

**FINANCIAL ASSISTANCE
FUNDING OPPORTUNITY ANNOUNCEMENT**



**U.S. Department of Energy
Office of Science**

**Office of Basic Energy Sciences (BES)
Office of Advanced Scientific Computing Research (ASCR)**

***Scientific Discovery through Advanced Computing:
Scientific Computation Application Partnership in Materials and
Chemical Sciences***

Funding Opportunity Number: DE-FOA-0000593

Announcement Type: **Amendment 2**

CFDA Number: 81.049

AMENDMENT ISSUED: October 7, 2011

ISSUE DATE: September 21, 2011

Pre-application Due Date: December 9, 2011, 11:59 PM Eastern Time
(Pre-applications are Required)

Application Due Date: March 12, 2012, 11:59 PM Eastern Time

Amendment 1: Correction of Program Manager's (Mark Pederson) phone number on pages 6 and 31. (Amendment 1 issued on October 5, 2011)

Amendment 2: This Funding Opportunity Announcement (FOA) was deleted from Grants.gov and reposted on October 7, 2011. A new Application Package (Forms) was posted at that time. The new Application Package is identical to the old one except it is encoded differently behind the scenes, so the information requested on the forms remains the same. Application Packages downloaded prior to October 7 will generate errors upon submission. If you downloaded the Application Package prior to October 7, please discard it, download a new Application Package, and use the new one for submitting your application. No other changes were made to this FOA on October 7. We apologize for the inconvenience.

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. 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 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

TABLE OF CONTENTS

PART I – FUNDING OPPORTUNITY DESCRIPTION

PART II – AWARD INFORMATION

- A. Type of Award Instrument**
- B. Estimated Funding**
- C. Maximum and Minimum Award Size**
- D. Expected Number of Awards**
- E. Anticipated Award Size**
- F. Period of Performance**
- G. Type of Application**

PART III – ELIGIBILITY INFORMATION

- A. Eligible Applicants**
- B. Cost Sharing or Matching**
- C. Other Eligibility Requirements**

PART IV – APPLICATION AND SUBMISSION INFORMATION

- A. Address to Request Application Package**
- B. Letter of Intent and Pre-Application**
- C. Content and Form of Application**
- D. Submissions from Successful Applicants**
- E. Submission Dates and Times**
- F. Intergovernmental Review**
- G. Funding Restrictions**
- H. Other Submission and Registration Requirements**

PART V – APPLICATION REVIEW INFORMATION

- A. Criteria**
- B. Review and Selection Process**
- C. Anticipated Notice of Selection and Award Dates**

PART VI – AWARD ADMINISTRATION INFORMATION

- A. Award Notices**
- B. Administrative and National Policy Requirements**
- C. Reporting**

PART VII – QUESTIONS/AGENCY CONTACTS

- A. Questions**
- B. Agency Contacts**

PART VIII – OTHER INFORMATION

- A. Modifications**
- B. Government Right to Reject or Negotiate**
- C. Commitment of Public Funds**
- D. Proprietary Application Information**
- E. Evaluation and Administration by Non-Federal Personnel**
- F. Intellectual Property Developed under this Program**
- G. Notice of Right to Request Patent Waiver**
- H. Notice Regarding Eligible/Ineligible Activities**
- I. Availability of Funds**

PART I – FUNDING OPPORTUNITY DESCRIPTION

GENERAL INQUIRIES ABOUT THIS FOA SHOULD BE DIRECTED TO:

Technical/Scientific Program Contacts:

Dr. James Davenport, Office of Basic Energy Sciences, SC-22.2

PHONE: (301) 903-0035

E-MAIL: James.Davenport@science.doe.gov

Dr. Mark Pederson, Office of Basic Energy Sciences, SC-22.1

PHONE: (301) 903-9956

E-MAIL: Mark.Pederson@science.doe.gov

Dr. Ceren Susut, Office of Advanced Scientific Computing Research, SC-21.1

PHONE: (301) 903-0366

E-MAIL: Ceren.Susut-Bennett@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 Basic Energy Sciences (BES) and the Office of Advanced Scientific Computing Research (ASCR) of the Office of Science (SC), U.S. Department of Energy (DOE), hereby announce their interest in receiving applications from interdisciplinary teams to the Scientific Discovery through Advanced Computing (SciDAC) program, for Scientific Computation Application Partnerships (hereafter, Partnerships) in the area of Materials and Chemical Sciences.

BES supports fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels in order to provide the foundations for new energy technologies and to support DOE missions in energy, environment, and national security.

The BES SciDAC Partnership portfolio will focus on the development of new algorithms and computational approaches which could dramatically accelerate the discovery of new materials and processes as well as provide fundamental understanding and improvement of current materials and processes. These elements are critical to the recently announced Materials Genome

Initiative (www.whitehouse.gov/sites/default/files/microsites/ostp/materials_genome_initiative-final.pdf). Implementing these new algorithms on current and next generation massively parallel computers requires a team approach which includes materials and chemical scientists, applied mathematicians and computer scientists.

As background, BES/ASCR workshops held in the past two years have outlined a number of priority research directions any of which could form a basis for a SciDAC Partnership project. (*Discovery in Basic Energy Sciences: The Role of Computing at the Extreme Scale*, Edited by G. Galli and T. Dunning (2010) http://science.energy.gov/~media/ascr/pdf/program-documents/docs/Bes_exascale_report.pdf and *Computational Materials Sciences and Chemistry: Accelerating Discovery and Innovation through Simulation-Based Engineering and Science*, Edited by G. Crabtree, S. Glotzer, B. McCurdy and J. Roberto (2011) http://science.energy.gov/~media/bes/pdf/reports/files/cmssc_rpt.pdf).

These are:

- Capturing Solar Energy
- Chemical Reactions
- Magnetism and Superconductivity
- Materials Under Extreme Environments
- Separations
- Energy Storage

Additional guidance may be found in BES Basic Research Needs Reports (Basic Research Needs Reports. <http://science.energy.gov/bes/besac/reports/>) and the recently announced Materials Genome Initiative (www.whitehouse.gov/sites/default/files/microsites/ostp/materials_genome_initiative-final.pdf).

While all of these areas are important to BES two overarching challenges that are especially relevant for SciDAC Partnership are 1) the development of first-principles treatments of excited states and excited-state processes, and 2) electron correlation in finite and extended systems.

It is expected that SciDAC Partnership projects will utilize the computational power available in DOE's Leadership Class machines. Projects may include requests to support software development.

More specific information on each area of interest is included in the Description of Topical Areas section under SUPPLEMENTARY INFORMATION.

A companion Program Announcement to DOE National Laboratories, LAB 11-593, will be posted on the SC Grants and Contracts web site at: <http://www.science.doe.gov/grants>

SUPPLEMENTARY INFORMATION:

Scientific Discovery through Advanced Computing

The Scientific Discovery through Advanced Computing (SciDAC) program accelerates progress in computational science by breaking down the barriers between disciplines and fostering productive partnerships between domain scientists and applied mathematicians and computer scientists who are capable of exploiting the capabilities of leadership class computational systems (by which we mean those existing at or planned in the next five years for the Oak Ridge and Argonne Leadership Computing Facilities, or the high performance production computational systems at the National Energy Research Scientific Computing Center, or similar computing facilities.) These partnerships enable scientists to conduct complex scientific and engineering computations at a level of fidelity needed to simulate real-world conditions. In particular, the key components of SciDAC are SciDAC Institutes and SciDAC Partnerships; the latter is addressed in this FOA. The Institutes will be the foundation for efforts by applied mathematicians and computer scientists to systematically address technical challenges that are inherent to the scale of new architectures and that are common across a wide range of science applications. The Institutes are responsible for developing new methods, algorithms and libraries spanning a wide range of SciDAC applications. The recently awarded SciDAC Institutes (see <http://science.energy.gov/ascr/research/scidac/scidac-institutes/>) are as follows:

- **FASTMath:** Frameworks, Algorithms, and Scalable Technologies for Mathematics (Director: Lori Diachin, Lawrence Livermore National Laboratory). Topics covered include structured and unstructured mesh tools and mesh-solver interfaces, particle methods, linear and nonlinear solvers, time integration, eigensolvers, and differential variational inequalities.
- **SUPER:** Sustained Performance, Energy and Resilience (Director: Robert Lucas, University of Southern California). Topics covered include performance engineering (including modeling and autotuning), energy efficiency, resilience, and optimization.
- **QUEST:** Quantification of Uncertainty in Extreme Scale Computations (Director: Habib Najm, Sandia National Laboratories). Topics covered include inverse problems, reduced stochastic representations, forward uncertainty propagation, fault tolerance, and experimental design and model validation.

A successful Partnership will:

1. Exploit leadership class computing resources to advance scientific frontiers in an area of strategic importance to the Office of Science, and
2. Effectively link to the intellectual resources in applied mathematics and computer science, expertise in algorithms and methods, and scientific software tools at one, or more, SciDAC Institutes.

Although not required, it is expected that all Partnerships funded under this FOA, will request, and will receive funds from both BES and ASCR to meet proposed objectives.

Reviewers of Applications submitted to this FOA will be asked to comment upon the feasibility, benefits, and management of the proposed collaborations between the materials and chemical

scientists supported by BES on the one hand, and the computational scientists (i.e., applied mathematicians and computer scientists/engineers) supported by ASCR on the other.

Description of Topical Areas

In terms of the overarching challenges (see **Summary** above), it is noted that developing next-generation technologies for capturing, converting and subsequently utilizing alternative forms of energy requires vast improvements in capabilities for predicting and understanding all types of excited-state properties and processes in solids, molecules and atoms. This includes electron and energy transfer, polarization and plasmonic effects and could have major impact on solar harvesting and conversion to fuel and electricity.

In order to enable future computational materials and chemical sciences approaches, automated excited-state methods: (1) incorporate potentially unforeseen and/or motivate improvements in mathematical approaches (2) provide controllable numerical precision (3) scale more favorably as a function of system size and (4) are computationally formulated in a manner that allows optimal use on current and next-generation HPC platforms will be required. Many BES reports in the Basic Research Needs Series

(http://science.energy.gov/~media/bes/pdf/reports/files/cmssc_rpt.pdf) as well as joint BES ASCR workshop reports

(www.whitehouse.gov/sites/default/files/microsites/ostp/materials_genome_initiative-final.pdf

and http://science.energy.gov/~media/ascr/pdf/program-documents/docs/Bes_exascale_report.pdf) assert that accelerated predictive advances in excited-state properties and dynamics represent one of the highest-priority needs of the computational sciences community.

Similar challenges are found for understanding correlation effects in extended systems. This topic underlies many technologically relevant research areas in materials science including magnetism and superconductivity, oxides, and actinides, as well as emerging materials such as graphene and topological insulators. There is a close connection between excited state properties, including quantum transport (conductivity, thermoelectric properties), and time dependent response. Advances in recent years have included Quantum Monte Carlo techniques, dynamical mean field theory, density matrix renormalization group, and exact diagonalization of many-body Hamiltonians. These techniques have been applied to simple model systems but there is an opportunity to extend these to important, complex systems, especially those which require a multi-orbital description.

Additional Considerations

Verification and Validation and Data Sharing

A strong verification and validation (V&V) component is essential for these efforts and therefore applicants should discuss their V&V plans in sufficient detail. In addition, since cross-benchmarking of different codes is an indispensable and often-used verification tool for large-scale simulation codes, successful applicants are expected to share data and other supporting information in a timely fashion with other researchers.

Coordination with SciDAC Institutes and other Program Elements

Applicants must provide specific plans for establishing partnerships with the SciDAC Institutes to systematically address the applied math and computer science challenges that are inherent to the scale of new architectures or common across applications.

In addition, applicants are encouraged to leverage other BES supported efforts, such as theory and computational groups and Computational Materials and Chemical Sciences Network (CMCSN) projects. Applicants must be explicit about the benefits that they expect to receive from these engagements. Finally, reviewers will examine (see Merit Review Criteria Part V) the collaborations for, among others, duplication of effort.

Management Structure

The applicants must identify a management structure that enables an effective collaboration among the participants from various disciplines. The structure and management must be sufficiently flexible to adapt quickly to changing technical challenges and scientific needs. To that end, the applicants must identify a Lead Principal Investigator, Principal Investigator(s), and Senior/Key Personnel. Furthermore, they should specify the requested level of support from BES or ASCR for each task. Note that some tasks may have both science and computational science components. Typical duties, responsibilities and authorities for each category are provided below:

- **Lead Principal Investigator** - The Lead Principal Investigator must be employed by the Lead institution and will serve as the primary contact responsible for communications with the DOE Program Officers on behalf of all of the Principal Investigators in the Partnership.
- **Principal Investigator** - A Principal Investigator (PI) is the individual designated by the collaborating institution and empowered with the appropriate level of authority and responsibility for the proper conduct of the research within that organization. These authorities and responsibilities include the appropriate use of funds and administrative requirements such as the submission of scientific progress reports to DOE.
- **Senior/Key Personnel** - A senior/key person is an individual who contributes in a substantive, measurable way to the scientific or technical development or execution of the project.

Additional Guidance to Applicants

- Leadership class computation should accelerate scientific discovery in areas of strategic importance to DOE
 - Applicants must explain the benefits from leadership class computation
 - Impacts on Science (*how does it advance the BES mission?*)
 - Advancements in Computational Science (*how does it advance the ASCR mission?*)
 - Is the whole result larger than the sum of its parts?
 - Proposed research must employ state-of-the-art approaches enabling the effective use of the DOE leadership class computing resources

- Applicants must identify metrics that will allow progress and contributions to be measured
- To that end, applicants must build and manage interdisciplinary, multi-institutional collaborations; in particular:
 - Applicants are encouraged to identify collaborations with researchers in the recently selected SciDAC Institutes, avoiding duplication of resources available at the Institutes; the goal is to build the functionality of a vertically integrated enterprise but with common resources found in the SciDAC Institutes
 - Alternatively, applicants may propose non-duplicative Applied Math/Computer Science expertise to supplement topics for which resources are provided by the Institutes, as well as expertise in topics for which no resources were provided by the Institutes.

Post-Award Process

Upon notification of award, the Lead Principal Investigators of the successful projects will be asked to join the Executive Council of the SciDAC Institutes Directors (see DE-FOA-0000505, <http://www.sc.doe.gov/grants/pdf/SC-FOA-0000505.pdf> or LAB 11-505, http://www.sc.doe.gov/grants/pdf/LAB_11-505.pdf for a further description of the Executive Council). This group will be chartered to develop and submit an operating plan to DOE that will describe the processes, procedures, and metrics to be used for coordination and communication between the Partnership and the Institutes. The operating plan will also include processes for the review and, as appropriate, redirection and reprioritization of tasks within the Partnership. Additional guidance will be provided in the award notification letter.

Collaboration

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 encouraged under this FOA. Collaborative applications submitted from different institutions, which are directed toward a single SciDAC Partnership, should clearly indicate they are part of a proposed collaboration and contain the Abstract for that SciDAC Partnership 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.

Collaborative applications should all have the same title as the lead. Each collaborating institution submitting an application must use the same title in Block 11 of the SF 424 (R&R) form. The narrative should include a summary of the main contributions from each of the collaborating institutions and each application must have their own budget and budget justification.

PART II – AWARD INFORMATION

A. TYPE OF AWARD INSTRUMENT.

DOE anticipates awarding Cooperative Agreements under this Funding Opportunity Announcement (FOA).

B. ESTIMATED FUNDING.

It is anticipated that up to \$6,000,000 per year will be available for 5-12 awards to be made in Fiscal Year 2012 contingent on the availability of appropriated funds. Awards 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. Funding for the final two years is contingent upon satisfactory completion of a progress review during the third year of each project. DOE is under no obligation to pay for any costs associated with preparation or submission of applications. DOE reserves the right to fund in whole or part, any, all or none of the applications submitted to this FOA. Although a SciDAC Partnership may be supported by a single award, BES and ASCR expect each Partnership to be a collaboration comprised of several separate awards. BES and ASCR reserve the right to make fewer awards than would be possible at \$6,000,000 per year, if an insufficient number of applications are judged to be of suitable scientific quality or of sufficient relevance to the programs.

C. MAXIMUM AND MINIMUM AWARD SIZE.

The award size will depend on the number of meritorious applications and the availability of appropriated funds.

D. EXPECTED NUMBER OF AWARDS.

BES and ASCR expect to support between five and twelve SciDAC Partnerships. The exact number of awards will depend on the number of meritorious applications and the availability of appropriated funds.

E. ANTICIPATED AWARD SIZE.

The award size will depend on the number of meritorious applications and the availability of appropriated funds.

F. PERIOD OF PERFORMANCE.

A maximum of five years will be considered. Out-year funding will depend upon suitable progress and the availability of appropriated funds. Funding for the final two years is contingent upon satisfactory completion of a progress review during the third year of each project.

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.

Letters of Intent are not required.

2. Pre-Application.

Pre-applications are **REQUIRED** and must be submitted by December 9, 2011, 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 Partnership should submit the pre-application. Pre-applications should be submitted by email to james.davenport@science.doe.gov or mark.pederson@science.doe.gov . **Please include "Pre-application for DE-FOA-0000593" in the subject line.**

Pre-applications should include cover page information, a brief description of the proposed work (2-3 pages, including text with minimum font size 11 point, figures, and references), and a one-page curriculum vitae from each Principal Investigator (PI), co-Principal Investigator (co-PI), and senior collaborator or consultant. The cover page should include: (a) A statement that the document is a pre-application in response to Funding Opportunity Announcement DE-FOA-0000593; (b) Lead PI information: name, institutional affiliation, telephone number, fax number, and e-mail address; and, (c) names and institutions of all Institutional PIs, and senior collaborators or consultants (excluding postdoctoral associates). Since among the purposes of the pre-application is to facilitate BES and 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.

Pre-applications will be reviewed by BES and ASCR program officials for responsiveness to this Funding Opportunity Announcement and the SciDAC program, eligibility of the applicant organization, and qualification of the applicant's personnel for carrying out a large-scale computational research activity. A response to the pre-applications encouraging or discouraging formal applications will be communicated to the applicants by December 30, 2011. 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 their status. **Only those applicants who receive notification from DOE encouraging a full application may submit a formal application. No other formal applications will be considered.**

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.

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. 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.”

Letters of endorsement from unfunded collaborators should also be included, if applicable. 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.

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-0000593

DOE/Office of Science Program Office: Office of Basic Energy Sciences

DOE/Office of Science Program Office Technical Contact: Dr. James Davenport, Dr. Mark Pederson, Dr. Ceren Susut

Is this a Collaboration? If yes, please list ALL Collaborating Institutions/Pis and indicate which ones will also be submitting applications. Also indicate the Lead PI who will be the point of contact and coordinator for the combined research activity. The Lead Application must contain an additional page with a budget table (see example below) that shows the requested annual budgets for each collaborating institution and an explanation (with another, e.g., chart, table) of which tasks will expect BES support and which tasks will expect ASCR support (some tasks may require both BES and ASCR support).

Partnership	Year 1	Year 2	Year 3	Year 4	Year 5	Total
(Start by Lead Institution)	\$(BES)/\$(ASCR)	\$(BES)/\$(ASCR)	\$(BES)/\$(ASCR)	\$(BES)/\$(ASCR)	\$(BES)/\$(ASCR)	\$(BES)/\$(ASCR)
Name of the Institution and the Principal Investigator						
Name of the Institution and the Principal Investigator	\$(BES)/\$(ASCR)	\$(BES)/\$(ASCR)	\$(BES)/\$(ASCR)	\$(BES)/\$(ASCR)	\$(BES)/\$(ASCR)	\$(BES)/\$(ASCR)
Name of the Institution and the Principal Investigator	\$(BES)/\$(ASCR)	\$(BES)/\$(ASCR)	\$(BES)/\$(ASCR)	\$(BES)/\$(ASCR)	\$(BES)/\$(ASCR)	\$(BES)/\$(ASCR)
Name of the Institution and the Principal Investigator	\$(BES)/\$(ASCR)	\$(BES)/\$(ASCR)	\$(BES)/\$(ASCR)	\$(BES)/\$(ASCR)	\$(BES)/\$(ASCR)	\$(BES)/\$(ASCR)
Total	\$(BES)/\$(ASCR)	\$(BES)/\$(ASCR)	\$(BES)/\$(ASCR)	\$(BES)/\$(ASCR)	\$(BES)/\$(ASCR)	\$(BES)/\$(ASCR)

Example budget table (\$ in thousands)

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. **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:

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

Letters of Intent are not required.

2. Pre-application.

Pre-applications are **REQUIRED** and must be submitted by December 9, 2011, 11:59 PM Eastern Time.

Failure to submit a pre-application by an applicant will preclude the full application from due consideration. The pre-application should be submitted electronically by

E-mail to james.davenport@science.doe.gov or mark.pederson@science.doe.gov. **Please include "Pre-application for DE-FOA-0000593" in the subject line.**

Pre-applications should include cover page information, a brief description of the proposed work (2-3 pages, including text with minimum font size 11 point, figures, and references), and a one-page curriculum vitae from each Principal Investigator (PI), co- Principal Investigator (co-PI), and senior collaborator or consultant. The cover page should include: (a) A statement that the document is a pre-application in response to Funding Opportunity Announcement DE-FOA-0000593; (b) Lead PI information: name, institutional affiliation, telephone number, fax number, and e-mail address; and, (c) names and institutions of all Institutional PIs, and senior collaborators or consultants (excluding postdoctoral associates). Since among the purposes of the pre-application is to facilitate BES and 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.

Pre-applications will be reviewed by BES and ASCR program officials for responsiveness to this Funding Opportunity Announcement and the SciDAC program, eligibility of the applicant organization, and qualification of the applicant's personnel for carrying out a large-scale computational research activity. A response to the pre-applications encouraging or discouraging formal applications will be communicated to the applicants by December 30, 2011. 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 their status. Only those applicants who receive notification from DOE encouraging a full application may submit a formal application. **No other formal applications will be considered.**

3. Formal Applications.

APPLICATION DUE DATE: March 12, 2012 11:59 PM Eastern Time

Formal applications submitted in response to this FOA must be received by March 12, 2012 11:59 PM Eastern Time, to permit timely consideration of awards in Fiscal Year 2012. **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. 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.

2. Registration Process.

You must COMPLETE the one-time registration process (all steps) before you can submit your first application through Grants.gov (See www.grants.gov/GetStarted). We recommend that you start this process at least three weeks before the application due date. It may take 21 days or more to complete the entire process. To register with Grants.gov go to "Get Registered" at 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. IMPORTANT: During the CCR registration process, you will be asked to designate an E-Business Point of Contact (EBIZ POC). The EBIZ POC must obtain a special password called "Marketing Partner Identification Number" (MPIN). 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).

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.

3. 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 Funding Opportunity Announcement. 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). Examples of specific questions that might be considered within each criterion are also given:

1. Scientific and/or Technical Merit of the Project;

- a. Does the proposed research address an important and relevant problem in basic energy science where breakthrough advances can be enabled by the use of leadership class computing resources?
- b. What science will become feasible with this collaboration that is not feasible now?
- c. Does the project demonstrate a functional partnership among the indicated domain scientists, applied mathematicians, and computer scientists?
- d. Does the research plan contain appropriate performance metrics that will allow progress and contributions to be measured?
- e. Does the project lead to new algorithms and/or software that will be made available to a broader community?

2. Appropriateness of the Proposed Method or Approach;

- a. Are the methods and approaches to be used in the conduct of the proposed research technically sound and feasible?
- b. Does the proposed research employ or lead to state-of-the-art approaches that effectively exploit leadership class computing resources available to DOE researchers?
- c. Are there significant potential problems in the proposed method or approach? If so, are the applicant's plans to address these problems—including the consideration of alternative strategies—adequate?
- d. Does the proposed research recognize mathematical, algorithmic, or architectural challenges arising in computations at this scale?

3. **Competency of Applicant's Personnel and Adequacy of Proposed Resources; and**
 - a. How strong is the background, past performance, and potential of the lead principal investigators for successful execution of the proposed project?
 - b. Does the applicant have a proven record of success in managing diverse teams of scientific and technical experts and delivering results for advanced computational science research?
 - c. Has the applicant identified a credible and fruitful collaboration between domain scientists and applied mathematicians and computer scientists?
 - d. Is the work of any of the applied mathematicians and computer scientists identified in the proposal (regardless of their affiliation with the SciDAC Institutes) duplicative of work going on in the Institutes?
 - e. Are the roles and intellectual contributions of the Lead Principal Investigator and the BES/ASCR Principal Investigators and each senior/key personnel adequately described?
4. **Reasonableness and Appropriateness of the Proposed Budget.**
 - a. Is the applicant's requested budget appropriate?
 - b. Does the requested budget support the applicant's specified management structure in a meaningful way?

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.

B. REVIEW AND SELECTION PROCESS.

1. Merit Review.

Applications that pass the initial review will be subjected to a merit review in accordance with the guidance provided in the "Office of Science Merit Review System for Financial Assistance." This Merit Review System is available at <http://www.science.doe.gov/grants/process.asp>.

2. Selection.

The Selection Official will consider the merit review recommendation, program policy factors, and the amount of funds available.

3. Discussion and Award.

Government Discussion with Applicant: The Government may enter into discussions with a selected applicant for any reason deemed necessary, including but not limited to: (1) the budget is not appropriate or reasonable for the requirement; (2) only a portion of the

application is selected for award; (3) the Government needs additional information to determine that the recipient is capable of complying with the requirements in 10 CFR part 600 and 605; and/or (4) special terms and conditions are required. Failure to resolve satisfactorily the issues identified by the Government will preclude award to the applicant.

C. ANTICIPATED NOTICE OF SELECTION AND AWARD DATES.

It is anticipated that selections will be completed by May 15, 2012. University and Private Industry awards will be made in Fiscal Year 2012.

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>.

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> under Award 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.

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. DOE cannot answer these questions.

B. AGENCY CONTACTS:

Technical/Scientific Program Contacts:

Dr. James Davenport, Office of Basic Energy Sciences, SC-22.2

PHONE: (301) 903-0035

E-MAIL: James.Davenport@science.doe.gov

Dr. Mark Pederson, Office of Basic Energy Sciences, SC-22.1

PHONE: (301) 903-9956

E-MAIL: Mark.Pederson@science.doe.gov

Dr. Ceren Susut, Office of Advanced Scientific Computing Research, SC-21.1

PHONE: (301) 903-0366

E-MAIL: Ceren.Susut-Bennett@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, 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.