# Office of Science
# Notice DE-FG01-05ER05-11

# *Scientific Discovery through Advanced Computing - Fusion Simulation Prototype Centers*

**Department of Energy**

**Office of Science Financial Assistance Program Notice DE-FG01-05ER05-11: Scientific Discovery through Advanced Computing - Fusion Simulation Prototype Centers**

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

**ACTION:** Notice inviting grant applications.

**SUMMARY:**The SciDAC Program, the Office of Fusion Energy Sciences (OFES) and the Office of Advanced Scientific Computing Research (OASCR) of the Office of Science (SC), U.S. Department of Energy (DOE), hereby announce their interest in receiving cooperative agreement applications for the development of specific scientific simulation codes that can become components of an integrated fusion plasma simulation. These integrated fusion plasma simulation prototype codes should focus on the development of new capabilities that couple together a wider range of physical phenomena in an integrated package of simulation codes (or code suite) than is currently being done.

The SciDAC Program, the Office of Fusion Energy Sciences and the Office of Advanced Scientific Computing Research are planning a multi-institutional Fusion Simulation Project (FSP) to develop an advanced integrated simulation capability for both existing magnetic fusion experiments and next-generation burning plasma experiments such as the International Thermonuclear Experimental Reactor (ITER). As a first step toward the initiation of the FSP, SciDAC, OFES and OASCR are seeking focused integration initiatives in topical areas that are particularly important to ITER. The goal of each initiative is to develop an integrated predictive modeling capability for a specific topical area while, at the same time, dealing with the integration issues that will be faced by the FSP. The experience with mathematical tools, innovative algorithms and high- performance computer architectures that is gained during these initiatives will be important in later phases of the FSP. Thus, close collaboration among fusion scientists, applied mathematicians and computer scientists is essential for the success of this initiative. The specific areas of interest are:

1) An integrated simulation of the edge/boundary region of a fusion plasma: The plasma edge is defined as the region from the top of the pedestal-a narrow region in the outer part of plasmas in high confinement regimes just inside the separatrix, characterized by sharp temperature and density gradients-to the material wall. The properties of the plasma edge have a strong influence on core confinement and, hence, on the overall performance of the device. In addition, edge

conditions have a strong impact on power and particle exhaust and fueling and determine the level of plasma-wall interactions. The multitude of physical processes affecting the properties of the plasma edge (turbulent and collisional transport, MHD, stochasticity, interactions with neutral atoms, molecules and impurities, plasma-wall interactions including sheath effects) with their different spatiotemporal scales evolving on complicated magnetic geometries, make predictive modeling of this region especially challenging and most likely to benefit from an integrated simulation.

A specific topic that should be addressed by an edge initiative is the self-consistent simulation of a full Edge Localized Mode (ELM) cycle and its effect on the pedestal formation, dynamic evolution and characteristics, such as width and height. Applications should address all relevant physical processes on all spatiotemporal scales, except for interactions with material walls. The formalism should be valid for the expected range of collisionality in present and next-generation experiments from the top of the pedestal to the material wall. This would require extending the present generation of gyrokinetic equations and codes to edge-relevant regimes and developing techniques to bridge the expected collisionality range.

2) An integrated understanding of how electromagnetic waves affect plasma profiles and plasma stability: Experiments over the past 20 years have shown that electromagnetic waves can provide local heating and current drive in plasmas, which in turn can affect the equilibrium, stability, and transport properties of a magnetically confined plasma. Localized wave driven currents have been produced by a wide variety of plasma waves, including electron cyclotron waves, lower hybrid waves, and ion cyclotron frequency waves, and several validated, quantitative current drive simulation codes have been developed. Further, stabilization of magnetohydrodynamic (MHD) modes and modification of plasma flows have been observed in experiments using radio-frequency waves. At the present time, the development of integrated simulation codes and the required physical models and algorithms is at the conceptual stage. The primary goal of this focused integration initiative is to understand how electromagnetic waves affect MHD stability of a fusion plasma and how these effects can be used to optimize the performance of a burning plasma.

A specific product of this focused integration initiative would be a suite of simulation codes that self-consistently couples the time evolution of the plasma equilibrium with the wave-driven modifications of the current, temperature, and flow profiles and includes the analysis of stability limits. Since one objective of this initiative is integration, existing codes or code modules may be used where appropriate. For example, an existing transport code could be used to evolve the plasma profiles and equilibrium. However, since a number of new codes or code modules will be needed, it is expected that the software and algorithm development environment and the code framework will be flexible enough to facilitate recombining of software components into new code capabilities as additional physics is added to the mathematical models. This code suite should be benchmarked against profile control experiments with pulse lengths that are long compared to the magnetic field diffusion times. Such an integrated simulation capability will allow the development of optimized burning plasma scenarios.

**DATES: A Letter-of-Intent (LOI) to submit an application is REQUIRED and should be submitted by February 23, 2005. Failure to submit a Letter-of-Intent by an applicant may preclude the full application from due consideration.**

To permit timely consideration for awards in FY 2005, formal applications submitted in response to this notice must be received by DOE no later than 4:30 p.m., Eastern Time, March 23, 2005.

Please see the "Addresses" section below for further instructions on the method of submission for the Letter-of-Intent and formal application.

Please see the "Supplementary Information" section below for further instructions on the preparation of the Letter-of-Intent and the full application. Electronic submission of the Letter-of-Intent and the formal application in PDF format are required. It is important that the submission be in a single PDF file.

**ADDRESSES:** The Letter-of-Intent should be submitted electronically by email to John.Sauter@science.doe.gov, Michael.Strayer@science.doe.gov and Steve.Eckstrand@science.doe.gov. Please include "Letter-of- Intent for Notice DE- FG01-05ER05-11" in the subject line.

Formal applications from universities and the private sector referencing Program Notice DE-FG01-05ER05-11 must be sent electronically by an authorized institutional business official through DOE's Industry Interactive Procurement System (IIPS) at: http://e-center.doe.gov (see also http://www.science.doe.gov/grants/). 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. **Although IIPS offers the option of using multiple files, it is important that all applications submitted to this Program Notice be in a single PDF file.** 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. 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 or you may call the help desk at (800) 683-0751. Further information on the use of IIPS by the Office of Science is available at: http://www.science.doe.gov/grants/IIPS-Instructions.html.

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) 903-3064, 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:** Office of Fusion Energy Sciences, U.S. Department of Energy, SC-55/Germantown Building, 1000 Independence Avenue, SW, Washington, DC 20585-1290. Dr. Stephen Eckstrand, SC-55, (301) 903-5546, steve.eckstrand@science.doe.gov, is the Program Manager for the OFES SciDAC Program, and

may be contacted for technical information. Mr. John Sauter, SC-55, (301) 903-3287, john.sauter@science.doe.gov may be contacted for administrative information relating to the submission of the application and Letter-of-Intent.

**SUPPLEMENTARY INFORMATION:**

**Background: Scientific Discovery through Advanced Computing**

In addition to scientific computing and computational science research included 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 eventually petascale, computing under the collective title of Scientific Discovery through Advanced Computing (SciDAC). The research projects in the SciDAC portfolio are addressing the extraordinary difficulties of achieving sustained peak performance on modern supercomputers for scientific applications, such as simulating supernovas, making multi-century climate predictions, and understanding and controlling a burning plasma. In recognition of these difficulties, the SciDAC research projects are collaborative efforts involving teams of physical scientists, applied mathematicians, computer scientists, and computational scientists working on major software and algorithm development to solve complex problems important to 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 facing 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/.

**Collaboration and Coordination**

It is expected that all applications submitted in response to this notice will be for collaborative centers involving multidisciplinary teams from more than one institution. Each institution involved in a proposed collaborative research project must submit a separate application. The application from the lead institution must identify the lead Principal Investigator (PI) who is responsible for the overall project, and the applications from the other institutions must identify the co-PI who is responsible for the part of the research to be carried out at his/her 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 may include a common technical description of the overall research project, but if the distinct scope of the work that will be carried out by the institution submitting the application is not indicated in the common scope of work, it must be summarized in a 1-2 page appendix to the common technical description. The lead PI for the project should also include a summary budget for the entire project, including the annual funding proposed for each institution. 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. A separate Laboratory solicitation will be posted **(Program Announcement LAB 05-11)**.

Further information on preparation of collaborative applications 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/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 processes established by the Office of Advanced Scientific Computing Research and the Office of Fusion Energy Sciences at the beginning of the SciDAC program. This includes 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.

**Letter-of-Intent**

The primary purpose of the Letter-of-Intent (LOI) is to assist the OFES and OASCR in planning the review and the selection of potential reviewers for the application. 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 reveal any potential conflict of interest in the selection of reviewers for the application.

**Since we expect that some reviewers will be asked to review several applications, all applications should be limited to a maximum of thirty five (35) pages (including text and figures) of technical information (sections two through seven below). Applications exceeding these page limits may be rejected without review.** The PDF file may also include a few selected publications in an Appendix as background information. In addition, please limit biographical and publication information for the principal investigator and key personnel to no more than two pages each. Each principal investigator should provide an e-mail address. The page count of 35 does not include the DOE Face Page and Budget Pages, the Title Page, the biographical material and publication information, or any Appendices. However, it is important that the 35 page technical information section provide a complete description of the proposed work, since reviewers are not obliged to read the Appendices.

**Application**

**The application should be written in strict compliance with the following format:**

1. Abstract - brief description of the project purpose and goals in no more than 250 words

2. Executive Summary - summary of the application in one to two pages

3. Background and Recent Accomplishments

    3.1. Background - explanation of the importance and relevance of the proposed work
    3.2. Recent Accomplishments - description of relevant work carried out by the PI and/or co-PIs during the past two years

4. Proposed research
    4.1. Detailed project description
    4.2. Project schedules, milestones, and deliverables, including plans for comparison with experimental results
    4.3. Description of work assignments (e.g. Work Breakdown Structure (WBS) with WBS managers and resource allocations)

5. Textual summary of the overall budget (in addition to the formal budget pages in each institution's application) showing how the budget relates to the proposed work assignments

6. Management plan - description of management structure and processes

7. Description of facilities, resources, and personnel

    7.1 Estimates of the amount of computational resources required, including processor hours and storage requirements
    7.2. Discussion about other SciDAC and base program support that is assumed in developing budget estimates

8. Other current and pending support.

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 Financial Assistance Program and 10 CFR Part 605. Electronic access to SC's Financial Assistance Guide and required forms is possible via the Internet using the following Web site address: http://www.science.doe.gov/grants/. DOE is under no obligation to pay for any costs associated with the preparation or submission of an application if an award is not made. The information required by 10 CFR Part 605 should be conveyed by the application using the above format wherever possible.

In selecting applications for funding, the DOE Office of Fusion Energy Sciences will give priority to applications that can produce results within three to four years after grant initiation. Preferred applications in this category would typically have a performance period of five years, assuming successful completion of a merit review during the third year.

As noted in the section on "Collaboration and Coordination" above, each institution involved in a collaborative research project must submit a separate application specifying the principal investigator who is responsible for the research to be performed at his or her institution. The description of the work to be carried out by each institution should be clearly described in section 4.3 of the application.

**Program Funding**

This is a new initiative. DOE identified total funding up to an amount of $1,200,000 in FY 2005 for this initiative. In addition, approximately $1,200,000 will be available for competition by DOE National Laboratories under a separate solicitation **(Program Announcement LAB 05-11).**

Awards are expected to be made for a period of five years, with out-year support contingent on the availability of funds and satisfactory progress. Funding for the final two years is contingent on satisfactory completion of a merit review during the third year of the project. OFES reserves the right not to make any awards if no application is judged to be of suitable scientific quality or of sufficient relevance to the SciDAC program.

The cost-effectiveness of an application will be considered when comparing applications with differing funding requirements. One or two awards may be made depending on the number and quality of the applications received and favorably reviewed. It is anticipated that total project awards may range from $1,500,000 to $2,000,000 per year.

**Merit Review**

Applications will be subjected to formal merit review and will be evaluated against the following criteria, which are listed in descending order of importance as set forth in 10 CFR Part 605. ( http://www.science.doe.gov/grants/605index.html). Included with each criteria are the detailed questions that are asked of the reviewers.

1. Scientific and/or technical merit of the project;

    o Does this application address an important problem in plasma science that is relevant to integrated simulation of fusion plasmas in the long term?
    o What is the likelihood that it will lead to new or fundamental advances in its field?
    o How well does the application demonstrate the need for extraordinary computing resources?
    o What is the potential of the proposed research to advance the state-of-the- art in computational modeling and simulation of plasma behavior?
    o How does the proposed research compare with other research in its field, both in terms of scientific and/or technical merit and originality?

2. Appropriateness of the proposed method or approach;
    o Are the conceptual framework, methods, and analyses adequately developed and sound?
    o Is the proposed method or approach likely to lead to scientifically valid conclusions or advances in the field?
    o How sound is the plan for managing the project? Is the balance between computational plasma physicists, computer scientists, and applied mathematicians appropriate for the proposed scope of work?
    o How good is the plan for verifying and validating the models developed, including close coupling with experiments for ultimate validation?
    o Are there significant potential problems and how well does the applicant address these problems?

3. Competency of the applicant's personnel and adequacy of the proposed resources;
    - o How well qualified are the applicant's personnel to carry out the proposed research? (If appropriate, please comment on the scientific reputation and quality of recent research by the principal investigator and other key personnel.)
    - o Do the applicants have demonstrated abilities to use terascale computers?
    - o Please assess the reasonableness of the estimates of the required computational resources.
    - o Does the proposed work take advantage of unique facilities and capabilities and/or make good use of collaborative arrangements?
4. Reasonableness and appropriateness of the proposed budget.

The reviewers are also asked to comment on Other Appropriate Factors:

- o Could the proposed research make a significant contribution to another field?
- o If applicable, please comment on the educational benefits of the proposed activity.

The Office of Fusion Energy Sciences and the Office of Advanced Scientific Computing Research will also consider, as part of the evaluation, other available advice or information as well as program policy factors such as ensuring an appropriate balance among the program areas and within the program areas and quality of previous performance. Selection of applications for award will be based upon the findings of the technical evaluations, the importance and relevance of the proposed research to the missions of the Office of Fusion Energy Sciences and the Office of Advanced Scientific Computing Research in fusion plasma simulation, and funding availability. Funding under this Notice is limited to supporting research activities based in the U.S., though subcontracts with limited funding for collaborators outside the U.S. may be allowed with appropriate justifications.

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

Martin Rubinstein
Grants and Contracts Division
Office of Science

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