Program Announcement
To DOE National Laboratories
LAB 09-23

Mathematics for Complex, Distributed, Interconnected Systems

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 the modeling, simulation and analysis of complex, distributed, interconnected systems.

Critical to the Department of Energy is understanding the behavior of large-scale complex, distributed, interconnected systems, such as Supervisory Control And Data Acquisition (SCADA) systems, electric power distribution networks, and other distributed, interconnected complex systems. The Department extensively utilizes distributed, collaborative systems with a significant fraction involving "open science" research in which significant amounts of information are shared among institutions and over networks around the world. These systems operating within the purview of the DOE involve networks and heterogeneous assemblies of different system types, which collectively operate as a whole. While integrating disparate models may capture some of the complex dynamics, often these integrated capabilities lack the ability to support policy-making and overall system control due to the decentralized nature of the component models. The benefits of better modeling, simulation and analysis of complex, distributed, interconnected systems range from improved strategies underlying policy and priority decision-making to forming the basis for building predictive capabilities.

Proposals should address the mathematical research challenges associated with the modeling, simulation and analysis of complex, distributed, interconnected systems.

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

PROPOSAL DUE DATE: June 12, 2009, 8 PM Eastern Time.

Formal proposals submitted in response to this Announcement must be received by June 12, 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 (https://www.osti.gov/fwp). 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 09-23

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: A strong mathematical foundation is essential in formulating realistic models for the simulation and analysis of critically important infrastructure systems operating within the purview of the DOE. Understanding real-world data based on observation and measurements are also important complements to this research. However, the size, heterogeneity, complexity and real-time characteristics of these systems lead to new challenges in modeling, simulation and analysis. Simple integration of existing modeling and simulation capabilities is not likely to capture the emergent and dynamic behavior of these large-scale systems. The DOE needs to address the daunting challenges of modeling, simulation and analysis of complex, distributed, interconnected systems. 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.

Prospective research should observe that:

- Collaborative proposals may include multiple DOE National Laboratories.
- Proposed research activities should be relevant to the mission of the Office of Science and, in particular, to the long-term goals of its research programs.
- Funds may be provided to universities through subcontracts.
- Researchers may request a period of performance of up to three (3) years.

This announcement seeks proposals for basic research in mathematical models, methods and tools for the modeling, simulation and analysis of complex, distributed, interconnected systems. Particularly innovative approaches for supporting mathematical research efforts will be considered under this solicitation. Areas of interest include, but are not limited to:

- Real-world, real-time data generated by complex, distributed, interconnected systems and associated novel data analysis techniques and methods for advanced situational awareness, including:
    - Mathematical methods that ensure the confidentiality, integrity, and availability of massive amounts of distributed real-world data in real, or near-real time, on which to base model development and analysis
    - Mathematical and statistical techniques that can operate in real-time on large-scale, distributed data to characterize normal behavior and to distinguish between harmless anomalies and malicious attacks
    - Novel techniques addressing the challenges associated with missing values and modeling uncertainty associated with complex interconnected systems
    - Statistical approaches for exploration, characterization and analysis of complex system activity.
- Modeling and simulation of the key properties and emergent behavior on large-scale complex distributed interconnected systems, including:
    - Mathematical and statistical techniques that faithfully reproduce the observed emergent behavior of the complex interconnected system as a whole while preserving the essential characteristics of its components
    - Large-scale complex system emulation capability that reproduces observed behavior to inform the development of mathematics, algorithms and models for complex interconnected systems
    - Approaches for large-scale realistic network simulations at different scales, including development of reasonable proxies and understanding the relations among different levels of modeling and their ability to predict emergent behavior
    - Rigorous methods to assess and validate computational models of large-scale complex systems incorporating robustness to adversarial environments
    - Quantification of uncertainty of large-scale complex distributed interconnected systems
- Mathematical methods for modeling and analysis of the dynamics and evolution of large-scale, complex, distributed interconnected systems, including
    - Techniques for discovering threats to complex distributed interconnected systems including malicious code and behavior detection.

For more information on complex, distributed, interconnected system research challenges and scientific examples of interest to DOE, see the following reports:

- National Cyber Security Research and Development Challenges http://www.thei3p.org/docs/publications/i3pnationalcybersecurity.pdf
- Transforming DOE CyberSecurity wiki https://wiki.cac.washington.edu/display/doe/Home
- A Scientific Research and Development Approach to Cyber Security http://www.science.doe.gov/ascr/ProgramDocuments/Docs/CyberSecurityScienceDec2008.pdf
- Mathematical Challenges in Cyber Security https://wiki.cac.washington.edu/download/attachments/7478403/Dunlavy-Hendrickson-Kolda-Mathematical-Challenges-in-Cybersecurity.pdf?version=1

- Report of the Cyber Security Research Needs for Open Science Workshop http://www.sc.doe.gov/ascr/Misc/CSWorkshopFinalReport.pdf

Collaboration and Communication

Proposals should identify potential collaborations or other interactions that will facilitate the exchange of ideas and dissemination of information among researchers in industry, universities, and/or other laboratories. Synergistic collaborations with researchers at universities and in industry will be achieved through subcontracts.

All awardees will be required to submit a management plan on how their team will interact with other awardees and the greater research community. The goal is to enhance collaborations among researchers and to build community support for the long-term sustainment of this effort. Long-term research may be achieved through an integrated center addressing mathematics, computer science, networking, and hardware research challenges associated with complex, distributed, interconnected systems.

ESTIMATED FUNDING

It is anticipated that up to $3.5 million total will be available for research projects 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 solicitation.

SUBMISSION INFORMATION

The instructions and format described below must be followed. You must reference Program Announcement LAB 09-23 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 (https://www.osti.gov/fwp). 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:

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Office of Advanced Scientific Computing Research, SC-21.1
Office of Science
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, 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 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 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."

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.

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

Publications. 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.

Synergistic Activities. 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.