE F 4650.2), Budget Page (DOE F 4620.1), Assurance of Compliance (DOE F 1600.5), and FA CERTS for the institution. These collaborative research applications must include a common technical description of the overall research project, but must also specify the distinct scope of the work that will be carried out at each institution. The primary PI for the collaborative research project should include a summary budget for the entire project, including annual funding proposed for each institution and the annual funding proposed for Scientific Application Partnership Program activities. Synergistic collaborations with researchers in federal laboratories and Federally Funded Research and Development Centers (FFRDCs), including the DOE National Laboratories are encouraged, though no funds will be provided to these organizations under this Notice.

Further information on preparation of collaborative proposals is available in the Application Guide for the Office of Science Financial Assistance Program that is available via the Internet at: <http://www.science.doe.gov/production/grants/Colab.html>.

Since each center will be developing new physics models and computational tools that are needed for an integrated fusion simulation capability, it is important that there be good communication between the different centers. It is also important to have guidance on code capabilities and development priorities from the broader fusion, scientific and computational communities. Thus, all successful projects should plan to work with the SciDAC management structure established by the Office of Science and the Office of Fusion Energy Sciences at the beginning of the SciDAC program. The SC SciDAC management team holds an annual principal investigators meeting to ensure good communication between the SciDAC applications projects and the SciDAC applied mathematics and computer science projects. The Office of Fusion Energy Sciences' oversight of the fusion SciDAC projects includes a program advisory committee, which holds an annual coordination meeting to review the progress of each of the fusion SciDAC projects and to develop priorities for future work.

## **Program Funding**

Approximately \$1,700,000 of Fiscal Year 2004 funding will be available for grant awards in FY 2004. Additional funding for the proposed project may be available through the Office of Advanced Scientific Computing Research for closely related research in computer science and/or applied mathematics. Applications may request support for up to three years, with out-year support contingent on the availability of funds and satisfactory progress. To support multi-disciplinary, multi-institutional efforts, annual funding levels of up to \$1 million may be requested for the scientific application work and up to \$200,000 per year for the Scientific Application Partnership Program work.

As required by the SC grant application guide, applicants must submit their budgets using the Budget Page (DOE Form 4620.1) with one Budget Page for each year of requested funding. The requested funding for the proposed work in computer science and applied mathematics should be included on a separate Budget Page. However, applicants are also requested to list the proposed computer science and applied mathematics costs separately in an appendix, as the Office of Advanced Scientific Computing Research may support this part of the work (up to about 20 percent of the total project cost). The Office of Fusion Energy Sciences expects to fund two or three centers, depending on the size of the awards.

## **Applications**

Applications will be subjected to scientific merit review (peer review) and will be evaluated against the following criteria listed in descending order of importance as codified in 10 CFR 605.10(d) (<http://www.science.doe.gov/production/grants/605index.html>):

1. Scientific and/or technical merit of the project;
2. Appropriateness of the proposed method or approach;
3. Competency of the applicant's personnel and adequacy of the proposed resources; and
4. Reasonableness and appropriateness of the proposed budget.

The evaluation under the first criterion in 10 CFR Part 605.10(d), Scientific and Technical Merit, will pay particular attention to:

- a) The importance of the proposed project to the mission of the Office of Fusion Energy Sciences;
- b) The potential of the proposed project to advance the state-of-the-art in computational modeling and simulation of plasma behavior; and
- c) The need for extraordinary computing resources to address problems of critical scientific importance to the fusion program and the demonstrated abilities of the applicants to use terascale computers.

The evaluation under item 2, Appropriateness of the Proposed Method or Approach, will also consider the following elements related to quality of planning and management:

- a) If the project involves more than one scientific code, how the use of multiple codes will contribute to a coherent set of scientific objectives that are more readily achieved through the use of multiple codes;
- b) Soundness of the plan for effective management of the project;
- c) Quality of plan for ensuring communication with math and computer science projects and with other relevant SciDAC projects;
- d) Viability of plan for verifying and validating the models developed, including close coupling with experiments for ultimate validation; and
- e) Quality and clarity of proposed work schedule and deliverables.

Note that external peer reviewers are selected with regard to both their scientific expertise and the absence of conflict-of-interest issues. 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.

General information about development and submission of applications, eligibility, limitations, evaluations and selection processes, and other policies and procedures may be found in the Application Guide for the Office of Science (SC) Financial Assistance Program and in 10 CFR Part 605. Electronic access to SC's Financial Assistance Guide and required forms is made available via the Internet using the following Web site address:  
<http://www.science.doe.gov/production/grants/grants.html>.

In addition, for this notice, project descriptions must be 25 pages or less, including tables and figures, but excluding attachments. The application must also contain an abstract or project summary on a separate page with the name of the principal investigator, mailing address, phone, FAX, and email listed. The application must also include letters of commitment from all non-funded collaborators (briefly describing the intended contribution of each to the research), and short curriculum vitae for the principal investigator and any co-PIs.

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

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Director  
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