

**FINANCIAL ASSISTANCE  
FUNDING OPPORTUNITY ANNOUNCEMENT**



**U.S. Department of Energy**

**Office of Science**

**Office of Advanced Scientific Computing Research (ASCR)**

*2012 Mathematical Multifaceted Integrated Capability Centers (MMICCs)*

**Funding Opportunity Number: DE-FOA-0000698**

**Announcement Type: Initial**

**CFDA Number: 81.049**

**ISSUE DATE: April 4, 2012**

**Pre-Application Due Date: April 30, 2012**  
**(Pre-Applications are required)**

**Application Due Date: June 1, 2012, 11:59 p.m. Eastern Time**

## NOTE: REQUIREMENTS FOR GRANTS.GOV

**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 Central Contract Registry (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 (i.e., obtain a Dun and Bradstreet Data Universal Numbering System (DUNS) number, register with the CCR, register with the credential provider, and register with Grants.gov). To register with Grants.gov go to “Get Registered” at [http://grants.gov/applicants/get\\_registered.jsp](http://grants.gov/applicants/get_registered.jsp). 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](mailto:support@grants.gov). Part VII of this Funding Opportunity Announcement (FOA) explains how to submit other questions to the Department of Energy (DOE).

### Application Receipt Notices

After an application is submitted, the Authorized Organization Representative (AOR) will receive a series of four e-mails. It is extremely important that the AOR watch for and save each of the emails. It may take up to two (2) business days from application submission to receipt of email Number 2. The titles of the four e-mails are:

- Number 1 - Grants.gov Submission Receipt Number
- Number 2 - Grants.gov Submission Validation Receipt for Application Number
- Number 3 - Grants.gov Grantor Agency Retrieval Receipt for Application Number
- Number 4 - Grants.gov Agency Tracking Number Assignment for Application Number

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## PART I – FUNDING OPPORTUNITY DESCRIPTION

### GENERAL INQUIRIES ABOUT THIS FOA SHOULD BE DIRECTED TO:

Technical/Scientific Program Contacts:

**Program Manager:** Sandy Landsberg, (301) 903-8507  
Office of Advanced Scientific Computing Research, SC-21.1  
**E-mail:** [Sandy.Landsberg@science.doe.gov](mailto:Sandy.Landsberg@science.doe.gov)

**Program Manager:** Dr. Steven L. Lee, (301) 903-5710  
Office of Advanced Scientific Computing Research, SC-21.1  
**E-mail:** [Steven.Lee@science.doe.gov](mailto:Steven.Lee@science.doe.gov)

### STATUTORY AUTHORITY

Public Law 95-91, US Department of Energy Organization Act  
Public Law 109-58, Energy Policy Act of 2005

### APPLICABLE REGULATIONS

U.S. Department of Energy Financial Assistance Rules, codified at 10 CFR Part 600  
U.S. Department of Energy, Office of Science Financial Assistance Program Rule, codified at 10 CFR Part 605

### SUMMARY:

The Office of Advanced Scientific Computing Research (ASCR) of the Office of Science (SC), U.S. Department of Energy (DOE), hereby invites applications for basic research that addresses grand challenges of increasing complexity within DOE's mission areas of energy, environment and security, from a mathematical perspective that require new integrated, iterative processes across multiple mathematical disciplines. This Funding Opportunity Announcement (FOA) will holistically address mathematics for increasingly complex DOE-relevant systems for scientific discovery, design, optimization and risk assessment – this will be achieved through *Mathematical Multifaceted Integrated Capability Centers* (MMICCs).

This FOA is *seeking applications for Mathematical Multifaceted Integrated Capability Centers addressing the long-term mathematical challenges* for one or more DOE grand challenges of increasing complexity. These science and engineering challenges must be abstracted into an interrelated set of mathematical research challenges that require new integrated, iterative processes across multiple mathematical disciplines. Applications focused on solution of a specific application problem will be considered outside the scope of this FOA.

These MMICCs will enable applied mathematics researchers to work together in large, collaborative teams to more effectively address DOE grand challenge problems from a mathematical perspective much earlier in the problem solving process. The MMICCs allow researchers to take a broader view of the problem as a whole, and devise solution strategies that

attack the problem in its entirety by building fundamental, multidisciplinary mathematical capabilities and tools. The MMICCs will have the flexibility and technical expertise to simultaneously consider all aspects of the problem-solving process ranging from the mathematical formulation to the development, analysis, and integration of appropriate models and methods to the demonstration of results and capabilities. The goal is to determine the most effective combination of the various mathematical components, as such, an iterative process will be necessary. These Centers will help serve as entry points for applied mathematicians and other researchers to more readily understand the mathematical challenges of DOE-relevant problems.

More specific information is included under SUPPLEMENTARY INFORMATION below.

A companion Program Announcement to DOE National Laboratories, LAB 12-698, will be posted on the SC Grants and Contracts web site at: <http://www.science.doe.gov/grants>

#### **SUPPLEMENTARY INFORMATION:**

##### **Mathematical Multifaceted Integrated Capability Centers**

The “Grand Challenges” were U.S. policy terms set in the 1980’s as goals for funding high-performance computing and communications research in response to foreign competition. They were described as “fundamental problems of science and engineering, with broad applications, whose solution would be enabled by high-performance computing resources...”. Grand Challenges today are interpreted in a much broader sense with the realization that they cannot be solved by advances in high performance computing alone; they also require breakthroughs in computational models, algorithms, data and visualization technologies, software and collaborative organizations uniting diverse disciplines.

This FOA is seeking applications that address grand challenges of increasing complexity within DOE’s mission areas of energy, environment and security, from a mathematical perspective that require new integrated, iterative processes across multiple mathematical disciplines. This new paradigm will holistically address mathematics for increasingly complex DOE-relevant systems for scientific discovery, design, optimization and risk assessment – this will be achieved through *Mathematical Multifaceted Integrated Capability Centers* (MMICCs). These MMICCs will enable applied mathematics researchers to work together in large, collaborative teams to more effectively address grand challenge problems from a mathematical perspective much earlier in the problem solving process. The MMICCs allow researchers to take a broader view of the problem as a whole, and devise solution strategies that attack the problem in its entirety by building fundamental, multidisciplinary mathematical capabilities and tools. The MMICCs will have the flexibility and technical expertise to simultaneously consider all aspects of the problem-solving process ranging from the mathematical formulation to the development, analysis, and integration of appropriate models and methods to the demonstration of results and capabilities. The goal is to determine the most effective combination of the various mathematical components, as such, an iterative process will be necessary. These Centers will help serve as entry points for applied mathematicians and other researchers to more readily understand the mathematical challenges of DOE-relevant problems.

The DOE Applied Math Summit [1], the DOE ASCR 2012 **Workshop for Mathematics for the Analysis, Simulation, and Optimization of Complex Systems** [2], and workshop report, *A Multifaceted Mathematical Approach for Complex Systems* [3] all concluded that future DOE challenges will require the ability to model systems of unprecedented complexity. Dealing with these increasingly complex systems will require new types of models that couple a broad array of diverse processes spanning a wide range of spatial and temporal scales. The models will likely combine both deterministic and stochastic elements; they are likely to have multiple representations; and they are likely to have dynamic properties. The goal is not to simply produce a simulation of the system, or couple existing models and methods, but rather to answer difficult questions regarding design, risk analysis, or optimization, while quantifying errors and uncertainties. These types of highly complex systems cannot be analyzed at the required fidelity with monolithic mathematical models. Effective models will be hierarchical and include multiple sub-models that represent different phenomena with vastly differing scales. These models can range from the representation of detailed physical processes to the description of complex engineered systems that must be optimized to obtain desired performance. This will require new approaches for understanding the impact on system behavior based on the interplay between sub-models at different physical resolutions or between decision points in an engineered system. Answering key questions about these systems may also require a much tighter coupling between data and simulation, and require new approaches to aggregate information from multiple sources.

The goal is to have researchers simultaneously examine, in an integrated form, all of the mathematical elements needed to make significant advances in the analysis, simulation, and optimization of a complex system. This holistic approach to problem solving is not a linear process of working from formulation to discretization to algorithm but rather an iterative one considering all aspects of the solution process. It is through this iteration that researchers will arrive at the combination of formulation, discretization, and solution methodologies that will enable the most effective combination of the various mathematical components to construct the tools needed to answer important questions about systems of increasing complexity while making efficient use of emerging computer architectures.

Applications for a Mathematical Multifaceted Integrated Capability Center must:

1. Advance multifaceted, integrated mathematics that spans, as appropriate, novel formulations, discretizations, algorithm development, data analysis techniques, uncertainty quantification methodologies, optimization techniques, and other mathematical approaches;
2. Address one or more Grand Challenge problems with clear relevance and impact to the DOE; and
3. Advance the field of applied and computational mathematics.

This FOA includes four illustrative DOE examples for MMICCs and the organizational structure and management plan of a MMICC.

## **Four Illustrative DOE Examples for MMICCs**

Grand Challenges for MMICCs include defining one or more DOE-relevant scientific or engineering challenges; these are then abstracted into an interrelated set of mathematical research challenges that must be addressed through an integrated, iterative process. MMICC grand challenges are multifaceted: they may involve complex continuous and discrete phenomena with both stochastic and deterministic elements; they may involve coupled models from multiple scientific disciplines; they may require integration of simulation and data; and they may be characterized by pervasive uncertainties. The multifaceted nature of these problems demands a new mode of operation for applied mathematicians; researchers are going to have to cut across the boundaries of traditional development of mathematical methods and tools. To contribute towards solving problems of major importance to DOE, applied mathematics researchers must consider new research directions not just within traditional mathematical topic areas such as modeling, discretizations, linear algebra, optimization, stochastics, and data analysis, but how these interact in an overall integrated problem-solving process.

The MMICCs will provide an opportunity to enhance the impact of applied mathematics on solving problems of critical importance to the DOE. These centers will also produce high-impact, lasting contributions to applied mathematics. The process of developing integrated problem-solving strategies for complex systems will lead to the creation of a far richer, deeper set of mathematical tools in areas ranging from basic analysis to software development. These tools will, in turn, lead to improved theoretical understanding and computational methodologies for systems of increasing complexity.

One of the goals of the MMICCs is to have some level of buy-in from DOE application domains. A letter of endorsement is not required; however, a clear explanation of long-term potential impact to DOE is required. The application will need to discuss one or more scientific or engineering grand challenges and identify an interrelated set of mathematics research challenges that represent abstractions of the grand challenges. These abstractions would then be optimally addressed through a multifaceted, integrated approach. The results of MMICC research should have potential impact to the DOE mission in the 5-10+ year timeframe by transitioning to SciDAC Partnerships, SciDAC Institutes, Co-Design Centers, and/or directly to DOE application scientists. Application drivers of importance for MMICCs are:

### **I. Mathematical Challenges from Materials and Chemistry for Energy Applications**

These long-term mathematical challenges potentially include bridging multiple scales, incorporating theory and experimental data, characterizing and propagating uncertainty, validation, and optimizing material design. The development of new models, methods, and computational approaches will dramatically accelerate the discovery of new materials and processes as well as provide fundamental understanding and improvement of current materials and processes. A series of workshops and reports discuss many of the associated challenges [4-6]. Most recently, the *Materials Genome Initiative for Global Competitiveness* [7] was announced. The long-term goal is to generate computational methods and tools that enable real-world materials development, that optimize or minimize traditional experimental testing, and that predict materials performance under diverse product conditions. One challenge is that current predictive algorithms do not have the ability to model behavior and properties across multiple spatial and temporal scales.

Another illustrative example is understanding and predicting the properties of catalysts and designing them for achieving the full potential of novel fuels [3,10]. Modeling and simulation built upon multifaceted integrated mathematics can help assess the technological feasibility of the resulting catalyst, has the potential of incorporating data from high-resolution experimental capabilities, and to significantly enhance predictability on multiple coupled scales. Mathematically this may include, but is not limited to, research in dynamical systems, partial differential and integral operators; optimization methods for inverse problems and energy minimization; and data analysis techniques.

## **II. Mathematical Challenges from Complex Engineered Systems for Energy Applications**

These long-term mathematical challenges potentially include, but are not limited to, new algorithms that are scalable and robust for solving large nonlinear mixed-integer optimization problems and methods for efficiently solving, in real-time, large sets of differential equations with constraints, parameter uncertainties, and incorporating sensor data. One illustrative example is the US electricity grid which is the world's largest engineered system. It consists of a dynamic collection of interacting components, operated under an enormous range of physical, reliability, economic, social, and political constraints that need to be satisfied over time scales ranging from seconds for relay-action and closed-loop control to decades for transmission siting and construction. Fundamental advances are needed in the areas of algorithms, computer networking and architecture, data analysis, simulation and modeling, and computational security [9]. Novel mathematics is necessary for characterizing uncertainty in information created from large volumes of data as well as for characterizing uncertainty in models used for prediction. A MMICC may develop and analyze the coupling of new multiscale models of the components of the grid, allow for treatment and mitigation of uncertainties in the system, and provide mathematical analysis and insight into the interaction effects for better understanding of this complex system. These mathematical foundations support the DOE's goal of moving from a reactive environment to a real-time predictive one.

## **III. Mathematical Challenges from Subsurface Flow and Transport for Energy Applications**

These long-term mathematical challenges potentially include, but are not limited to, multiscale/multiphysics modeling, characterizing uncertainty, optimization, and data assimilation techniques. Accurate models for subsurface flow and transport are needed to design optimal and efficient remediation strategies [3] and address the challenges related to geological CO<sub>2</sub> sequestration [10]. There is a strong need for significant advances in multiscale/multiphysics models for subsurface flow and transport. Subsurface modeling can be highly uncertain, and characterization of the uncertainty becomes a crucial issue for decision-making and risk analysis in the design of remediation strategies. New optimization techniques and data assimilation strategies may be needed to make optimal use of available information. This will enable more accurate subsurface flow and transport modeling to develop more effective remediation strategies.

Another illustrative example is from geologic sequestration of large volumes of carbon dioxide, the challenge is that the relevant physical and chemical interactions occur on spatial scales that range from those of atoms, molecules, and mineral surfaces, up to tens of kilometers, and time scales that range from picoseconds to millennia and longer. Fundamental advances in the ability to simulate multiscale systems that may be perturbed during sequestration activities and for very long times afterward are needed. In addition, improved capabilities are needed to monitor those systems in real time with increasing spatial and temporal resolution. This will enable accurately predicting the performance of the subsurface storage systems building confidence to meet design targets.

#### **IV. Mathematical Challenges from Office of Science Facilities**

There is a rich set of mathematical challenges that has not been articulated or applied to enhancing scientific discovery at DOE Office of Science Facilities. A recent workshop and report on *Data and Communications in Basic Energy Sciences* [11] focused on identifying opportunities and needs for data analysis, ownership, storage, mining, provenance and data transfer at light sources, neutron sources, microscopy centers and other facilities. A MMICC addressing the broader long-term mathematical challenges, which potentially include both experimental and simulation information, may enable better understanding of future DOE Office of Science facility challenges.

#### **Organizational Structure and Management Plan for MMICCs**

Each MMICC will require expertise from a variety of different mathematical sub-disciplines. In addition, the MMICCs may require long-term engagement from problem inception to demonstration of results with domain scientists, computational scientists, and/or computer scientists in working towards the Grand Challenges. Applications may include funding for domain scientists or other expertise; the level of involvement or commitment is to be determined by the Center. Each MMICC must identify an appropriate team and organizational structure that enables it to function efficiently in a collaborative manner to address the multifaceted integrated mathematical research challenges and the associated grand challenges. The MMICC Director (“Center Director”) will serve as the primary contact responsible for communications with the DOE Program Office on behalf of all of the Principal Investigators in the MMICC. A lean management structure is sought; as such, it is expected that the Center Director will provide overall direction for the center ensuring internal coordination and collaboration as well as appropriate external outreach. The expectation is the Center Director will need to devote at least 33% of their time to the MMICC. The MMICC structure must be sufficiently flexible to adapt to changing technical challenges and scientific needs. In particular, it is expected that there will be changes in the multifaceted mathematics research plans as research progresses; equally likely are potential changes in the scientific challenges. Applications should identify key senior personnel who will contribute in a substantive, measurable way to the scientific/technical development or execution of the project. It is acceptable to not explicitly name all junior staff; however, the application should include a discussion of how the center will be fully staffed. Given the diversity of the expertise required for a successful MMICC, it is expected that MMICCs will involve more than one institution. Multi-institutional collaborations should be identified in the

application. The role of each institution should be discussed in terms of the contributions to the MMICC. Additional collaborations may form after an MMICC is established; applications should include a discussion of how this may be accomplished.

Applicants should identify key milestones of the research plan, including interactions among researchers, key dependencies (internal or external), and level of risk. It is expected that the MMICC will have multiple levels of risk. The milestones should:

1. Advance multifaceted, integrated mathematics that spans, as appropriate, novel formulations, discretizations, algorithm development, data analysis techniques, uncertainty quantification methodologies, optimization techniques, and other mathematical approaches;
2. Address one or more Grand Challenge problems with clear relevance and impact to the DOE; and
3. Advance the field of applied and computational mathematics.

The application must include a concise management plan that addresses the organization, communications, and coordination of the collaborating researchers. This plan should include mitigation strategies for foreseeable risks and explain how the project will have sufficient flexibility to adapt to changing priorities, challenges, and resources. Centers will be reviewed annually; additional informal reviews and reports will be conducted throughout the year. The application must contain a plan to support technical and programmatic review of the Center.

1. DOE 2012 Applied Math Summit, <http://science.energy.gov/ascr/news-and-resources/workshops-and-conferences/doe-applied-math-summit/>
2. DOE ASCR 2012 Workshop for Mathematics for the Analysis, Simulation, and Optimization of Complex Systems, <http://www.ornl.gov/mathworkshop2011/>
3. DOE ASCR 2012 A Multifaceted Mathematical Approach for Complex Systems Report, [http://science.energy.gov/~media/ascr/pdf/program-documents/docs/Multifaceted\\_Mathematical\\_Approach\\_for\\_Complex\\_Systems.pdf](http://science.energy.gov/~media/ascr/pdf/program-documents/docs/Multifaceted_Mathematical_Approach_for_Complex_Systems.pdf)
4. DOE Basic Energy Sciences: Basic Research Needs Reports, <http://science.energy.gov/bes/besac/reports>
5. DOE Basic Energy Sciences Report 2010: Discovery in Basic Energy Sciences: The Role of Computing at the Extreme Scale, [http://science.energy.gov/~media/ascr/pdf/program-documents/docs/Bes\\_exascale\\_report.pdf](http://science.energy.gov/~media/ascr/pdf/program-documents/docs/Bes_exascale_report.pdf)
6. DOE Basic Energy Sciences Report 2011: Computational Materials Sciences and Chemistry: Accelerating Discovery and Innovation through Simulation-Based Engineering and Science, [http://science.energy.gov/~media/bes/pdf/reports/files/cmssc\\_rpt.pdf](http://science.energy.gov/~media/bes/pdf/reports/files/cmssc_rpt.pdf)
7. National Science and Technology Council, Committee on Technology, Materials Genome Initiative, 2011, [http://www.whitehouse.gov/sites/default/files/microsites/ostp/materials\\_genome\\_initiative-final.pdf](http://www.whitehouse.gov/sites/default/files/microsites/ostp/materials_genome_initiative-final.pdf)
8. DOE Basic Energy Sciences Workshop Report 2007: Basic Research Needs: Catalysis for Energy, [http://science.energy.gov/~media/bes/pdf/reports/files/cat\\_rpt.pdf](http://science.energy.gov/~media/bes/pdf/reports/files/cat_rpt.pdf)

9. DOE Office of Electricity Delivery and Energy Reliability 2011 Report: Computational Needs for the Next Generation Electric Grid Proceedings,  
[http://energy.gov/sites/prod/files/FINAL\\_CompNeeds\\_Proceedings2011.pdf](http://energy.gov/sites/prod/files/FINAL_CompNeeds_Proceedings2011.pdf)
10. DOE Basic Energy Sciences Workshop Report: Basic Research Needs for Geosciences: Facilitating 21<sup>st</sup> Century Energy Systems.  
[http://science.energy.gov/~media/bes/pdf/reports/files/geo\\_rpt.pdf](http://science.energy.gov/~media/bes/pdf/reports/files/geo_rpt.pdf)
11. DOE Basic Energy Sciences Data Workshop 2011,  
<https://www.ornl.gov/dataworkshop2011/default1.htm>

## **Collaborations**

Collaborative research projects with other institutions, such as universities, industry, non-profit organizations, and Federally Funded Research and Development Centers (FFRDCs), including the DOE National Laboratories, are strongly encouraged. Collaborative applications submitted from different institutions should clearly indicate they are part of a proposed collaboration and contain the same title, abstract and narrative for that research project. In addition, such applications must describe the work and the associated budget for the research effort being performed under the leadership of the Principal Investigator at that participating institution.

These collaborative applications should all have the same title as the Lead Institution. Each collaborating institution submitting an application must use the same title in Block 11 of the SF 424 (R&R) form.

## **Additional Application Requirements**

We are seeking strong teams that address novel research requiring multifaceted, integrated mathematics. We will give priority to applications that clearly discuss one or more scientific or engineering grand challenges, abstract an interrelated set of mathematics research challenges that are optimally addressed through a multifaceted, integrated approach and have potential DOE impact in the 5-10+ year timeframe. Organizationally, the application must identify the Center Director, key personnel who will make significant technical contributions to the proposed research, and key collaborations.

## **PART II – AWARD INFORMATION**

### **A. TYPE OF AWARD INSTRUMENT.**

DOE anticipates awarding Cooperative Agreements under this FOA.

### **B. ESTIMATED FUNDING.**

Awards are expected to be made for a period of five years at a funding level of up to \$9,000,000 per year to support multiple awards in Fiscal Year 2013, with out-year support contingent on the availability of appropriated funds and satisfactory progress.

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.

### **C. MAXIMUM AND MINIMUM AWARD SIZE.**

The award size will depend on the number of meritorious applications and the availability of appropriated funds. However, it is anticipated that approximately 3 to 4 centers will be awarded with total project size ranging from \$2,000,000 to \$3,500,000 per year. It is anticipated that approximately 9 awards will be made with a range of \$250,000 to \$3,500,000 per year.

### **D. EXPECTED NUMBER OF AWARDS.**

The number of awards will depend on the number of meritorious applications and the availability of appropriated funds. However, it is anticipated that approximately 3 to 4 centers will be awarded with total project size ranging from \$2,000,000 to \$3,500,000 per year. It is anticipated that approximately 9 awards will be made with a range of \$250,000 to \$3,500,000 per year.

### **E. ANTICIPATED AWARD SIZE.**

The award size will depend on the number of meritorious applications and the availability of appropriated funds. However, it is anticipated that approximately 3 to 4 centers will be awarded with total project size ranging from \$2,000,000 to \$3,500,000 per year. It is anticipated that approximately 9 awards will be made with a range of \$250,000 to \$3,500,000 per year.

### **F. PERIOD OF PERFORMANCE.**

Cooperative Agreements are expected to be made for a period of five years at a funding level appropriate for the proposed scope, with out-year support contingent on the availability of appropriated funds and satisfactory progress.

### **G. TYPE OF APPLICATION.**

DOE will accept new applications under this FOA.

### **PART III - ELIGIBILITY INFORMATION**

#### **A. ELIGIBLE APPLICANTS.**

All types of domestic entities are eligible to apply, except other Federal agencies, Federally Funded Research and Development Center (FFRDC) Contractors, and nonprofit organizations described in section 501(c)(4) of the Internal Revenue Code of 1986 that engaged in lobbying activities after December 31, 1995.

#### **B. COST SHARING.**

Cost sharing is not required.

#### **C. OTHER ELIGIBILITY REQUIREMENTS.**

N/A

## PART IV – APPLICATION AND SUBMISSION INFORMATION

### A. ADDRESS TO REQUEST APPLICATION PACKAGE.

Application forms and instructions are available at Grants.gov. To access these materials, go to <http://www.grants.gov>, select "Apply for Grants", and then select "Download a Grant Application Package". Enter the CFDA and/or the funding opportunity number located on the cover of this FOA and then follow the prompts to download the application package.

### B. LETTER OF INTENT AND PRE-APPLICATION

#### 1. Letter of Intent.

N/A

#### 2. Pre-Application.

**PRE-APPLICATIONS DUE DATE: April 30, 2012**

Pre-applications are **REQUIRED** and must be submitted by April 30, 2012, 11:59 PM Eastern Time.

**Failure to submit a pre-application by an applicant will preclude the full application from due consideration.** Only the Lead institution of a Center should submit the pre-application. Pre-applications referencing Program Announcement LAB 12-698 should be submitted electronically by E-mail to [Sandy.Landsberg@science.doe.gov](mailto:Sandy.Landsberg@science.doe.gov) and [Steven.Lee@science.doe.gov](mailto:Steven.Lee@science.doe.gov). **No FAX or mail submission of pre-applications will be accepted.**

The pre-application will be reviewed for conformance with the guidelines presented in this FOA and suitability in the technical areas specified in this FOA. A response to the pre-application encouraging or discouraging formal applications will be communicated to the applicants by **May 4, 2012**. Applicants who have not received a response regarding the status of their pre-application by this date are responsible for contacting the program to confirm this status.

Only those pre-applications that receive notification from DOE encouraging a formal application may submit full applications. **No other formal applications will be considered.**

The intent in requesting a pre-application is to save the time and effort of applicants in preparing and submitting a formal project application that may be inappropriate for the program. Pre-applications will be reviewed relative to the scope and research needs as outlined in the summary paragraph and in the SUPPLEMENTARY INFORMATION. The pre-application should contain (1) a cover sheet and (2) a technical narrative.

The cover sheet identifies the name, institutional affiliation, e-mail address, and telephone number of the Center Director, Senior/Key personnel expected to be involved in the planned application, and an estimated amount of funding requested for each year for the project for each funded institution. No biographical data need be included. Since among the purposes of the pre-application is to facilitate ASCR in planning the merit review and the selection of peer-reviewers without conflicts of interest, it is important that applicants ensure their list of supported or unsupported participants is as comprehensive as possible.

The technical narrative should be no more than three pages in length and briefly discuss one or more scientific or engineering grand challenges and identify an interrelated set of mathematics research challenges that represent abstractions of the grand challenges. These abstractions would then be optimally addressed through a multifaceted, integrated approach. The narrative should also include a brief summary of the multifaceted, integrated approach, the proposed team members, and their expertise.

### **C. CONTENT AND FORM OF APPLICATION – SF 424 (R&R)**

You must complete the mandatory forms and any applicable optional forms (e.g., SF-LLL-Disclosure of Lobbying Activities) in accordance with the instructions on the forms and the additional instructions below. **Files that are attached to the forms must be in Adobe Portable Document Format (PDF) unless otherwise specified in this FOA.**

#### **1. SF 424 (R&R)**

Complete this form first to populate data in other forms. Complete all the required fields in accordance with the pop-up instructions on the form. The list of certifications and assurances referenced in Field 17 can be found on the DOE Financial Assistance Forms Page at <http://energy.gov/management/office-management/operational-management/financial-assistance/financial-assistance-forms> under Certifications and Assurances.

By submitting an application in response to this FOA the Applicant certifies that:

- It is **not** a corporation that has been convicted (or had an officer or agent of such corporation acting on behalf of the corporation convicted) of a felony criminal violation under any Federal law within the preceding 24 months,
- It is **not** a corporation that has any unpaid Federal tax liability that has been assessed, for which all judicial and administrative remedies have been exhausted or have lapsed, and that is not being paid in a timely manner pursuant to an agreement with the authority responsible for collecting the tax liability,
- If the Applicant's financial assistance application is chosen for award and the award is in excess of \$1,000,000, the applicant will, by the end of the fiscal year, upgrade the efficiency of their facilities by replacing any lighting that does not meet or exceed the energy efficiency standard for incandescent light bulbs set forth in Section 325 of the Energy Policy and Conservation Act (42 U.S.C. 6295).

## **2. RESEARCH AND RELATED Other Project Information.**

Complete questions 1 through 6 and attach files. The files must comply with the following instructions:

### **Project Summary/Abstract (Field 7 on the Form).**

The project summary/abstract must contain a summary of the proposed activity suitable for dissemination to the public. It should be a self-contained document that identifies the name of the applicant, the project director/principal investigator(s) (PD/PI), the project title, the objectives of the project, a description of the project, including methods to be employed, the potential impact of the project (i.e., benefits, outcomes), and major participants (for collaborative projects). This document must not include any proprietary or sensitive business information as the Department may make it available to the public. The project summary must not exceed 1 page when printed using standard 8.5" by 11" paper with 1" margins (top, bottom, left and right) with font not smaller than 11 point. To attach a Project Summary/Abstract, click "Add Attachment."

### **Project Narrative (Field 8 on the Form).**

The project narrative **must not exceed 20 pages** of technical information, including charts, graphs, maps, photographs, and other pictorial presentations, when printed using standard 8.5" by 11" paper with 1 inch margins (top, bottom, left, and right). **EVALUATORS WILL ONLY REVIEW THE NUMBER OF PAGES SPECIFIED IN THE PRECEDING SENTENCE.** The font must not be smaller than 11 point.

Please do not submit general letters of support as these are not used in making funding decisions and can interfere with the selection of peer reviewers.

Do not include any Internet addresses (URLs) that provide information necessary to review the application, because the information contained in these sites will not be reviewed. See Part VIII.D for instructions on how to mark proprietary application information. To attach a Project Narrative, click "Add Attachment."

The application narrative should begin with a cover page that includes: the project title, the Lead PI's name and complete contact information.

**The cover page must also include the following information (this page will not count in the project narrative page limitation):**

**Applicant/Institution:**

**Street Address/City/State/Zip:**

**Principal Investigator:**

**Postal Address:**

**Telephone Number:**

**Email:**

**Funding Opportunity Announcement Number:** DE-FOA-0000698

**DOE/Office of Science Program Office:** Office of Advanced Scientific Computing Research (ASCR)

**DOE/Office of Science Program Office Technical Contact:** Sandy Landsberg

**Is this a Collaboration?** If yes, please list ALL Collaborating Institutions/Pis\* and indicate which ones will also be submitting applications. Also indicate the PI who will be the point of contact and coordinator for the combined research activity.

**Sample Table for the Lead Institution (\$ in thousands)**

| <b>2012 MMICC</b>                                 | <b>Year 1</b> | <b>Year 2</b> | <b>Year 3</b> | <b>Year 4</b> | <b>Year 5</b> | <b>Total</b> |
|---|---------------|---------------|---------------|---------------|---------------|--------------|
| Name of the Center<br>Director and Institution    | \$            | \$            | \$            | \$            | \$            | \$           |
| <b>Collaborating Institutions</b>                 |               |               |               |               |               | <b>Total</b> |
| Name of Institution and<br>Principal Investigator | \$            | \$            | \$            | \$            | \$            | \$           |
| Name of Institution and<br>Principal Investigator | \$            | \$            | \$            | \$            | \$            | \$           |
| Name of Institution and<br>Principal Investigator | \$            | \$            | \$            | \$            | \$            | \$           |
| <b>TOTALS</b>                                     | \$            | \$            | \$            | \$            | \$            | \$           |

**Project Objectives:**

This section should provide a clear, concise statement of the specific objectives/aims of the proposed project.

The Project Narrative comprises the research plan for the project; 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 method 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.

**Appendix 1: Biographical Sketch.**

Provide a biographical sketch for the project director/principal investigator (PD/PI) and each senior/key person listed in Section A on the R&R Budget form. **Provide the Biographical Sketch information as an Appendix to your project narrative. Do not attach a separate file. The Biographical Sketch Appendix will not count in the project narrative page limitation.**

The biographical information (curriculum vitae) for each person must not exceed 2 pages when printed on 8.5” by 11” paper with 1 inch margins (top, bottom, left, and right) with font not smaller than 11 point 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.

*Identification of Potential Conflicts of Interest or Bias in Selection of Reviewers.* Provide the following information in this section:

*Collaborators and Co-editors:* List in alphabetical order all persons, including their current organizational affiliation, who are, or who have been, collaborators or co-authors with you on a research project, book or book article, report, abstract, or paper during the 48 months preceding the submission of this application. For publications or collaborations with more than 10 authors or participants, only list those individuals in the core group with whom the Principal Investigator interacted on a regular basis while the research was being done. Also, list any individuals who are currently, or have been, co-editors with you on a special issue of a journal, compendium, or conference proceedings during the 24 months preceding the submission of this application. If there are no collaborators or co-editors to report, state “None.”

*Graduate and Postdoctoral Advisors and Advisees:* List the names and current organizational affiliations of your graduate advisor(s) and principal postdoctoral sponsor(s) during the last 5 years. Also, list the names and current organizational affiliations of your graduate students and postdoctoral associates during the past 5 years.

## **Appendix 2: Current and Pending Support.**

Provide a list of all current and pending support (both Federal and non-Federal) for the Project Director/Principal Investigator(s) (PD/PI) and senior/key persons, including subawardees, for ongoing projects and pending applications. For each organization providing support, show the total award amount for the entire award period (including indirect costs) and the number of person-months per year to be devoted to the project by the senior/key

person. **Provide the Current and Pending Support as an Appendix to your project narrative. Do not attach a separate file. The Current and Pending Support Appendix will not count in the project narrative page limitation.** Concurrent submission of an application to other organizations for simultaneous consideration will not prejudice its review.

**Appendix 3: Bibliography and References Cited.**

Provide a bibliography of any references cited in the Project 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. Applicants should be especially careful to follow scholarly practices in providing citations for source materials relied upon when preparing any section of the application. **Provide the Bibliography and References Cited information as an Appendix to your project narrative. Do not attach a separate file. The Bibliography and References Cited Appendix will not count in the project narrative page limitation.**

**Appendix 4: Facilities and Other Resources.**

This information is used to assess the capability of the organizational resources, including subawardee resources, available to perform the effort proposed. Identify the facilities to be used (Laboratory, Animal, Computer, Office, Clinical and Other). If appropriate, indicate their capacities, pertinent capabilities, relative proximity, and extent of availability to the project. Describe only those resources that are directly applicable to the proposed work. Describe other resources available to the project (e.g., machine shop, electronic shop) and the extent to which they would be available to the project. **Provide the Facility and Other Resource information as an Appendix to your project narrative. Do not attach a separate file. The Facility and Other Resource Appendix will not count in the project narrative page limitation.**

**Appendix 5: Equipment.**

List major items of equipment already available for this project and, if appropriate identify location and pertinent capabilities. **Provide the Equipment information as an Appendix to your project narrative. Do not attach a separate file. The Equipment Appendix will not count in the project narrative page limitation.**

**Appendix 6: Other Attachment.**

If you need to elaborate on your responses to questions 1-6 on the “Other Project Information” document, **please provide the Other Attachment information as an Appendix to your project narrative. Do not attach a separate file. The Other Attachment Appendix will not count in the project narrative page limitation.**

**Do not attach any of the requested Appendices described above as files for fields 9, 10, 11, and 12. Instead follow the above instructions to include the information as Appendices to the project narrative file (these Appendices will not count in the project narrative page limitation).**

### **3. RESEARCH AND RELATED BUDGET.**

Complete the Research and Related Budget form in accordance with the instructions on the form and the following instructions. You must complete a separate budget for each year of support requested. The form will generate a cumulative budget for the total project period. You must complete all the mandatory information on the form before the NEXT PERIOD button is activated. You may request funds under any of the categories listed as long as the item and amount are necessary to perform the proposed work, meet all the criteria for allowability under the applicable Federal cost principles, and are not prohibited by the funding restrictions in this FOA (See PART IV, G).

#### **Budget Justification (Field K on the form).**

Provide the required supporting information for the following costs: equipment; domestic and foreign travel; participant/trainees; material and supplies; publication; consultant services; ADP/computer services; subaward/consortium/contractual; equipment or facility rental/user fees; alterations and renovations; and indirect cost type. Provide any other information you wish to submit to justify your budget request. **Attach a single budget justification file for the entire project period in Field K.** The file automatically carries over to each budget year.

### **4. R&R SUBAWARD BUDGET ATTACHMENT(S) FORM.**

**Budgets for Subawardees, other than DOE FFRDC Contractors.** You must provide a separate cumulative R&R budget for each subawardee that is expected to perform work estimated to be more than \$100,000 or 50 percent of the total work effort (whichever is less). If you are selected for award, you must submit a multi-year budget for each of these subawardees. Download the R&R Budget Attachment from the R&R SUBAWARD BUDGET ATTACHMENT(S) FORM and e-mail it to each subawardee that is required to submit a separate budget. After the Subawardee has e-mailed its completed budget back to you, attach it to one of the blocks provided on the form. Use up to 10 letters of the subawardee's name (plus .xfd) as the file name (e.g., ucla.xfd or energyres.xfd).

### **5. PROJECT/PERFORMANCE SITE LOCATION(s)**

Indicate the primary site where the work will be performed. If a portion of the project will be performed at any other site(s), identify the site location(s) in the blocks provided.

**Note that the Project/Performance Site Congressional District is entered in the format of the 2 digit state code followed by a dash and a 3 digit Congressional district code, for example VA-001. Hover over this field for additional instructions.**

Use the Next Site button to expand the form to add additional Project/Performance Site Locations.

### **6. SF-LLL Disclosure of Lobbying Activities**

If applicable, complete SF- LLL. Applicability: If any funds other than Federal appropriated funds have been paid or will be paid to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of

Congress, or an employee of a Member of Congress in connection with the grant, you must complete and submit Standard Form - LLL, "Disclosure Form to Report Lobbying."

**Summary of Required Forms/Files**

Your application must include the following documents:

| <b>Name of Document</b>  | <b>Format</b> | <b>Attach to</b> |
|--|---------------|------------------|
| <b>SF 424 (R&amp;R)</b>  | Form          | N/A              |
| <b>RESEARCH AND RELATED Other Project Information</b>          | Form          | N/A              |
| Project Summary/Abstract                                       | PDF           | Field 7          |
| Project Narrative, including required appendices               | PDF           | Field 8          |
| <b>RESEARCH &amp; RELATED BUDGET</b>                           | Form          | N/A              |
| Budget Justification   | PDF           | Field K          |
| <b>PROJECT/PERFORMANCE SITE LOCATION(S)</b>                    | Form          | N/A              |
| <b>SF-LLL Disclosure of Lobbying Activities, if applicable</b> | Form          | N/A              |

**D. SUBMISSIONS FROM SUCCESSFUL APPLICANTS.**

If selected for award, DOE reserves the right to request additional or clarifying information for any reason deemed necessary, including, but not limited to:

- Indirect cost information
- Other budget information
- Name and phone number of the Designated Responsible Employee for complying with national policies prohibiting discrimination (See 10 CFR 1040.5)
- Representation of Limited Rights Data and Restricted Software, if applicable
- Commitment Letter from Third Parties Contributing to Cost Sharing, if applicable.

**E. SUBMISSION DATES AND TIMES.**

**1. Letter of Intent.**

N/A

**2. Pre-Application.**

**PRE-APPLICATION DUE DATE: April 30, 2012**

Pre-applications are **REQUIRED** and must be submitted by April 30, 2012, 11:59 PM Eastern Time.

**Failure to submit a pre-application by an applicant will preclude the full application from due consideration.** Only the Lead institution of a Center should submit the pre-application. Pre-applications referencing Program Announcement LAB 12-698 should be submitted electronically by E-mail to [Sandy.Landsberg@science.doe.gov](mailto:Sandy.Landsberg@science.doe.gov) and [Steven.Lee@science.doe.gov](mailto:Steven.Lee@science.doe.gov). **No FAX or mail submission of pre-applications will be accepted.**

The pre-application will be reviewed for conformance with the guidelines presented in this Announcement and suitability in the technical areas specified in this Announcement. A response to the pre-application encouraging or discouraging formal applications will be communicated to the applicants by **May 4, 2012**. Applicants who have not received a response regarding the status of their pre-application by this date are responsible for contacting the program to confirm this status.

Only those pre-applications that receive notification from DOE encouraging a formal application may submit full applications. **No other formal applications will be considered.**

The intent in requesting a pre-application is to save the time and effort of applicants in preparing and submitting a formal project application that may be inappropriate for the program. Pre-applications will be reviewed relative to the scope and research needs as outlined in the summary paragraph and in the SUPPLEMENTARY INFORMATION. The pre-application should contain (1) a cover sheet and (2) a technical narrative.

The cover sheet identifies the name, institutional affiliation, e-mail address, and telephone number of the Center Director, Senior/Key personnel expected to be involved in the planned application, and an estimated amount of funding requested for each year for the project for each funded institution. No biographical data need be included. Since among the purposes of the pre-application is to facilitate ASCR in planning the merit review and the selection of peer-reviewers without conflicts of interest, it is important that applicants ensure their list of supported or unsupported participants is as comprehensive as possible.

The technical narrative should be no more than three pages in length and briefly discuss one or more scientific or engineering grand challenges and identify an interrelated set of mathematics research challenges that represent abstractions of the grand challenges. These abstractions would then be optimally addressed through a multifaceted, integrated approach. The narrative should also include a brief summary of the multifaceted, integrated approach, the proposed team members, and their expertise.

### **3. Formal Applications.**

**APPLICATION DUE DATE: June 1, 2012, 11:59 PM Eastern Time**

Formal applications submitted in response to this FOA must be received by **June 1, 2012, 11:59 PM Eastern Time**, to permit timely consideration of awards in Fiscal Year 2013. **You are encouraged to submit your application well before the deadline. APPLICATIONS**

**RECEIVED AFTER THE DEADLINE WILL NOT BE REVIEWED OR CONSIDERED FOR AWARD.**

**F. INTERGOVERNMENTAL REVIEW.**

This program is not subject to Executive Order 12372 Intergovernmental Review of Federal Programs.

**G. FUNDING RESTRICTIONS.**

Cost Principles. Costs must be allowable in accordance with the applicable Federal cost principles referenced in 10 CFR Part 600. The cost principles for commercial organization are in FAR Part 31.

Pre-award Costs. Recipients may charge to an award resulting from this FOA pre-award costs that were incurred within the ninety (90) calendar-day period immediately preceding the effective date of the award, if the costs are allowable in accordance with the applicable Federal cost principles referenced in 10 CFR Part 600. Recipients must obtain the prior approval of the contracting officer for any pre-award costs that are for periods greater than this 90-day calendar period.

Pre-award costs are incurred at the applicant's risk. DOE is under no obligation to reimburse such costs if for any reason the applicant does not receive an award or if the award is made for a lesser amount than the applicant expected.

**H. OTHER SUBMISSION AND REGISTRATION REQUIREMENTS.**

**1. Where to Submit.**

**APPLICATIONS MUST BE SUBMITTED THROUGH GRANTS.GOV TO BE CONSIDERED FOR AWARD.**

Submit electronic applications through the "Apply for Grants" function at [www.Grants.gov](http://www.Grants.gov). If you have problems completing the registration process or submitting your application, call Grants.gov at 1-800-518-4726 or send an email to [support@grants.gov](mailto:support@grants.gov).

**2. Registration Process.**

**Registration Requirements:** There are several one-time actions you must complete in order to submit an application through Grants.gov (i.e., obtain a Dun and Bradstreet Data Universal Numbering System (DUNS) number, register with the CCR, register with the credential provider, and register with Grants.gov). To register with Grants.gov go to "Get Registered" at [http://grants.gov/applicants/get\\_registered.jsp](http://grants.gov/applicants/get_registered.jsp). 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](mailto:support@grants.gov). Part VII of this Funding Opportunity Announcement (FOA) explains how to submit other questions to the Department of Energy (DOE).

### **Application Receipt Notices**

After an application is submitted, the Authorized Organization Representative (AOR) will receive a series of four e-mails. It is extremely important that the AOR watch for and save each of the emails. It may take up to two (2) business days from application submission to receipt of email Number 2. The titles of the four e-mails are:

Number 1 - Grants.gov Submission Receipt Number

Number 2 - Grants.gov Submission Validation Receipt for Application Number

Number 3 - Grants.gov Grantor Agency Retrieval Receipt for Application Number

Number 4 - Grants.gov Agency Tracking Number Assignment for Application Number

## **PART V - APPLICATION REVIEW INFORMATION**

### **A. CRITERIA**

#### **1. Initial Review Criteria.**

Prior to a comprehensive merit evaluation, DOE will perform an initial review in accordance with 10 CFR 605.10(b) to determine that (1) the applicant is eligible for the award; (2) the information required by the FOA has been submitted; (3) all mandatory requirements are satisfied; and (4) the proposed project is responsive to the objectives of the FOA. Applications that fail to pass the initial review will not be forwarded for merit review and will be eliminated from further consideration.

#### **2. Merit Review Criteria**

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). Included within each criterion are specific questions that the merit reviewers will be asked to consider.

##### **1. Scientific and/or Technical Merit of the Project**

- a. What compelling, scientific grand challenge problems are identified and to what extent are they relevant to the DOE mission? What is the potential long-term impact of the MMICC?
- b. What are the main technical challenges and how well does the application articulate the difficulties that bar scientific progress?
- c. What fundamental mathematical advances are needed to achieve the desired scientific discoveries and breakthroughs?
- d. What is the likelihood and to what extent can the proposed research overcome the main technical challenges to the scientific grand challenge problems?

##### **2. Appropriateness of the Proposed Method or Approach**

- a. How well does the application articulate a mathematical, multifaceted, integrated approach to addressing the scientific grand challenge problems?
- b. To what extent does the proposed research treat the grand challenges holistically and justify the choice of mathematical abstractions?
- c. To what extent does the proposed research identify novel mathematical models, methods and approaches of individual components as well as integrated approaches?
- d. How well does the research plan describe metrics that will allow research progress and contributions to be measured?
- e. To what extent does the application articulate a plan for effectively coordinating and managing the research activities of the Center?

##### **3. Competency of Applicant's Personnel and Adequacy of Proposed Resources**

- a. How well is the role of the Center Director articulated? What prior experience and success does the Center Director have in effectively managing collaborative teams?

- b. To what extent are the roles of key personnel adequately described? To what extent do key personnel have a proven record of success in delivering results in computational and applied mathematics?
- c. To what extent do key personnel have extensive research and development experience in the mathematical sub-disciplines needed for the success of the Center?

**4. Reasonableness and Appropriateness of the Proposed Budget**

- a. To what extent is the overall requested budget appropriate for the scope of the work proposed?
- b. Is the requested budget and level of effort of the Center Director and key personnel sufficient and appropriate to achieve success?
- c. How well does the requested budget support the Center's management structure? What Center procedures, if any, will be used to permit flexibility in staffing and allow for additional future collaborations?
- d. What Center procedures, if any, will be used for reallocating funds to address changing priorities?

**The selection official will consider the following program policy and management factors in the selection process:**

- Potential impact of proposed research activities on ASCR Exascale goals in the areas of this FOA.
- Potential for developing synergies and/or relation of the proposed research activities to other research efforts supported by ASCR, particularly co-design;
- Total amount of DOE funds available; and
- A management plan that addresses the organization, communications, and coordination of the collaborating researchers. This plan should include mitigation strategies for foreseeable risks and explain how the project will have sufficient flexibility to adapt to changing priorities, challenges, and resources.

**The selection official will also consider the following program policy and management factors in the selection process:**

- a. Potential impact of proposed research activities on DOE mission.
- b. Potential for developing synergies and/or relation of the proposed research activities to other research efforts supported by ASCR, for example, other applied mathematics projects, SciDAC Institutes, and/or SciDAC Partnerships; and
- c. Total amount of DOE funds available.

The evaluation process 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. Note that external peer reviewers are selected with regard to both their scientific expertise and the absence of conflict-of-interest issues. Both Federal and non-Federal reviewers may be used, and submission of an application constitutes agreement that this is acceptable to the investigator(s) and the submitting institution.

**C. ANTICIPATED NOTICE OF SELECTION AND AWARD DATES.**

It is anticipated that selections will be completed by July 6, 2012. Awards will be made in Fiscal Year 2013.

## PART VI - AWARD ADMINISTRATION INFORMATION

### A. AWARD NOTICES.

#### 1. Notice of Selection.

**Selected Applicants Notification:** DOE will notify applicants selected for award. This notice of selection is not an authorization to begin performance. (See Part IV.G with respect to the allowability of pre-award costs.)

**Non-selected Notification:** Organizations whose applications have not been selected will be advised as promptly as possible. This notice will explain why the application was not selected.

#### 2. Notice of Award.

An Assistance Agreement issued by the contracting officer is the authorizing award document. It normally includes, either as an attachment or by reference: 1. Special Terms and Conditions; 2. Applicable program regulations, if any; 3. Application as approved by DOE; 4. DOE assistance regulations at 10 CFR Part 600; 5. National Policy Assurances to be Incorporated as Award Terms; 6. Budget Summary; and 7. Federal Assistance Reporting Checklist, which identifies the reporting requirements.

For grants and cooperative agreements made to universities, non-profits and other entities subject to Title 2 CFR the Award also includes the Research Terms and Conditions located at: <http://www.nsf.gov/bfa/dias/policy rtc/index.jsp>.

### B. ADMINISTRATIVE AND NATIONAL POLICY REQUIREMENTS.

#### 1. Administrative Requirements.

The administrative requirements for DOE grants and cooperative agreements are contained in 10 CFR 600 and 10 CFR Part 605 (See: <http://ecfr.gpoaccess.gov>). Grants and cooperative agreements made to universities, non-profits and other entities subject to Title 2 CFR are subject to the Research Terms and Conditions located on the National Science Foundation web site at: <http://www.nsf.gov/bfa/dias/policy rtc/index.jsp>.

#### DUNS and CCR Requirements

Additional administrative requirements for DOE grants and cooperative agreements are contained in 2 CFR, Part 25 (See: <http://ecfr.gpoaccess.gov>). Prime awardees must keep their data at CCR current. Subawardees at all tiers must obtain DUNS numbers and provide the DUNS to the prime awardee before the subaward can be issued.

## **Subaward and Executive Reporting**

Additional administrative requirements necessary for DOE grants and cooperative agreements to comply with the Federal Funding and Transparency Act of 2006 (FFATA) are contained in 2 CFR, Part 170. (See: <http://ecfr.gpoaccess.gov>). Prime awardees must register with the new FSRS database and report the required data on their first tier subawardees. Prime awardees must report the executive compensation for their own executives as part of their registration profile in the CCR.

### **2. Special Terms and Conditions and National Policy Requirements.**

The DOE Special Terms and Conditions for Use in Most Grants and Cooperative Agreements are located at: <http://energy.gov/management/office-management/operational-management/financial-assistance/financial-assistance-forms> under Award Terms. The National Policy Assurances to be Incorporated as Award Terms are located at: <http://www.nsf.gov/bfa/dias/policy/rtc/appc.pdf>.

### **Intellectual Property Provisions.**

The standard DOE financial assistance intellectual property provisions applicable to the various types of recipients are located at: <http://energy.gov/gc/standard-intellectual-property-ip-provisions-financial-assistance-awards>.

### **Statement of Substantial Involvement**

Either a grant or cooperative agreement may be awarded under this FOA. If the award is a cooperative agreement, the DOE Contract Specialist and DOE Project Officer will negotiate a Statement of Substantial Involvement prior to award.

## **C. REPORTING.**

Reporting requirements are identified on the Federal Assistance Reporting Checklist, DOE F4600.2, attached to the award agreement. For a sample Checklist, see <http://energy.gov/management/office-management/operational-management/financial-assistance/financial-assistance-forms>.

## PART VII - QUESTIONS/AGENCY CONTACTS

### A. QUESTIONS

Questions regarding the content of the FOA must be submitted through the FedConnect portal. You must register with FedConnect to respond as an interested party to submit questions, and to view responses to questions. It is recommended that you register as soon after release of the FOA as possible to have the benefit of all responses. More information is available at:

[https://www.fedconnect.net/FedConnect/PublicPages/FedConnect\\_Ready\\_Set\\_Go.pdf](https://www.fedconnect.net/FedConnect/PublicPages/FedConnect_Ready_Set_Go.pdf).

DOE will try to respond to a question within 3 business days, unless a similar question and answer have already been posted on the website.

**Applications submitted through FedConnect will not be accepted.**

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](mailto:support@grants.gov). DOE cannot answer these questions.

### B. AGENCY CONTACTS:

Technical/Scientific Program Contacts:

**Program Manager:** Sandy Landsberg, (301) 903-8507  
Office of Advanced Scientific Computing Research, SC-21.1  
**E-mail:** [Sandy.Landsberg@science.doe.gov](mailto:Sandy.Landsberg@science.doe.gov)

**Program Manager:** Dr. Steven L. Lee, (301) 903-5710  
Office of Advanced Scientific Computing Research, SC-21.1  
**E-mail:** [Steven.Lee@science.doe.gov](mailto:Steven.Lee@science.doe.gov)

## **PART VIII - OTHER INFORMATION**

### **A. MODIFICATIONS.**

Notices of any modifications to this FOA will be posted on Grants.gov and the FedConnect portal. You can receive an email when a modification or an FOA message is posted by registering with FedConnect as an interested party for this FOA. It is recommended that you register as soon after release of the FOA as possible to ensure you receive timely notice of any modifications or other FOAs. More information is available at <http://www.fedconnect.net>.

### **B. GOVERNMENT RIGHT TO REJECT OR NEGOTIATE.**

DOE reserves the right, without qualification, to reject any or all applications received in response to this FOA and to select any application, in whole or in part, as a basis for negotiation and/or award.

### **C. COMMITMENT OF PUBLIC FUNDS.**

The Contracting Officer is the only individual who can make awards or commit the Government to the expenditure of public funds. A commitment by other than the Contracting Officer, either explicit or implied, is invalid.

### **D. PROPRIETARY APPLICATION INFORMATION.**

Patentable ideas, trade secrets, proprietary or confidential commercial or financial information, disclosure of which may harm the applicant, should be included in an application only when such information is necessary to convey an understanding of the proposed project. The use and disclosure of such data may be restricted, provided the applicant includes the following legend on the first page of the project narrative and specifies the pages of the application which are to be restricted:

“The data contained in pages \_\_\_\_\_ of this application have been submitted in confidence and contain trade secrets or proprietary information, and such data shall be used or disclosed only for evaluation purposes, provided that if this applicant receives an award as a result of or in connection with the submission of this application, DOE shall have the right to use or disclose the data herein to the extent provided in the award. This restriction does not limit the government’s right to use or disclose data obtained without restriction from any source, including the applicant.”

To protect such data, each line or paragraph on the pages containing such data must be specifically identified and marked with a legend similar to the following:

“The following contains proprietary information that (name of applicant) requests not be released to persons outside the Government, except for purposes of review and evaluation.”

## **E. EVALUATION AND ADMINISTRATION BY NON-FEDERAL PERSONNEL.**

In conducting the merit review evaluation, the Government may seek the advice of qualified non-Federal personnel as reviewers. The Government may also use non-Federal personnel to conduct routine, nondiscretionary administrative activities. The applicant, by submitting its application, consents to the use of non-Federal reviewers/administrators. Non-Federal reviewers must sign conflict of interest and non-disclosure agreements prior to reviewing an application. Non-Federal personnel conducting administrative activities must sign a non-disclosure agreement.

## **F. INTELLECTUAL PROPERTY DEVELOPED UNDER THIS PROGRAM.**

Patent Rights. The government will have certain statutory rights in an invention that is conceived or first actually reduced to practice under a DOE award. 42 U.S.C. 5908 provides that title to such inventions vests in the United States, except where 35 U.S.C. 202 provides otherwise for nonprofit organizations or small business firms. However, the Secretary of Energy may waive all or any part of the rights of the United States subject to certain conditions. (See “Notice of Right to Request Patent Waiver” in paragraph G below.)

Rights in Technical Data. Normally, the government has unlimited rights in technical data created under a DOE agreement. Delivery or third party licensing of proprietary software or data developed solely at private expense will not normally be required except as specifically negotiated in a particular agreement to satisfy DOE’s own needs or to insure the commercialization of technology developed under a DOE agreement.

## **G. NOTICE OF RIGHT TO REQUEST PATENT WAIVER.**

Applicants may request a waiver of all or any part of the rights of the United States in inventions conceived or first actually reduced to practice in performance of an agreement as a result of this FOA, in advance of or within 30 days after the effective date of the award. Even if such advance waiver is not requested or the request is denied, the recipient will have a continuing right under the award to request a waiver of the rights of the United States in identified inventions, i.e., individual inventions conceived or first actually reduced to practice in performance of the award. Any patent waiver that may be granted is subject to certain terms and conditions in 10 CFR 784.12, [http://ecfr.gpoaccess.gov/cgi/t/text/text-idx?c=ecfr&tpl=/ecfrbrowse/Title10/10cfr784\\_main\\_02.tpl](http://ecfr.gpoaccess.gov/cgi/t/text/text-idx?c=ecfr&tpl=/ecfrbrowse/Title10/10cfr784_main_02.tpl).

Domestic small businesses and domestic nonprofit organizations will receive the patent rights clause at 37 CFR 401.14, i.e., the implementation of the Bayh-Dole Act. This clause permits domestic small business and domestic nonprofit organizations to retain title to subject inventions. Therefore, small businesses and nonprofit organizations do not need to request a waiver.

## **H. NOTICE REGARDING ELIGIBLE/INELIGIBLE ACTIVITIES.**

N/A

## **I. AVAILABILITY OF FUNDS.**

Funds are not presently available for this award. The Government's obligation under this award is contingent upon the availability of appropriated funds from which payment for award purposes can be made. No legal liability on the part of the Government for any payment may arise until funds are made available to the Contracting Officer for this award and until the awardee receives notice of such availability, to be confirmed in writing by the Contracting Officer.