

**Program Announcement
To DOE National Laboratories
LAB 07-22**

***Scientific Discovery Through Advanced Computing:
Computational Physics of Energetic Particles In 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 and application of high performance scientific simulation codes on topical areas that are important to burning plasma physics experiments, such as ITER, and which will contribute to establishing the scientific foundation for an integrated fusion simulation in the future. The goal is the creation of codes that achieve high performance on a single node, scale to thousands of nodes and tens-of-thousands of processors, and have the potential to be ported to future generations of high performance computers.

DATES: A Letter of Intent (LOI) to submit a proposal is **REQUIRED** and should be submitted by April 23, 2007. **Failure to submit a Letter of Intent by a proposer may preclude the full proposal from due consideration.**

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

Full proposals submitted in response to this Announcement must be submitted to the DOE Electronic Proposal Management Application (ePMA) system (<https://epma.doe.gov>) no later than 8:00 p.m., Eastern Time, June 4, 2007, to be accepted for merit review and to permit timely consideration for award in Fiscal Year 2008. It is important that the entire peer reviewable proposal be submitted to the ePMA system as a single PDF file attachment.

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

ADDRESSES: Letters-of-Intent, referencing Program Announcement LAB 07-22 should be sent to Mr. John Sauter by E-mail: John.Sauter@science.doe.gov, with a copy to Dr. Curtis Bolton at Curt.Bolton@science.doe.gov. Please use "Program Announcement LAB 07-22 Letter-of-Intent" as the subject of the email.

A complete formal FWP in a single Portable Document Format (PDF) file must be submitted through the DOE ePMA system (<https://epma.doe.gov>) as an attachment. To identify that the

FWP is responding to this program announcement, please fill in the following fields in the "ePMA Create Proposal Admin Information" screen as shown:

Proposal Short Name:

Fiscal Year:

Proposal Reason:

Program Announcement Number: LAB 07-22 *

Program announcement Title: Scientific Discovery Through Advanced Computing: Computational Physics of Energetic Particles In Plasmas *

Proposal Purpose:

Estimated Proposal Begin Date:

HQ Program Manager Organization:

* Please use the wording shown when filling in these fields to identify that the FWP is responding to this Program Announcement.

In order to expedite the review process, please submit a CD and one paper copy of the proposal and FWP using the following address by U.S. Postal Service Express Mail, any commercial mail delivery service, or when hand-carried.

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 07-22

DOE National Laboratories should submit using ePMA as instructed above. **Researchers from other Federal agencies** and Non-DOE Federally Funded Research and Development Centers (FFRDCs) should follow the format at http://www.science.doe.gov/grants/fed_prop.html and submit the proposal as a CD and one paper copy using the above address, by U.S. Postal Service Express Mail, any commercial mail delivery service, or when hand-carried.

In the proposal package, include an extra copy of the one-page abstract.

FOR FURTHER INFORMATION CONTACT: Dr. Curtis Bolton, Research Division, SC-24.2/Germantown Building, Office of Fusion Energy Sciences, Office of Science, U.S. Department of Energy, 1000 Independence Ave., SW, Washington, D.C. 20585- 1290, telephone: 301-903- 4914, e-mail: Curt.Bolton@science.doe.gov, fax: (301) 903- 4716. Communications related to the formal proposal should use "Program Announcement LAB 07-22 FORMAL" in the subject line.

Communications related to the formal proposal should use "Program Announcement LAB 07-22" in the subject line.

SUPPLEMENTARY INFORMATION:

Proposals in this area should focus on developing a predictive understanding of the effects of energetic particles, including runaway electron effects, on plasma performance in regimes relevant to burning plasma experiments. Such particles can be introduced either by auxiliary heating mechanisms--such as neutral beam injection or the launching of RF waves--or created by the fusion reaction itself, and their nonlinear interaction with the background thermal plasma and various excited modes is expected to be of fundamental importance for the macroscopic stability, confinement, and performance of burning plasmas.

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

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

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

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

Scientific Discovery through Advanced Computing

Beyond the scientific computing and computational science research embedded in the Office of Science (SC) core research programs, SC invests in a portfolio of coordinated research efforts directed at exploiting the emerging capabilities of terascale and petascale computing under the collective title of Scientific Discovery through Advanced Computing (SciDAC). The research projects in the SciDAC portfolio respond to the extraordinary difficulties of realizing sustained peak performance for scientific applications, such as simulating combustion, making 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.scidac.gov/>

Background: Advanced Simulation of Fusion Plasmas

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

Following the signing of the ITER agreement, the Office of Fusion Energy Sciences decided to focus its part of the SciDAC program on burning plasma physics needs. Accordingly, the new and renewal 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.

Collaboration

Collaborative research projects with other institutions, such as universities, industry, non-profit organizations, and Federally Funded Research and Development Centers (FFRDCs), including the DOE National Laboratories, are encouraged under this Announcement. Proposals submitted from different institutions, which are directed at a single research activity, should clearly indicate they are part of a proposed collaboration and contain a brief description of the overall research project. However, each proposal must have a distinct scope of work and a qualified principal

investigator who is responsible for the research effort being performed at his or her institution. Further information on preparation of collaborative proposals may be accessed via the Internet at: <http://www.science.doe.gov/grants/Colab.html>.

Program Funding

It is anticipated that up to \$300,000 will be available for awards to be made in Fiscal Year 2008, contingent on the availability of appropriated funds. Proposals may request project support up to three years, with out-year support contingent on the availability of funds, progress of the research and programmatic needs. The number of awards will depend on the number of proposals received and selected for award and the availability of appropriated funds, but it is likely that only one project will be funded. DOE is under no obligation to pay for any costs associated with preparation or submission of proposals.

Formal Proposals

The research project description must be **25** pages or less, exclusive of attachments and must contain an abstract or summary of the proposed research. All collaborators should be listed with the abstract or summary. Attachments include curriculum vitae, a listing of all current and pending federal support and letters of intent when collaborations are part of the proposed research. Curriculum vitae should be limited to no more than two pages per individual.

Full proposals adhering to DOE Field Work Proposal format (Reference DOE Order 412.1) are to be prepared and submitted consistent with policies of the investigator's laboratory and the local DOE Operations Office. Laboratories may submit proposals directly to the SC Program Office listed above. A copy should also be provided to the appropriate DOE Operations Office.

The instructions and format described below should be followed. You must reference Program Announcement LAB 07-22 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

1. Scientific and/or technical merit of the project

- What is the potential of the proposed research to advance the state-of-the art in computational modeling and predictive simulation of plasma behavior?
- How is the proposed research relevant to burning plasmas and ITER?
- How does the proposed research compare with other research in its field, both in terms of scientific and/or technical merit, originality and likelihood for fundamental advances in the field?

2. Appropriateness of the proposed method or approach

- Does the proposed research make use of the best available mathematical algorithms, computer science methods and state-of-the-art data management and visualization techniques?
- Have the researchers demonstrated that their codes can effectively use the Office of Science's High Performance Computing resources and lead to scientifically valid conclusions or advances in the field?
- How good is the proposed verification and validation plan?
- Are there significant potential problems in the proposed method or approach and how well does the researcher address these problems?

3. Competency of the researcher's personnel and adequacy of the proposed resources

- How well qualified are the researchers' 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.)
- Please assess the reasonableness of the estimates of the required computational resources.
- What is the quality of the plan for effective collaboration and communication among participants as well as for forming substantive partnerships with applied mathematicians and computer scientists?
- Does the proposed work take advantage of unique facilities and capabilities and/or make good use of collaborative arrangements?

4. Performance under existing award (for renewal proposals):

- Assess the progress the researchers made toward their research goals during the most recent performance period and the impact of the research on the fusion program.
- Have the researchers disseminated the results of their research through publications in peer-reviewed journals, meeting and conference presentations, workshops, or other appropriate means?
- How successful have the researchers' efforts been to verify and validate the predictions of their simulation codes?
- How effective have the researchers' partnerships been with applied mathematics and computer science groups?

5. Reasonableness and appropriateness of the proposed budget.

- Are the proposed staffing levels and budget appropriate for carrying out the proposed research?

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

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

The evaluation process will include program policy factors such as the relevance of the proposed research to the terms of the announcement and the agencies' programmatic needs. Note that 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 an 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 O 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, 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)

2.1 Number of Copies to Submit

A complete formal FWP in a single Portable Document Format (PDF) file must be submitted through the DOE ePMA system (<https://epma.doe.gov>) as an attachment. To identify that the FWP is responding to this program announcement, please fill in the following fields in the "ePMA Create Proposal Admin Information" screen as shown:

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In order to expedite the review process, please submit a CD and one paper copy of the proposal and FWP using the following address by U.S. Postal Service Express Mail, any commercial mail delivery service, or when hand-carried.

Mr. John Sauter
U.S. Department of Energy
Office of Fusion Energy Sciences, SC-24.2/GTN
19901 Germantown Road
Germantown, MD 20874-1290
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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, or 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 the entire project period 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.science.doe.gov/grants/budgetform.pdf>

3.5 Abstract

Provide an abstract of less than 400 words. 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 **25 pages (maximum)**. 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.

More specifically, the project narrative must include:

Executive Summary

- Summarize the proposal in no more than two pages

Background and Recent Accomplishments

- Background - explanation of the importance and relevance of the proposed work
- Recent Accomplishments - this subsection is mandatory for renewal proposals and should summarize the proposed work and the actual progress made during the previous funding period.

Proposed Research and Tasks

In addition to the technical description of the proposed work and tasks, include a discussion of the following:

- Verification and Validation (V&V) plans
- Estimate of required high performance computing resources
- Impact of the proposed research on other fields of science, if appropriate

- Project timeline, milestones and deliverables, including tables of quarterly milestones from each collaborating Institution and for each year of the proposed work

Management plan, including work breakdown structure showing the level of effort for each task.

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 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.

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.

To assist in the identification of potential conflicts of interest or bias in the selection of reviewers, the following information **must 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.

3.9 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 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.