

**Program Announcement
To DOE National Laboratories
LAB 04-09**

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

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 proposals 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.

More specific information on this Announcement is outlined in the Supplementary Information section below.

DATES: Researchers are requested to submit a letter of intent by February 16, 2004. This letter should include the name of the Principal Investigator(s)/project director, the email address and address of the PI, the title of the project, 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 effect a responsive application submitted in a timely fashion. The letter of intent should be sent by E-mail to john.sauter@science.doe.gov, and the subject line should state: Letter-of-Intent regarding Program Announcement LAB 04-09.

Formal proposals 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 proposals in PDF format is encouraged.

ADDRESSES: Letters of Intent should be sent by E-mail to John Sauter at john.sauter@science.doe.gov, and the subject line should state: Letter-of-Intent regarding Program Announcement LAB 04-09.

Formal proposals, referencing Program Announcement LAB 04-09, should also be submitted by E-mail to: John Sauter at john.sauter@science.doe.gov. If necessary, proposals may be submitted on CD-ROM to John Sauter, U.S. Department of Energy, Office of Fusion Energy Sciences, SC-55/Germantown Building, 1000 Independence Avenue, SW, Washington DC 20585-1290. ATTN: Program Announcement LAB 04-09.

When submitting proposals by U.S. Postal Service Express Mail, any commercial mail delivery service, or when hand carried by the proposer, the following address must be used: U.S. Department of Energy, Office Fusion Energy Sciences, SC-55, 19901 Germantown Road, Germantown, MD 20874-1290, ATTN: Program Announcement LAB 04-09.

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

Arnold Kritz: telephone (301) 903-2027, e-mail arnold.kritz@science.doe.gov

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 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 proposals 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 proposal. 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. Researchers may request designated funding for associated applied mathematics or computer science work that is needed to support the development of the scientific application codes as part of Scientific Application Partnership Program.

Proposals are being sought in the following four topical areas:

1. Macroscopic Equilibrium and Stability: Proposals 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 non-linear evolution, 6) two-fluid and kinetic effects on MHD modes, and 7) the onset and evolution of major disruptions.

2. Turbulence and Transport: Proposals 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: Proposals 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, diverter 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: Proposals 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 proposals 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 proposal, 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 and budget page for the institution. These collaborative research proposals 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 at other federal laboratories, universities, industry, and non-profit organizations are encouraged.

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 awards in FY 2004. Additional funding for the proposed project may be available through the Office of Advanced Scientific Computing Research Scientific Application Partnership Program for closely related research in computer science and/or applied mathematics. Proposals 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. Since these projects are expected to be multi-institution and multi-disciplinary projects, awards under this announcement would range from \$100,000 to \$400,000 per participating institution.

Submission Information

The Project Description must be 25 pages or less, exclusive of attachments. It must 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 proposal must include letters of intent from 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 instructions and format described below should be followed. Reference Program Announcement LAB 04-09 on all submissions and inquiries about this program.

OFFICE OF SCIENCE GUIDE FOR PREPARATION OF SCIENTIFIC/TECHNICAL PROPOSALS TO BE SUBMITTED BY NATIONAL LABORATORIES

Proposals from National Laboratories submitted to the Office of Science (SC) as a result of this program announcement will follow the Department of Energy Field Work Proposal process with additional information requested to allow for scientific/technical merit review. The following guidelines for content and format are intended to facilitate an understanding of the requirements necessary for SC to conduct a merit review of a proposal. Please follow the guidelines carefully, as deviations could be cause for declination of a proposal without merit review.

1. Evaluation Criteria Proposals will be subjected to scientific merit review (peer review) and will be evaluated against the following criteria, which are listed in descending order of importance:

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, 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 will the use of multiple codes 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.

The evaluation will also include program policy factors such as the relevance of the proposed research to the terms of the announcement, the uniqueness of the proposer's capabilities, and prior performance on DOE funded work.

2. Summary of Proposal Contents

Field Work Proposal (FWP) Format (Reference DOE Order 5700.7C) (DOE ONLY)
Proposal Cover Page
Table of Contents
Abstract
Narrative
Literature Cited
Budget and Budget Explanation
Other support of investigators
Biographical Sketches
Description of facilities and resources
Appendix

2.1 Number of Copies to Submit

Formal proposals 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 proposals in PDF format is encouraged.

3. Detailed Contents of the Proposal

Proposals must be readily legible, when photocopied, and must conform to the following three requirements: the height of the letters must be no smaller than 10 point with at least 2 points of spacing between lines (leading); the type density must average no more than 17 characters per inch; the margins must be at least one-half inch on all sides. Figures, charts, tables, figure legends, etc., may include type smaller than these requirements so long as they are still fully legible.

3.1 Field Work Proposal Format (Reference DOE Order 5700.7C) (DOE ONLY)

The Field Work Proposal (FWP) is to be prepared and submitted consistent with policies of the investigator's laboratory and the local DOE Operations Office. Additional information is also requested to allow for scientific/technical merit review.

Laboratories may submit proposals directly to the SC Program office listed above. A copy should also be provided to the appropriate DOE operations office.

3.2 Proposal Cover Page

The following proposal cover page information may be placed on plain paper. No form is required.

Title of proposed project
SC Program announcement title
Name of laboratory
Name of principal investigator (PI)
Position title of PI
Mailing address of PI
Telephone of PI
Fax number of PI
Electronic mail address of PI
Name of official signing for laboratory*
Title of official
Fax number of official
Telephone of official
Electronic mail address of official
Requested funding for each year; total request
Use of human subjects in proposed project:

If activities involving human subjects are not planned at any time during the proposed project period, state "No"; otherwise state "Yes", provide the IRB

Approval date and Assurance of Compliance Number and include all necessary information with the proposal should human subjects be involved.

Use of vertebrate animals in proposed project:

If activities involving vertebrate animals are not planned at any time during this project, state "No"; otherwise state "Yes" and provide the IACUC Approval date and Animal Welfare Assurance number from NIH and include all necessary information with the proposal.

Signature of PI, date of signature

Signature of official, date of signature*

*The signature certifies that personnel and facilities are available as stated in the proposal, if the project is funded.

3.3 Table of Contents

Provide the initial page number for each of the sections of the proposal. Number pages consecutively at the bottom of each page throughout the proposal. Start each major section at the top of a new page. Do not use unnumbered pages and do not use suffices, such as 5a, 5b.

3.4 Abstract

Provide an abstract of no more than 250 words. Give the broad, long-term objectives and what the specific research proposed is intended to accomplish. State the hypotheses to be tested. Indicate how the proposed research addresses the SC scientific/technical area specifically described in this announcement.

3.5 Narrative

The narrative comprises the research plan for the project and is limited to 5 pages per task. It should contain the following subsections:

Background and Significance: Briefly sketch the background leading to the present proposal, critically evaluate existing knowledge, and specifically identify the gaps which the project is intended to fill. State concisely the importance of the research described in the proposal. Explain the relevance of the project to the research needs identified by the Office of Science. Include references to relevant published literature, both to work of the investigators and to work done by other researchers.

Preliminary Studies: Use this section to provide an account of any preliminary studies that may be pertinent to the proposal. Include any other information that will help to establish the experience and competence of the investigators to pursue the proposed project. References to appropriate publications and manuscripts submitted or accepted for publication may be included.

Research Design and Methods: Describe the research design and the procedures to be used to accomplish the specific aims of the project. Describe new techniques and methodologies and

explain the advantages over existing techniques and methodologies. As part of this section, provide a tentative sequence or timetable for the project.

Subcontract or Consortium Arrangements: If any portion of the project described under "Research Design and Methods" is to be done in collaboration with another institution, provide information on the institution and why it is to do the specific component of the project. Further information on any such arrangements is to be given in the sections "Budget and Budget Explanation", "Biographical Sketches", and "Description of Facilities and Resources".

3.6 Literature Cited

List all references cited in the narrative. Limit citations to current literature relevant to the proposed research. Information about each reference should be sufficient for it to be located by a reviewer of the proposal.

3.7 Budget and Budget Explanation

A detailed budget is required for the entire project period, which normally will be three years, and for each fiscal year. It is preferred that DOE's budget page, Form 4620.1 be used for providing budget information*. Modifications of categories are permissible to comply with institutional practices, for example with regard to overhead costs.

A written justification of each budget item is to follow the budget pages. For personnel this should take the form of a one-sentence statement of the role of the person in the project. Provide a detailed justification of the need for each item of permanent equipment. Explain each of the other direct costs in sufficient detail for reviewers to be able to judge the appropriateness of the amount requested.

Further instructions regarding the budget are given in section 4 of this guide.

* Form 4620.1 is available at web site: <http://www.sc.doe.gov/production/grants/Forms-E.html>

3.8 Other Support of Investigators

Other support is defined as all financial resources, whether Federal, non-Federal, commercial or institutional, available in direct support of an individual's research endeavors. Information on active and pending other support is required for all senior personnel, including investigators at collaborating institutions to be funded by a subcontract. For each item of other support, give the organization or agency, inclusive dates of the project or proposed project, annual funding, and level of effort devoted to the project.

3.9 Biographical Sketches

This information is required for senior personnel at the laboratory submitting the proposal and at all subcontracting institutions. The biographical sketch is limited to a maximum of two pages for each investigator.

3.10 Description of Facilities and Resources

Describe briefly the facilities to be used for the conduct of the proposed research. Indicate the performance sites and describe pertinent capabilities, including support facilities (such as machine shops) that will be used during the project. List the most important equipment items already available for the project and their pertinent capabilities. Include this information for each subcontracting institution, if any.

3.11 Appendix

Include collated sets of all appendix materials with each copy of the proposal. Do not use the appendix to circumvent the page limitations of the proposal. Information should be included that may not be easily accessible to a reviewer.

Reviewers are not required to consider information in the Appendix, only that in the body of the proposal. Reviewers may not have time to read extensive appendix materials with the same care as they will read the proposal proper.

The appendix may contain the following items: up to five publications, manuscripts (accepted for publication), abstracts, patents, or other printed materials directly relevant to this project, but not generally available to the scientific community; and letters from investigators at other institutions stating their agreement to participate in the project (do not include letters of endorsement of the project).

4. Detailed Instructions for the Budget

(DOE Form 4620.1 "Budget Page" may be used)

4.1 Salaries and Wages

List the names of the principal investigator and other key personnel and the estimated number of person-months for which DOE funding is requested. Proposers should list the number of postdoctoral associates and other professional positions included in the proposal and indicate the number of full-time-equivalent (FTE) person-months and rate of pay (hourly, monthly or annually). For graduate and undergraduate students and all other personnel categories such as secretarial, clerical, technical, etc., show the total number of people needed in each job title and total salaries needed. Salaries requested must be consistent with the institution's regular practices. The budget explanation should define concisely the role of each position in the overall project.

4.2 Equipment

DOE defines equipment as "an item of tangible personal property that has a useful life of more than two years and an acquisition cost of \$25,000 or more." Special purpose equipment means equipment which is used only for research, scientific or other technical activities. Items of needed equipment should be individually listed by description and estimated cost, including tax, and adequately justified. Allowable items ordinarily will be limited to scientific equipment that is

not already available for the conduct of the work. General purpose office equipment normally will not be considered eligible for support.

4.3 Domestic Travel

The type and extent of travel and its relation to the research should be specified. Funds may be requested for attendance at meetings and conferences, other travel associated with the work and subsistence. In order to qualify for support, attendance at meetings or conferences must enhance the investigator's capability to perform the research, plan extensions of it, or disseminate its results. Consultant's travel costs also may be requested.

4.4 Foreign Travel

Foreign travel is any travel outside Canada and the United States and its territories and possessions. Foreign travel may be approved only if it is directly related to project objectives.

4.5 Other Direct Costs

The budget should itemize other anticipated direct costs not included under the headings above, including materials and supplies, publication costs, computer services, and consultant services (which are discussed below). Other examples are: aircraft rental, space rental at research establishments away from the institution, minor building alterations, service charges, and fabrication of equipment or systems not available off-the-shelf. Reference books and periodicals may be charged to the project only if they are specifically related to the research.

a. Materials and Supplies

The budget should indicate in general terms the type of required expendable materials and supplies with their estimated costs. The breakdown should be more detailed when the cost is substantial.

b. Publication Costs/Page Charges

The budget may request funds for the costs of preparing and publishing the results of research, including costs of reports, reprints page charges, or other journal costs (except costs for prior or early publication), and necessary illustrations.

c. Consultant Services

Anticipated consultant services should be justified and information furnished on each individual's expertise, primary organizational affiliation, daily compensation rate and number of days expected service. Consultant's travel costs should be listed separately under travel in the budget.

d. Computer Services

The cost of computer services, including computer-based retrieval of scientific and technical information, may be requested. A justification based on the established computer service rates should be included.

e. Subcontracts

Subcontracts should be listed so that they can be properly evaluated. There should be an anticipated cost and an explanation of that cost for each subcontract. The total amount of each subcontract should also appear as a budget item.

4.6 Indirect Costs

Explain the basis for each overhead and indirect cost. Include the current rates.