

**Program Announcement
To DOE National Laboratories
LAB 10-315**

***Advancing Uncertainty Quantification (UQ)
in Modeling, Simulation, and Analysis
of Complex 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 Field Work Proposals (FWPs) for research addressing the mathematical and computational challenges of uncertainty quantification in the modeling and simulation of complex natural and engineered systems.

Simulation plays a key role in addressing scientific and technical issues concerning DOE mission-relevant complex systems such as climate, carbon capture and storage, nuclear energy, and other energy applications. A central challenge in the predictive modeling, simulation, and analysis of these complex systems is Uncertainty Quantification (UQ). Uncertainty quantification refers to the broad range of activities aimed at assessing and improving confidence in simulation. There are many different sources of uncertainty and error that arise in the modeling and simulation of complex systems. For increasing the confidence of simulations, it is important to accurately characterize and quantify the effects of uncertainties and errors on mathematical models and computational algorithms.

Understanding and predicting the behavior of complex multiphysics, multiscale systems typical of those within the DOE mission, represents a portfolio of challenges for modern science and engineering. Uncertainty and error are inherent in the study of systems of this level of complexity. Overall success depends on a fusion of data (experimental, observational) and models (physics, computation), within practical limitations:

- The available physical data (observational or experimental) may vary greatly in terms of its type, quality and quantity;
- The computational demands of the model limit the number of simulations that can be carried out;
- The computational models are not perfect representations of physical reality – they have inadequacies, approximations, missing physics, etc.;
- The computational models may represent single realizations of inherently stochastic systems;
- The computational models typically have unknown parameters and boundary conditions which need to be adjusted for the application at hand;

- The computing environment on which the models execute may not be deterministic due to silent errors, and differing hardware and software configurations;
- Scientists often wish to use such models in extrapolative conditions, where we have little or no physical observations to validate model output.

This Program Announcement calls for research in applied mathematics on Uncertainty Quantification in complex systems of interest to the DOE, scalable UQ methods, and UQ relevant to the simulation and analysis of complex systems on high-concurrency, extreme-scale computing architectures.

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

SUPPLEMENTARY INFORMATION:

Scientists are being asked to identify or provide technology, or to give expert analysis to inform policy-makers that requires the scientific understanding of increasingly complex natural and engineered systems. Simulations of complex systems are often our only tool for such analysis, where experimentation is neither feasible nor possible. However, scientists often lack quantitative estimates of the limits of applicability in these models, nor do they have a full, quantitative understanding of the sources of uncertainty and the subsequent propagation of uncertainty in these models.

Uncertainty quantification (UQ) broadly refers to the assessment of confidence of simulation predictions based on all available information including: accuracy of physical measurements; incomplete understanding of the underlying physical processes; the complexity of coupling different physical processes across large-scale differences; numerical errors associated with simulations of complex models; and the sensitivity of simulation output to inputs.

As most DOE high-end application science codes currently do not incorporate UQ technology, the anticipated re-engineering of application codes presents an opportunity for the research, design, and implementation of advanced, scalable UQ methods for next-generation scientific simulation codes. Incorporating errors from software and hardware characteristics, e.g. resulting from trading accuracy for speed, may become more significant in future application codes and advanced architectures.

This Program Announcement calls for research in advanced Uncertainty Quantification techniques for complex systems with future computing architectures in mind. Areas of interest include, but are not limited to:

- Mathematical, statistical and hybrid approaches for quantifying and describing the effects and interactions of uncertainty and errors, potentially from multiple sources and with multiple representations
- Mathematical and computational frameworks for integrating statistical and deterministic analysis

- Mathematical theory and/or implementation of algorithms that demonstrably circumvent the “curse of dimensionality” in UQ analysis for complex system simulations
- Mathematical theory and/or algorithms for reduced-order modeling, inference, and inverse problems
- Scalable algorithms for numerical solutions of stochastic differential equations
- Tractable UQ treatment (intrusive or non-intrusive) for high-concurrency architectures
- Memory-access-efficient algorithms that match current and emerging computer architectures and allow for efficient and tractable sampling-based approaches

For more information, please see the following workshops and reports:

- Modeling and Simulation at the Exascale for Energy and the Environment Town Hall Meetings, April 17-18, 2007, May 17-18, 2007, and May 31-June 1, 2007.
<http://www.sc.doe.gov/ascr/ProgramDocuments/Docs/TownHall.pdf>
- “Scientific Grand Challenges: Challenges in Climate Change Science and the Role of Computing at the Extreme Scale.” Workshop, November 6-7, 2008 in Washington, DC.
<http://www.sc.doe.gov/ascr/ProgramDocuments/Docs/ClimateReport.pdf>
- “Science Based Nuclear Energy Systems enabled by Advanced Modeling and simulation at the Extreme Scale”, Workshop, May 11-12, 2009 in Washington, DC.
<http://www.sc.doe.gov/ascr/ProgramDocuments/Docs/Nuclear%20Workshop%20Report%20.pdf>
- “Scientific Grand Challenges in National Security: the Role of Computing at the Extreme Scale.” Workshop, October 6-8, 2009 in Washington, DC.
- “Evaluation of Quantification of Margins and Uncertainties (QMU) for Assessing and Certifying the Reliability of the Nuclear Stockpile,” National Academies Report, November 11, 2008. http://www.nap.edu/catalog.php?record_id=12531#toc
- “Applied Mathematics at the U.S. Department of Energy: Past, present, and a view to the Future”, May 2008.
http://www.sc.doe.gov/ascr/ProgramDocuments/Docs/Brown_Report_May_08.pdf

Collaboration and Communication

The FWP 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: <http://www.sc.doe.gov/grants/Colab.html>. An important aspect of this program announcement is to build and foster an active, integrated research community to understand the most promising scalable uncertainty quantification methods and influence the design of next-generation science codes. Accordingly, the FWP should include plans for the dissemination of research results with relevance to DOE complex systems. The FWP should also clearly identify the roles and responsibilities of each senior project personnel and articulate how their research advances the use of UQ as an essential element in the modeling and simulation of complex systems.

DATES:

Full proposals submitted in response to this Announcement must be received no later than 11:59 pm ET, **Monday, April 26, 2010**, to be accepted for merit review and to permit timely consideration for award in Fiscal Year 2010.

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

ADDRESSES and SUBMISSION INSTRUCTIONS:

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.

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. This will assist in expediting the review process.

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 10-315

FOR FURTHER INFORMATION CONTACT:

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PROGRAM FUNDING:

It is anticipated that up to a total of \$3 million annually will be available for multiple awards in this program announcement. Awards are planned to be made in Fiscal Year 2010, and FWPs

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 FWP. DOE reserves the right to fund, in whole or in part, any, all, or none of the FWPs submitted in response to this Announcement.

Eligibility:

This is a DOE LAB-only Announcement. FFRDCs from other federal agencies are not eligible to submit in response to this Announcement. Partnerships between DOE LABs and other appropriate institutions are encouraged, as appropriate. For multi-lab proposals, a complete proposal with all collaborating parts should be submitted by the lead LAB. No individual submissions by university partnerships should be sent via grants.gov at this stage.

SUBMISSION INFORMATION:

The instructions and format described below must be followed. All submissions and inquiries about this Program Announcement must reference Program Announcement Lab 10-315.

The research project description must be **20 pages or less**, exclusive of attachments and the required one-page abstract (see below). 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.

The following is a list of essential items that a proposal must contain:

- 1. Field Work Proposal (FWP) Format** - Complete and signed by appropriate officials.
- 2. Proposal Cover Page**
- 3. Table of Contents**
- 4. Budget Page(s)** (Form DOE F 4620.1) - Complete a separate Budget Page for the entire multi-year period for each separate participating institution, if applicable.
<http://www.science.doe.gov/grants/budgetform.pdf>
- 5. Budget Description and Justification** - Separately for each collaborating institution if applicable.
- 6. Other Project Information**
 - a. A one-page abstract** (on a page by itself): The abstract must include, at the top of the page: the (lead) DOE National Laboratory, title of the project, name of the principal investigator (PI), the PI's telephone number and e-mail address, and a list of all collaborating investigators (if any) and their institutions. The abstract must provide a

summary of the project narrative, including the technical qualifications of the principal investigator.

b. Project Narrative (20 pages maximum): The project narrative must include a detailed description of the proposed research project, which must include a list of project milestones, a timeline of key activities, and clear statements of which project personnel will be responsible for each key activity.

c. Bibliography: A complete bibliographic listing of all the published scientific and engineering literature referred to in the project narrative.

d. Biographical Sketches: Relevant information about the background and experience of the principal investigator and co-principal investigators or collaborators (if any). Biographical sketches are limited to two pages per individual.

e. Facilities and Resources: Include information on the experience of the proposing institution(s), their facilities, and the available resources that would be relevant to successful completion of the project.

f. Statement of all current and pending support for the principal investigator and co-principal investigators and collaborators (if any), including the time devoted (each year) to each project by each named individual.

The instructions and format described below must be followed. You must reference Program Announcement LAB 10-315 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 this Announcement, proposals will be subjected to a formal 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 Researcher's Personnel and Adequacy of Proposed Resources; and
- 4) Reasonableness and Appropriateness of the Proposed Budget.

The evaluation process will include program policy factors such as the relevance of the proposed research to the terms of the Announcement and the agency's 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 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 - 20-page limit)
- Literature Cited
- Biographical Sketch(es)
- Description of Facilities and Resources
- Other Support of Investigator(s)
- Appendix (optional)

2.1 Submission Instructions

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.

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. This will assist in expediting the review process.

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

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Computational Science Research & Partnerships Division, SC-21.1
Office of Advanced Scientific Computing Research
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19901 Germantown Road
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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 his or her proposal. 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.

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 lead DOE national Laboratory, 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 **20 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. It is important that the 20-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 or the first 20 pages may be reviewed without regard to the remainder.

All proposals submitted in response to this LAB Announcement must explicitly state how the proposed project will support the accomplishment of the program goals and the ASCR mission, including the project's impact on applications of interest to the Office of Science.

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. 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 five 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. Finally, list any individuals who are not listed in the previous categories with whom you are discussing future collaborations. 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.