Program Announcement To DOE National Laboratories LAB 09-04

Fusion Simulation Program

SUMMARY: 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 proposals for carrying out a detailed planning study for the Fusion Simulation Program (FSP). The goal of the FSP is to develop a world-leading, experimentally validated predictive simulation capability for fusion plasmas in the regimes and geometries relevant for practical fusion energy. To accomplish this objective, the FSP will take advantage of the emergence of petascale computing capabilities and the scientific knowledge enabled by the OFES and OASCR research programs, in particular those under the auspices of the Scientific Discovery through Advanced Computing (SciDAC) program.

The purpose of the present Program Announcement is to competitively select a nationally coordinated interdisciplinary team consisting of fusion scientists and technologists, applied mathematicians, computer scientists, and computational scientists to carry out a one- to two-year detailed planning study for the FSP. The results of this study will help OFES and OASCR proceed with the full FSP, subject to the results of an independent review at the end of the planning period and the availability of appropriated funds. In addition to the technical and scientific issues expected to be addressed by this study, a detailed management plan will also be a key deliverable. The plan should define the simplest management structure that could effectively address the challenges of a geographically dispersed, multi-institutional research program with focused deliverables which engages diverse scientific communities. It should also consider how principles and concepts from project management can be used to help dealing with issues such as flexibility in resource allocation for maintaining the appropriate balance among the various tasks throughout the duration of this research activity.

The team selected for carrying out the planning activity is expected to form the core of the FSP management structure, once the full program is authorized.

PREPROPOSALS DUE DATE: October 31, 2008, 8:00 PM Eastern Time

Potential Researchers are **REQUIRED** to submit a brief preproposal referencing Program Announcement LAB 09-04 by 8:00 PM, October 31, 2008 Eastern Time. Preproposals should be submitted electronically to john.mandrekas@science.doe.gov and john.sauter@science.doe.gov.

Preproposals should include cover page information, a brief description of the proposed work (3-5 pages, including text with minimum font size 11 point, figures, and references), and one-page curriculum vitae from each Principal Investigator (PI) and senior collaborator. The cover page should include: (a) A statement that the document is a preproposal in response to Program Announcement LAB 09-04; (b) PI information: name, institutional affiliation, telephone number, fax number, and e-mail address; and, (c) Names and Institutions of all co-Principal Investigators and senior collaborators (excluding postdoctoral associates). The description of the proposed work should include the vision of the Researcher(s) for the planning stage of the FSP, the approach to be taken, program schedule, and information regarding the experience of the Applicant(s) in managing large, multi-institutional, research projects.

Preproposals will be reviewed by OFES and OASCR program officials for responsiveness to this Announcement, eligibility of the Researcher organization, and qualification of the Researcher's personnel for carrying out a planning study for a large- scale computational research activity. Only those Researchers who receive notification from DOE encouraging a full proposal may submit a formal proposal. **No other formal proposals will be considered.**

DATES: Proposals submitted in response to this Announcement must be received no later than **December 10, 2008**, 8:00 PM Eastern Time to be accepted for merit review and to permit timely consideration for award.

Please see the "Addresses" section below for further instructions on the method of submission for the proposal.

ADDRESSES: A complete formal FWP in a single Portable Document Format (PDF) document that has 'formatted text and graphics' (also known as "native" PDF) must be submitted. (This submission process includes sending the FWP via CD using Federal Express).

Send CD via Federal Express to:

Mr. John Sauter U.S. Department of Energy Office of Fusion Energy Sciences, SC-24.2/GTN 19901 Germantown Road Germantown, MD 20874-1290 ATTN: Program Announcement LAB 09-04

To identify that the FWP is responding to this Program Announcement, when sending your CD please identify the Program Announcement Title and Program Announcement number on the Federal Express package.

In addition, please submit via email, a single PDF file of the entire LAB proposal and FWP. This will assist in expediting the review process. Please send the email to: john.sauter@science.doe.gov. Please include "Proposal for LAB 09-04" in the subject line of the email.

DOE National Laboratories should submit as instructed above. Researchers from other Federal agencies and Non-DOE Federally Funded Research and Development Centers (FFRDCs) should follow the format at <u>http://www.science.doe.gov/grants/fed_prop.html</u> and also submit via email as stated above.

FOR FURTHER INFORMATION CONTACT:

PROGRAM MANAGER: Dr. John Mandrekas, Office of Fusion Energy Sciences
PHONE: (301) 903-0552
FAX: (301) 903-4716
E-MAIL: john.mandrekas@science.doe.gov

Communications related to the formal proposal should use "Program Announcement LAB 09-04" in the subject line.

SUPPLEMENTARY INFORMATION:

Program Objective:

The potential of integrated simulations to significantly contribute toward the FES mission of establishing the scientific basis for fusion energy as well as its long term goal of developing a predictive capability for burning plasmas was recognized early by the fusion community. In 2001, the Integrated Simulation and Optimization of Fusion Systems (ISOFS) subcommittee of the Fusion Energy Sciences Advisory Committee (FESAC) recommended the initiation of a Fusion Simulation Project with the objective of developing an advanced simulation capability to reliably predict the behavior of plasma discharges in toroidal magnetic fusion devices on all relevant time and space scales. More recently, a community workshop - co-sponsored by OFES and OASCR - was held in May 2007 to refine the long term vision of the FSP and develop a detailed roadmap. The report which emerged from this workshop was recently evaluated by FESAC and the Advanced Scientific Computing Advisory Committee (ASCAC). These reports may be found at:

http://www.science.doe.gov/ofes/programdocuments/reports/FSPWorkshopReport.pdf http://www.ofes.fusion.doe.gov/FESAC/Oct-2007/FESAC_FSP_report.pdf http://www.sc.doe.gov/ascr/ASCAC/Reports/ASCAC_FSP_REPORT_FINAL.pdf

A major focus of the 2007 FSP workshop was the potential impact of the FSP on the U.S. participation in ITER - the FSP will be an important asset for maximizing the return of our investment in ITER while, at the same time, benefiting from this participation through the validation opportunities offered by the anticipated data from ITER, the world's first burning plasma experiment. However the scope of the FSP is much wider as it is being envisioned as a tool that embodies our predictive understanding of magnetically confined plasmas in regimes and geometries relevant for practical fusion energy, and properly coordinated and integrated with theory and experiment. In addition, for the FSP to deliver a true "whole device" modeling capability, its scope should include the entire region from the core of the plasma to the first wall, including the closely coupled plasma-materials interactions.

The FSP will also be a critical component of the initiative toward predictive plasma modeling and validation, as described in the recent Priorities, Gaps, and Opportunities FESAC report. (<u>http://www.ofes.fusion.doe.gov/FESAC/Oct-2007/FESAC_Planning_Report.pdf</u>)

Program Funding:

Approximately \$2,000,000 will be available for this initiative in FY 2009. Additional funding may be available in FY 2010, subject to satisfactory progress during the first year of this activity and on the availability of appropriated funds. It is anticipated that one award will be made under this announcement. DOE is under no obligation to pay for any costs associated with the preparation or submission of proposals. DOE reserves the right to fund, in whole or in part, any, all, or none of the proposals submitted.

Formal Proposals:

Proposals should identify the key members of the proposed planning study team (the lead PI, institutional co-investigators, and senior collaborators) and include information about their experience in managing large multi-institutional and multidisciplinary research projects. The proposals should also include detailed information on how the applicants propose to address the following issues during the detailed planning activity of the FSP:

- FSP Deliverables the detailed planning study should consider the list of prioritized deliverables outlined in the 2007 FSP workshop report for each of the three five-year periods of the program. The study should critically evaluate and modify, if warranted, the original list of deliverables, taking into consideration both the near-term focus of this research effort (the ITER needs) and the long term vision for the FSP as outlined in the previous section. The planning study should include a credible assessment of the resources (in terms of Full Time Equivalent [FTE]) and mix of expertise (plasma physics, material science, applied math, and computer science) necessary to successfully complete each task or group of tasks. Accordingly, the proposals should describe in detail the method or approach that will be followed for determining the required resources and reassessing the list of deliverables for the FSP, as well as for developing clear and compelling Work Breakdown Structures
- Comprehensive assessment of the present computational capabilities of the fusion community in terms of major simulation codes, numerical algorithms, computational science tools (data management, visualization, code performance tools, etc.), computational frameworks, interface standards, code scalability, and other related issues. Identification of major gaps and weaknesses, and suggestions for the path forward should also be addressed
- Integration and coordination of the FSP with the projects in the FES SciDAC portfolio, including the process for incorporating results from the FES SciDAC Centers into the FSP
- Integration and coordination of the FSP with other SciDAC (non-FES) Centers, and in particular with SciDAC Institutes and Centers for Enabling Technologies (CETs), as well as with efforts supported by the OASCR Applied Mathematics program
- Integration and coordination with the FES analytic theory and modeling program, including the process for incorporating improved theoretical models into the FSP simulation codes and engaging the help of the FES theory community to address gaps in the physics models implemented in the FSP codes
- Integration and coordination with the materials community for the purpose of addressing the plasma-materials interaction challenges

- Details of the researchers' vision and approach for developing a successful and credible Verification and Validation plan, including interaction and coordination with the FES experimental and diagnostic communities
- Interaction and coordination with international integrated modeling efforts-in particular those undertaken by our ITER partners in support of the needs of the international ITER Organization (IO)
- Management Issues:
 - The Researchers' vision and approach for developing a management plan that could effectively address the challenges of a geographically dispersed, multi-institutional research program with focused deliverables which engages diverse scientific communities. Researchs should also consider how principles and concepts from project management can be used to help dealing with issues such as flexibility in resource allocation for maintaining the appropriate balance among the various tasks throughout the duration of this research activity, while providing clear accountability and oversight and being responsive to the needs of the main stakeholders
 - Researchers should detail their approach for identifying the key-technical and non-technical-risks associated with a large-scale computational research effort such as the FSP, and outline their plans for developing risk mitigation strategies
- High Performance Computing (HPC) Resource Requirements-as a major computational activity, the success of the FSP will critically depend on the availability of HPC resources. Researchers should describe in sufficient detail their approach for determining the required HPC resources for carrying out the various FSP tasks, including the appropriate mix of capacity and capability resources. Resources to be considered should include the-current and projected- capabilities at the SC leadership computing facilities, as well as other resources (national or local) that can be reasonably expected to be available to the FSP researchers

The expertise of the existing SciDAC teams is an important resource for the success of the FSP detailed planning study. Accordingly, the PIs of the existing FES SciDAC Centers will be available to support the FSP planning team.

Funding under this Announcement is limited to supporting research activities based in the U.S. Proposals from non-U.S. institutions will be declined.

The research project description must be **30 pages** or less, exclusive of attachments and appendices and must contain an abstract or summary of the proposed research. All collaborators should be listed with the abstract or summary. Attachments include literature cited, biographical sketches, description of facilities and resources, letters of endorsement from unfunded collaborators, and a listing of all current and pending federal support. Please do not submit general letters of support as these are not used in making funding decisions. Biographical sketches should be limited to no more than two pages per individual.

The instructions and format described below should be followed. You must reference Program Announcement LAB 09-04 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

After an initial screening for eligibility and responsiveness to the solicitation, proposals will be subjected to scientific merit review (peer review). The proposals 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 applicant's personnel and adequacy of proposed resources; and
- 4. Reasonableness and appropriateness of the proposed budget.

The OFES 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 within the program and quality of previous performance. The selected projects will be required to acknowledge support by DOE in all public communication of the research results.

External peer reviewers are selected with regard to both their scientific expertise and the absence of conflict-of-interest issues. Both Federal and non-Federal reviewers may be used, and submission of a proposal constitutes agreement that this is acceptable to the investigator(s) and the submitting institution.

2. Summary of Proposal Contents

- Field Work Proposal (FWP) Format (Reference DOE Order 412.1A) (DOE ONLY)
- Proposal Cover Page
- Table of Contents
- Budget (DOE Form 4620.1) and Budget Explanation
- Abstract (one page)
- Narrative (main technical portion of the proposal, including background/introduction, recent accomplishments, proposed research and methods, timetable of activities, and responsibilities of key project personnel)
- Literature Cited
- Biographical Sketch(es)
- Description of Facilities and Resources
- Other Support of Investigator(s)
- Appendix (optional)

3. Detailed Contents of the Proposal

Adherence to type size and line spacing requirements is necessary for several reasons. No researcher should have the advantage, by using small type, of providing more text in their proposals. Small type may also make it difficult for reviewers to read the proposal. Proposals must have 1-inch margins at the top, bottom, and on each side. Type sizes must be at least 11 point. Line spacing is at the discretion of the researcher, but there must be no more than 6 lines per vertical inch of text. Pages should be standard 8 1/2" x 11" (or metric A4, i.e., 210 mm x 297 mm).

3.1 Field Work Proposal Format (Reference DOE Order 412.1A)(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 Budget and Budget Explanation

A detailed budget is required 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.science.doe.gov/grants/budgetform.pdf

3.5 Abstract

Summarize the proposal in no more than two pages. Give the project objectives (in broad scientific terms), the approach to be used, and what the research is intended to accomplish. State the hypotheses to be tested (if any). At the top of the abstract give the project title, names of all the investigators and their institutions, and contact information for the principal investigator, including e-mail address.

3.6 Narrative (main technical portion of the proposal, including background/introduction, proposed research and methods, timetable of activities, and responsibilities of key project personnel).

The narrative comprises the research plan for the project and is limited to 30 pages (maximum), including text and figures, when printed using standard 8.5" by 11" paper with 1 inch margins (top, bottom, left, and right) and font not smaller than 11 point. It should contain enough background material in the Introduction, including review of the relevant literature, to demonstrate sufficient knowledge of the state of the science. The major part of the narrative

should be devoted to a description and justification of the proposed project, including details of the methods to be used. It should also include a timeline for the major activities of the proposed project, and should indicate which project personnel will be responsible for which activities.

It is important that the 30-page technical information section provide a complete description of the proposed work, because reviewers are not obliged to read the Appendices. Proposals exceeding these page limits may be rejected without review.

If any portion of the project is to be done in collaboration with another institution (or institutions), provide information on the institution(s) and what part(s) of the project it will carry out. 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

3.7 Literature Cited

Give full bibliographic entries for each publication cited in the narrative. Each reference must include the names of all authors (in the same sequence in which they appear in the publication), the article and journal title, book title, volume number, page numbers, and year of publication. Include only bibliographic citations. Principal investigators should be especially careful to follow scholarly practices in providing citations for source materials relied upon when preparing any section of the proposal.

3.8 Biographical Sketches

This information is required for senior personnel at the institution submitting the proposal and at all subcontracting institutions (if any). The biographical sketch is limited to a maximum of two pages for each investigator and must include:

Education and Training. Undergraduate, graduate and postdoctoral training, provide institution, major/area, degree and year.

<u>Research and Professional Experience</u>. Beginning with the current position list, in chronological order, professional/academic positions with a brief description.

<u>Publications</u>. Provide a list of up to 10 publications most closely related to the proposed project. For each publication, identify the names of all authors (in the same sequence in which they appear in the publication), the article title, book or journal title, volume number, page numbers, year of publication, and website address if available electronically. Patents, copyrights and software systems developed may be provided in addition to or substituted for publications.

<u>Synergistic Activities</u>. List no more than 5 professional and scholarly activities related to the effort proposed.

To assist in the identification of potential conflicts of interest or bias in the selection of reviewers, the following information must also be provided in each biographical sketch.

Collaborators and Co-editors: A list of all persons in alphabetical order (including their current organizational affiliations) who are currently, or who have been, collaborators or co- authors with the investigator on a research project, book or book article, report, abstract, or paper during the 48 months preceding the submission of the proposal. Also include those individuals who are currently or have been co-editors of a special issue of a journal, compendium, or conference proceedings during the 24 months preceding the submission of the proposal. If there are no collaborators or co- editors to report, this should be so indicated.

Graduate and Postdoctoral Advisors and Advisees: A list of the names of the individual's own graduate advisor(s) and principal postdoctoral sponsor(s), and their current organizational affiliations. A list of the names of the individual's graduate students and postdoctoral associates during the past five years, and their current organizational affiliations.

3.8 Description of Facilities and Resources

Facilities to be used for the conduct of the proposed research should be briefly described. Indicate the pertinent capabilities of the institution, 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).

3.10 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 (months per year or percentage of the year) devoted to the project.

3.11 Appendix

Information not easily accessible to a reviewer may be included in an appendix, but do not use the appendix to circumvent the page limitations of the proposal. Reviewers are not required to consider information in an appendix, and reviewers may not have time to read extensive appendix materials with the same care they would use with 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 general 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.