Office of Science
Financial Assistance
Funding Opportunity Announcement
DE-FOA-0000315

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 applications 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 Funding Opportunity Announcement (FOA) 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.

APPLICATION DUE DATE: April 26, 2010, 11:59 p.m. Eastern Time

Formal applications submitted in response to this FOA must be received by April 26, 2010, 11:59 p.m. Eastern time, to permit timely consideration of awards. **APPLICATIONS RECEIVED AFTER THE DEADLINE WILL NOT BE REVIEWED OR CONSIDERED FOR AWARD.**

IMPORTANT SUBMISSION INFORMATION:

The full text of the Funding Opportunity Announcement (FOA) is located on FedConnect. Instructions for completing the Grant Application Package are contained in the full text of the FOA which can be obtained at: https://www.fedconnect.net/FedConnect/?doc=DE-FOA-0000315&agency=DOE. To search for the FOA in FedConnect click on "Search Public Opportunities". Under "Search Criteria", select "Advanced Options", enter a portion of the title "Advancing Uncertainty Quantification (UQ) in Modeling,Simulation, and Analsyis of Complex Systems", then click on "Search". Once the screen comes up, locate the appropriate Announcement.

In order to be considered for award, Applicants must follow the instructions contained in the Funding Opportunity Announcement.

WHERE TO SUBMIT: Applications must be submitted through Grants.gov to be considered for award.

You cannot submit an application through Grants.gov unless you are registered. Please read the registration requirements carefully and start the process immediately. Remember you have to update your CCR registration annually. If you have any questions about your registration, you should contact the Grants.gov Helpdesk at 1-800-518-4726 to verify that you are still registered in Grants.gov.

Registration Requirements: There are several one-time actions you must complete in order to submit an application through Grants.gov (e.g., obtain a Dun and Bradstreet Data Universal Numbering System (DUNS) number, register with the Central Contract Registry (CCR), register with the credential provider, and register with Grants.gov). See http://www.grants.gov/GetStarted. Use the Grants.gov Organization Registration Checklist at http://www.grants.gov/assets/OrganizationRegCheck.pdf to guide you through the process.

Designating an E-Business Point of Contact (EBiz POC) and obtaining a special password called an MPIN are important steps in the CCR registration process. Applicants, who are not registered with CCR and Grants.gov, should allow at least 21 days to complete these requirements. It is suggested that the process be started as soon as possible.

IMPORTANT NOTICE TO POTENTIAL APPLICANTS:
When you have completed the process, you should call the Grants.gov Helpdesk at 1-800-518-4726 to verify that you have completed the final step (i.e. Grants.gov registration).

Questions: Questions relating to the registration process, system requirements, how an application form works, or the submittal process must be directed to Grants.gov at 1-800-518-4726 or support@grants.gov. Part VII of the FOA explains how to submit other questions to the Department of Energy (DOE).

GENERAL INQUIRIES ABOUT THIS FOA SHOULD BE DIRECTED TO:

Technical/Scientific Program Contact:

Program Manager: Dr. Karen Pao
Office of Advanced Scientific Computing Research
U. S. Department of Energy
Telephone: (301) 903-5384
E-mail: Karen.Pao@science.doe.gov

Program Manager: Alexandra Landsberg
Office of Advanced Scientific Computing Research
U. S. Department of Energy
Telephone: (301) 903-8507
E-mail: Sandy.Landsberg@science.doe.gov

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 FOA 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.

Program Funding

It is anticipated that up to a total of $3 million annually will be available for multiple awards in this solicitation. Awards are planned to be made in Fiscal Year 2010, and applications 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 an application. DOE reserves the right to fund, in whole or in part, any, all, or none of the applications submitted in response to this Notice.

DOE is under no obligation to pay for any costs associated with the preparation or submission of an application. DOE reserves the right to fund, in whole or in part, any, all, or none of the applications submitted in response to this FOA.

Merit Review

Applications will be subjected to scientific merit review (peer review) and will be evaluated against the following evaluation criteria which are listed in descending order of importance codified at 10 CFR 605.10(d):

1. Scientific and/or Technical Merit of the Project;
2. Appropriateness of the Proposed Method or Approach;

3. Competency of Applicant's Personnel and Adequacy of Proposed Resources; and
4. Reasonableness and Appropriateness of the Proposed Budget.

The evaluation will include program policy factors such as the relevance of the proposed research to the terms of the FOA and the agency's programmatic needs. It should be noted that external peer reviewers are selected on the basis of their scientific expertise and the absence of conflict- of-interest issues. Both Federal and non-Federal reviewers may be used, and submission of an application constitutes agreement that this review process is acceptable to the investigator(s) and the submitting institution.

The Catalog of Federal Domestic Assistance (CFDA) number for this program is 81.049, and the solicitation control number is ERFAP 10 CFR Part 605.

Posted on the Office of Science Grants and Contracts Web Site
March 16, 2010.