# Program Announcement To DOE National Laboratories LAB 09-10

# Mathematics for Analysis of Petascale Data

## **SUMMARY:**

The Office of Advanced Scientific Computing Research (ASCR) of the Office of Science (SC), U.S. Department of Energy (DOE), hereby announces its interest in receiving proposals for research addressing the mathematical challenges involved in extracting insights from extremely large datasets ("petascale data") and investigating fundamental issues in finding key features and understanding the relationships between those features.

Petascale data may be produced by high-resolution simulations on massively parallel computers in complex applications, such as climate modeling, fusion, and other large-scale science and engineering calculations. They may also result from experiments and observational studies, such as those in high-energy physics and cosmology. The effective analysis of petascale data is often challenged by some combination of its large-scale, distributed, heterogeneous, and varying statistical properties. Novel mathematical models, methods, and tools are needed for the representation, analysis, and understanding of such large-scale datasets that come from scientific domains pertinent to the DOE.

All proposals should address the potential for advances in mathematical methods or numerical algorithms and not just the application of methods and algorithms to a specific science problem, no matter how challenging. Educational aspects, while always welcome, are neither required nor emphasized in this call.

More information on this solicitation is provided in the Supplementary Information below.

## LETTER OF INTENT DUE DATE: April 15, 2009, 4:30pm, Eastern Time

A one-page Letter of Intent (LOI) to submit a proposal **is REQUIRED** and must be received by April 15, 2009, 4:30pm Eastern Time. The Letter of Intent should be submitted by e-mail as a PDF file attachment to: appliedmath@ascr.doe.gov. Please use "Letter of Intent for Announcement LAB09-10" in the subject line.

The purpose of the Letter of Intent (LOI) is to facilitate the planning of the peer review process and the selection of reviewers, including identifying any potential conflicts of interest. The one-page LOI must include the following information:

- the announcement number LAB09-10;
- name, institutional affiliation, e-mail address, and phone number for the Principal Investigator (PI);

- name, institutional affiliation, and e-mail address of other PIs and senior personnel;
- project funding request (approximate);
- title of the proposed effort;
- and an abstract of the proposed research.

For collaborations involving multiple institutions, a single LOI should be submitted by the PI of the lead institution. An example of the format for the one-page LOI can be viewed at: <a href="http://www.science.doe.gov/ascr/Research/LOI\_MAPD.pdf">http://www.science.doe.gov/ascr/Research/LOI\_MAPD.pdf</a>

A response to the Letters of Intent encouraging or discouraging formal proposals will be communicated to the applicants by April 24, 2009. Formal proposals will be accepted only from those encouraged to submit. No other formal proposals will be considered.

#### PROPOSAL DUE DATE: May 29, 2009, 8 PM Eastern Time.

Formal proposals submitted in response to this Announcement must be received by May 29, 2009, 8:00 p.m. Eastern time, to permit timely consideration of awards. You are encouraged to transmit your proposal well before the deadline. PROPOSALS RECEIVED AFTER THE DEADLINE WILL NOT BE REVIEWED OR CONSIDERED FOR AWARD.

#### **ADDRESSES:**

Please have your lab administrator submit the entire lab proposal and FWP via Searchable FWP (<u>https://www.osti.gov/fwp</u>). If you have questions about who your lab administrator is or how to use Searchable FWP, please contact the Searchable FWP Support Center.

Also, to assist in expediting the review process, please submit via federal express, a single PDF file of the entire LAB proposal and FWP on a CD along with two hard copies to the address below.

#### Please send the CD and 2 hard copies via Federal Express to:

Teresa Beachley Office of Advanced Scientific Computing Research, SC-21.1 Office of Science 19901 Germantown Road Germantown, MD 20874-1290 ATTN: Program Announcement LAB 09-10

**FOR FURTHER INFORMATION CONTACT:** Alexandra Landsberg, Applied Mathematics Program, Telephone: (301) 903-8507, FAX: (301) 903-7774, E-mail: landsberg@ascr.doe.gov.

#### SUPPLEMENTARY INFORMATION:

The analysis of large-scale datasets has become increasingly difficult due to the complexity and enormous volume of data obtained from observatories, experimental facilities, and computational simulations. DOE scientists need to address the daunting challenges in extracting scientific

knowledge from petascale data, and mathematical methods have long been the mainstay for such efforts. Over the next decade, many existing approaches for data analysis will fail to provide adequate robustness, scalability, and combinatorial tractability. The Applied Mathematics Program within the Office of Advanced Scientific Computing Research supports basic research on the mathematical methods and numerical algorithms that address these long-term needs. This Notice solicits innovative basic research proposals in mathematics for petascale data analysis. Particularly innovative approaches for supporting mathematical research efforts, including but not limited to workshops and conferences, will also be considered under this solicitation.

Prospective research should observe that:

- Collaborative proposals involving multiple institutions, which may include universities, laboratories, and/or private institutions, are encouraged but not required.
- Proposed research activities should be relevant to the mission of the Department of Energy and, in particular, to the long-term goals of its research programs.
- Researchers may request a period of performance of up to three (3) years.

This solicitation seeks proposals for basic research in mathematical models, methods and tools for the representation, analysis, and understanding of petascale data. Areas of interest include, but are not limited to:

- Novel mathematical techniques and algorithmic approaches to build and evaluate appropriate models from large-scale, heterogeneous, high-dimensional data.
- New algorithms designed to scale with the size of the data, which is often independent of the number of model parameters, and so may require parallel, single-pass, or subsampling methodologies.
- Methodologies for analyzing data, distributed over space and time, with changing local properties that may not statistically resemble the global properties of the data.
- The development of real-time anomaly identification in streaming and evolving data for detecting and responding to interesting phenomena that may be short-lived or urgent.
- Novel mathematical approaches to improve the methods of collection for petascale data, and dimension reduction for extracting pertinent subsets, features of interest, or low-dimensional patterns.
- The development of rigorous mathematical approaches for combining data of different types and quality (e.g., noisy or incomplete data), and that can also quantify the various forms of uncertainties in the data.
- Rigorous mathematical methods for identifying important features in complex data, such as time-dependent scalar, vector, and tensor field data.

For more information on petascale data challenges and scientific examples of interest to DOE, see the following reports -

- Mathematics for Analysis of Petascale Data Workshop Report
  <u>http://www.sc.doe.gov/ascr/ProgramDocuments/Docs/PetascaleDataWorkshopReport.pdf</u>
- Visualization and Knowledge Discovery: Report from the DOE/ASCR Workshop on Visual Analysis and Data Exploration at Extreme Scale

http://www.sc.doe.gov/ascr/ProgramDocuments/Docs/DOE-Visualization-Report-2007.pdf

• Applied Mathematics at the U.S. Department of Energy: Past, present and a view to the future <a href="http://www.sc.doe.gov/ascr/ProgramDocuments/Docs/Brown\_Report\_May\_08.pdf">http://www.sc.doe.gov/ascr/ProgramDocuments/Docs/Brown\_Report\_May\_08.pdf</a>

#### **Collaboration and Communication**

The proposal should identify potential collaborations or other interactions that will facilitate the exchange of ideas and dissemination of information among research centers in industry, universities, and/or laboratories. Further information on preparation of collaborative proposals may be accessed via the Internet at <u>http://www.science.doe.gov/grants/colab.html</u>.

## **ESTIMATED FUNDING**

It is anticipated that up to \$4 million total will be available for multiple awards for this solicitation in Fiscal Year 2009. Proposers may request project support for up to three years. All awards are contingent on the availability of funds and programmatic needs. DOE is under no obligation to pay for any costs associated with the preparation or submission of a proposal. DOE reserves the right to fund, in whole or in part, any, all or none of the proposals submitted in response to the Notice.

#### SUBMISSION INFORMATION

The instructions and format described below must be followed. You must reference Program Announcement LAB 09-10 on all submissions and inquiries about this Program Announcement.

## 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. Included with each criteria are the detailed questions that will be asked of the reviewers.

- 1. Scientific and/or Technical Merit of the Proposed Research
- 2. Appropriateness of the Proposed Method or Approach

- 3. Competency of Applicant's Personnel and Adequacy of Proposed Resources
- 4. Reasonableness and Appropriateness of the Proposed Budget
- 5. Other Appropriate Factors

The evaluation process will include program policy factors such as the relevance of the proposed research to the terms of the Announcement and the Department's programmatic needs. 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 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, 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

Please have your lab administrator submit the entire lab proposal and FWP via Searchable FWP (<u>https://www.osti.gov/fwp</u>). If you have questions about who your lab administrator is or how to use Searchable FWP, please contact the Searchable FWP Support Center.

Also, to assist in expediting the review process, please submit via federal express, a single PDF file of the entire LAB proposal and FWP on a CD along with two hard copies to the address below.

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Teresa Beachley Office of Advanced Scientific Computing Research, SC-21.1 Office of Science 19901 Germantown Road Germantown, MD 20874-1290 ATTN: Program Announcement LAB 09-10

# 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 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**

Summarize the proposal in one page. 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 15 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.

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." Collaborative research projects with institutions that receive grants, such as universities, industry, and non-profit organizations, are allowed under this Announcement. See the section on Collaboration. Further information on collaboration may be accessed at <a href="http://www.science.doe.gov/grants/Colab.html">http://www.science.doe.gov/grants/Colab.html</a>.

# **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.

## **3.9 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 \$50,000 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.