Office of Science
Financial Assistance
Funding Opportunity Announcement
DE-FOA-0000505

Scientific Discovery through Advanced Computing Institutes

SUMMARY:

The Office of Advanced Scientific Computing Research (ASCR) of the Office of Science (SC), U.S. Department of Energy (DOE), hereby announces its interest in receiving grant applications to the Scientific Discovery through Advanced Computing (SciDAC) program for SciDAC Institutes.

A companion Program Announcement to DOE Laboratories (LAB 11-505) will be posted on the Office of Science Grants and Contracts web site at http://www.science.doe.gov/grants/

The mission of the SciDAC Institutes is to provide intellectual resources in applied mathematics and computer science, expertise in algorithms and methods, and scientific software tools to advance scientific discovery through modeling and simulation in areas of strategic importance to the Office of Science and the National Nuclear Security Administration (NNSA). Funding opportunities for SciDAC science domains will be announced through several forthcoming Funding Opportunity Announcements (FOAs) and Program Announcements. These Announcements, issued by ASCR's SciDAC partners, could include opportunities for linking applied mathematics and/or computer science research to science-domain specific challenges through science application partnerships.

The development of SciDAC tools and resources by the Institutes, funded under this FOA, is intended for computational systems such as those existing and planned for at the Oak Ridge and Argonne Leadership Computing Facilities, the National Energy Research Scientific Computing Center, and similar world-class computing facilities over the next 5 years. Specific goals and objectives for the SciDAC Institutes are:

- Tools and resources for lowering the barriers to effectively use state-of-the-art computational systems;
- Mechanisms for taking on computational grand challenges across different science application areas;
- Mechanisms for incorporating and demonstrating the value of basic research results from Applied Mathematics and Computer Science; and
- Plans for building up and engaging our nation's computational science research communities.

One of the primary metrics for the success of the SciDAC Institutes is the extent to which its deliverables are used by application scientists. An equally important metric is the extent to which Institute researchers actively collaborate and leverage their expertise in achieving that success. This FOA describes the process by which grant applications for individual SciDAC Institutes are to be developed, submitted, and merit reviewed. The overall portfolio and management of

Institute awards is expected to cover a significant portion of DOE computational science needs on current and emerging computational systems. Although the work of each proposed Institute is not science application-specific, it is likely – for the purposes of this FOA – to be application-, architecture-, and Institutes-aware.

Institutes-aware. It is most likely that several Institutes will be needed to provide a foundation for next-generation computational science advances for the DOE mission. Consequently, a proposed Institute must not only make a compelling case for its own intrinsic capabilities, but also describe processes for effectively leveraging results from other potential Institutes with complementary or related objectives. The needs of specific science applications will be addressed by science application partnerships through jointly-issued Announcements, which are being planned. New capabilities of strategic importance, or the tailored development of existing capabilities, would be funded by such partnerships. A key point of the Institutes and science application partnerships is that innovative science projects can be accommodated by the Institutes' pooling of a broad range of computational skills that is otherwise not readily available to DOE domain scientists.

Architecture-aware. Each SciDAC Institute should include areas of expertise in which an integrated mathematics and/or computer science effort is required to make an impact on science applications. Representative examples include, but are not limited to:

(a) Multi- and many-core aware algorithms, solution and code verification, uncertainty quantification;
(b) Portable programming models and execution models for many-core architectures, and efficient use of new and emerging memory systems;
(c) Data provenance and triage, data analytics and visualization;
(d) Application performance benchmarking, tuning and analysis, fault tolerance and resilience;
(e) Workflow management, rapid prototyping tools, and advanced debugging capabilities.

Cross-cutting efforts include data management, visualization tools, code profiling, code optimization, best software engineering practices, and model validation. The examples are representative in the sense that items (a)-(e) above and the cross-cuts are important, architecture-aware components in the end-to-end computational science pipeline. Over the next 5 years, the main architectural features of existing and planned computing environments include: heterogeneous nodes (CPUs, GPUs), different memory hierarchies, and varying trade-off costs for computation versus data movement. Tools and methodologies for coping with and taking full advantage of such architectural complexities are an important practical consideration. For example, the re-design and analysis of heavily used computational kernels, and systematic experimentation with algorithmic parameters, are potentially attractive strategies to develop classes of algorithms that can be adapted for optimal performance across a variety of architectures. Algorithm design and analysis is further aided by the development and use of computer science tools for code profiling and optimization, program debugging, and related tasks. The tailored development of efficient, architecture- and application-aware data analysis methods and visualization are examples of tools that are crucial to extracting scientific value from experiments, observations and/or simulations.

Application-aware. The application-aware features of the SciDAC Institutes are essential in ensuring that its deliverables are used by application scientists (a primary metric of success). Nevertheless, it is difficult to anticipate the near-term and changing computational science needs of domain scientists. This observation motivates the need to develop intellectual resources and tools to meet cross-cutting or core computational science needs for DOE and SC missions. Furthermore, to engage and attract domain scientists, applicants may propose proof-of-principle demonstrations of potential benefits – which may motivate the development of meaningful and credible suites of test applications or benchmark problems. The latter considerations are no substitute for realistic, full-scale applications or data sets, but may be useful for development purposes and for gaining experience with the most significant issues confronting domain scientists.

Management structure. Each Institute must identify a management structure that enables it to function efficiently and to collaborate effectively and quantifiably with the science applications as well as with each other (see Post Award below). Institute structure and management must be sufficiently flexible to adapt quickly to changing technical challenges and scientific needs. Each Institute must identify a Director, Principal Investigator(s), and Senior/Key Personnel. Typical duties, responsibilities and authorities for each category are provided below:

- **Institute Director** - The SciDAC Institute Director is the Lead Principal Investigator and must be employed by the Lead institution. The SciDAC Institute Director will serve as the primary contact responsible for communications with the DOE Program Officer on behalf of all of the Principal Investigators in the Institute.
- **Principal Investigator** - A Principal Investigator is the individual designated by the research organization 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. When an organization designates more than one Principal Investigator, it identifies them as individuals who share the authority and responsibility for leading and directing the research, intellectually and logistically.
- **Senior/Key Personnel** - A senior/key person is an individual who contributes in a substantive, measurable way to the scientific/technical development or execution of the project. This definition includes, but is not limited to, the SciDAC Institute Director and the Principal Investigator(s).

Post-Award process. Upon notification of award, the Institute Director for each successful applicant will be asked to serve with the other Institute Directors on a SciDAC Institute Directors Executive Council. This group will be chartered to develop and submit an operating plan for the SciDAC Institutes. The plan will describe the processes and procedures to be used for coordination and communication among the Institutes. The plan will also describe the process used by each Institute to review activities within that Institute, re-prioritize as appropriate and communicate those results to all of the Institutes, the Executive Council, and ASCR. As scientific application partnerships (i.e., ASCR and other DOE Programs) develop, the Executive Council will document its approach for working with these science application partnerships and present it to DOE. Additional guidance will be provided in the award notification letter.

Science application partnerships. Beginning in the mid-FY2011 timeframe, a series of focused, follow-on Announcements are planned for the domain science components of SciDAC. Current thinking about this series of Announcements can be found in the Supplementary Information section that follows.

Letter of Intent (LOI).

Applicants are strongly encouraged to submit a LOI by close of business **March 30, 2011.** The LOI should include the following:

a. A cover sheet containing the name and mailing address of the applicant Lead institution; the planned title of the SciDAC Institute; the estimated annual cost and total cost of the project over the five-year project period; the name, institutional affiliation, e-mail address, and telephone number of the SciDAC Institute Director, Principal Investigator(s), and Senior/Key personnel expected to be involved in the planned application.

b. A one-page overview of the strategic plan for the proposed SciDAC Institute, including the vision, goals and key objectives.

c. A one-page overview of the research plan.

Letters of Intent will be used to organize and expedite the merit review process. Consequently, the submission of a LOI is strongly encouraged but not required. The absence of a LOI will not negatively affect a thorough evaluation of a responsive formal application submitted in a timely fashion. The LOI should be sent by E-mail as a PDF file to: scidac-institutes@ascr.doe.gov. Please include the phrase "Letter of Intent" in the subject line.

APPLICATION DUE DATE: May 2, 2011, 11:59 p.m. Eastern Time

Formal applications submitted in response to this FOA must be received by **May 2, 2011, 11:59 PM Eastern Time**, to permit timely consideration of awards. **APPLICATIONS RECEIVED AFTER THE DEADLINE WILL NOT BE REVIEWED OR CONSIDERED FOR AWARD.**

IMPORTANT SUBMISSION INFORMATION:

The full text of the Funding Opportunity Announcement (FOA) is located on FedConnect. Instructions for completing the Grant Application Package are contained in the full text of the FOA which can be obtained at: https://www.fedconnect.net/FedConnect/?doc=DE-FOA-0000505&agency=DOE. To search for the FOA in FedConnect click on "Search Public Opportunities". Under "Search Criteria", select "Advanced Options", enter a portion of the title " Scientific Discovery through Advanced Computing Institutes". Once the screen comes up, locate the appropriate Announcement.

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

Applications must be submitted using Grants.gov.

Applications submitted through FedConnect will not be accepted.

WHERE TO SUBMIT: Where to Submit: Applications must be submitted through Grants.gov to be considered for award. You cannot submit an application through Grants.gov unless you are registered. Please read the registration requirements carefully and start the process immediately. Remember you have to update your CCR registration annually. If you have any questions about your registration, you should contact the Grants.gov Helpdesk at 1-800-518-4726 to verify that you are still registered in Grants.gov.

Registration Requirements: There are several one-time actions you must complete in order to submit an application through Grants.gov (e.g., obtain a Dun and Bradstreet Data Universal Numbering System (DUNS) number, register with the Central Contract Registry (CCR), register with the credential provider, and register with Grants.gov). See http://www.grants.gov/GetStarted. Use the Grants.gov Organization Registration Checklist at http://www.grants.gov/assets/OrganizationRegCheck.pdf to guide you through the process. Designating an E-Business Point of Contact (EBiz POC) and obtaining a special password called an MPIN are important steps in the CCR registration process. Applicants, who are not registered with CCR and Grants.gov, should allow at least 21 days to complete these requirements. It is suggested that the process be started as soon as possible.

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

Questions: Questions relating to the registration process, system requirements, how an application form works, or the submittal process must be directed to Grants.gov at 1-800-518-4726 or support@grants.gov. Part VII of this 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

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 http://www.compusearch.com/products/fedconnect/fedconnect.asp and

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.

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 and http://www.compusearch.com/products/fedconnect/fedconnect.asp.

All applications should be in a single PDF file.

GENERAL INQUIRIES ABOUT THIS FOA SHOULD BE DIRECTED TO:

Technical/Scientific Program Contact:

Program Manager: Dr. Walter M. Polansky, Office of Advanced Scientific Computing Research, U.S. Department of Energy
Telephone: (301) 903-5800
Fax: (301) 903-7774
E-mail: scidac-institutes@ascr.doe.gov

SUPPLEMENTARY INFORMATION:
The Scientific Discovery through Advanced Computing (SciDAC) program was initiated in 2001 as a partnership involving all of the Office of Science (SC) program offices to dramatically accelerate progress in scientific computing that delivers breakthrough scientific results through partnerships comprised of applied mathematicians, computer scientists, and scientists from other disciplines. The SciDAC program was re-competed in 2006, and the partnerships were extended to include the DOE National Nuclear Security Administration (NNSA) and the National Science Foundation (NSF). Through partnerships with ASCR-funded mathematicians and computer scientists, SciDAC applications pursued computational solutions to challenging problems in climate science, fusion research, high energy physics, nuclear physics, astrophysics, material science, chemistry, particle accelerators, biology and the reactive subsurface flow of contaminants through groundwater. Today the SciDAC program is recognized as the leader in accelerating the use of high-performance computing to advance the state of knowledge in science applications. These advances in applications would not have been possible without the expertise in applied mathematics and computer science provided to the application domain scientists.

Since the inception of the SciDAC Program, its Centers and Institutes (and their predecessors) have accelerated the process of transitioning basic research in applied mathematics and computer science to applications in targeted areas by direct engagement with the applications in the SciDAC Science Application partnerships. Both parties found the direct engagement beneficial: the domain scientists received better algorithms, faster codes, and vastly improved scientific insights, while the mathematicians and computer scientists gained a deeper understanding of the challenges associated with solving complex problems. There was, however, no prescribed procedure for this engagement. While many SciDAC application scientists regularly collaborated with the Centers and Institutes in their work, many others (for a variety of reasons) bypassed Centers and Institutes. A desired outcome of these new SciDAC projects is the marked improvement in collaborations among Institutes participants and their domain-science partners.

The SciDAC model has accelerated the pace of scientific discovery. With this new SciDAC funding opportunity and science application partnerships, scientifically sound and efficient approaches will be needed to address mathematical and computational challenges related to the generation and management of large data sets, the increased demand for scientific credibility, and the expected disruptions in computer architectures. Furthermore, the Institutes will employ best practices in software development, packaging, and distribution.

Below, ASCR's SciDAC science application partners identify areas of joint strategic importance that are positioned to be met through SciDAC over the next 5 years.

Basic Energy Sciences (BES)

Basic Energy 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. Underpinning these activities are needs to apply and continually improve computational methods for explaining, predicting, and optimizing materials and processes such as catalysis, materials under extreme environments, solar energy utilization, and superconductivity. Methods include simulations of chemically reacting flows; quantum calculations of the structure and electronic properties of atoms, molecules, and solids; simulation of reactive and non reactive dynamics, computation of mechanical and radiative energy transfer as well as charge and mass transport through a wide variety of materials and conditions and electromagnetic stimuli; macroscopic properties of materials such as strength, toughness, and ductility. Specific topical areas include, but are not limited to, Advanced Nuclear Systems, Catalysis, Clean and Efficient Combustion, Electrical Energy Storage, Geosciences and Geological Systems, Hydrogen Economy, Material under Extreme Environments, Solar Energy Utilization, Solid State Lighting, and Superconductivity. Additional information about modeling challenges in these areas can be found at: http://www.sc.doe.gov/bes/reports/list.html and http://www.sc.doe.gov/bes/BES.html

Biological and Environmental Research (BER)

Biological and environmental Research (BER) supports fundamental, interdisciplinary research to achieve a predictive systems-level understanding of climate change, contaminant fate and transport in complex subsurface environments and systems biology, which requires the

organization and integration of diverse interdisciplinary data and models in innovative ways. In particular, BER seeks to develop advanced computer models ranging from molecular to global scales and an ability to connect extremely large datasets from a wide variety of sources with models, which enables more holistic and robust predictions of complex system behavior. For example, both the Community Earth System Model (CESM; http://www.cesm.ucar.edu/) and BER's subsurface science modeling efforts will require the development of new model physics and numerical capabilities, manipulation and analysis of large and diverse data-sets, and frameworks for collaboration. Both also require conceptual and algorithmic frameworks for integrating the wide range of multi-physics over multi-scales that must be employed to provide understanding and prediction as well as innovative frameworks to quantify the uncertainty in prediction resulting from the model and observational uncertainties. Systems biology approaches facilitating genome-enabled, mechanistic descriptions of biological processes into multidisciplinary, multiscale environmental process models is a unique, key point of the integration for BER programs. Potential SciDAC Institutes and BER science application partnership projects for systems biology should be aware of the Systems Biology Knowledgebase (http://www.sc.doe.gov/ober/kbase_plan.pdf) efforts to address the enormous data storage, management, access, and utilization challenges for systems biology. Additional information about modeling challenges in the areas of climate, subsurface science, systems biology and BER programs in general can be found at:
http://www.sc.doe.gov/ober/BER_workshops.html and
http://www.sc.doe.gov/ober/ober_top.html

Fusion Energy Sciences (FES)

The Fusion Energy Sciences (FES) mission is to expand the fundamental understanding of matter at very high temperatures and densities and to build the scientific foundations needed to develop a fusion energy source. As fusion research enters the era of burning plasmas and ITER, large-scale simulations based on high fidelity physics models will be necessary to develop the validated predictive capability needed for meeting the FES mission. Modern fusion simulation codes are based on near first-principles or advanced reduced descriptions of the fundamental Maxwell-Boltzmann system of equations describing the properties and behavior of magnetically confined plasmas. The intrinsic nonlinearities, complicated geometries and magnetic topologies, extreme anisotropies, wide ranges of overlapping temporal and spatial scales, and multiphysics effects associated with a realistic description of the confined plasma state pose significant challenges to the solution of these equations. Contributions from the applied mathematics and computer science communities are essential for overcoming these challenges and accelerating progress in advanced fusion simulations. In particular, contributions in applied mathematics and computer science are needed to address challenges for nonlinear gyrokinetic simulations based on the particle-in-cell or continuum methodologies; macroscopic stability of magnetically confined plasmas including two-fluid and 3-D effects; 3-D simulations of RF wave propagation in magnetically confined plasmas, including coupling with Fokker-Planck solvers; and integrated multi-physics simulations on transport time scales. Additional information about modeling challenges in the area of fusion energy sciences can be found at:
http://extremecomputing.labworks.org/fusion/PNNL_Fusion_final19404.pdf and
http://www.ofes.fusion.doe.gov/ProgramDocuments/reports/FSPWorkshopReport.pdf

High Energy Physics (HEP) and Nuclear Physics (NP)

The mission of the High Energy Physics (HEP) and Nuclear Physics (NP) programs is to understand how our universe functions at the most fundamental level. HEP research does this by discovering the most elementary constituents of matter and energy, determining their properties and interactions, and exploring the basic nature of space and time itself. NP supported research is concerned with three broad, related research topics: the theory of Quantum Chromodynamics (QCD), which describes strongly interacting matter and the strong forces that bind nuclei; the structure and properties of atomic nuclei, and nuclear astrophysics, which addresses the origin of the elements; and extensions of the standard model of fundamental particles, which may explain the matter/antimatter asymmetry in the universe. As fundamental topics in HEP and NP, these areas underlie all of the physical sciences. Current major computational science research topics in HEP and NP include projects in the areas of QCD calculations, Astrophysics and Cosmology, Low Energy Nuclear Physics, and Particle Accelerator Design. Further topics may emerge as a result of scientific developments.

Additional information about modeling challenges in the area of high energy physics can be found at: http://www.science.doe.gov/hep/index.shtml.

Additional information about modeling challenges in the area of nuclear physics can be found at: http://www.science.doe.gov/np/index.shtml. Recent SciDAC projects with major NP participation are described at: http://www.scidac.gov/physics/physics.html.

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 Institute, should clearly indicate they are part of a proposed collaboration and contain the Abstract for that SciDAC Institute 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. Further information on preparation of collaborative applications may be accessed via the Internet at: http://www.sc.doe.gov/grants/colab.asp .

Program Funding

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 funds and satisfactory progress. Five-year SC-total funding up to $13,000,000 per year is expected to be available to support the DOE-laboratory and non-DOE-laboratory portions of this FOA subject to appropriation of funds by the Congress. 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.

ASCR expects to support between 1 and 5 SciDAC Institutes through the DOE-laboratory and non-DOE laboratory portions of this FOA. Although a SciDAC Institute may be supported by a single award, ASCR expects each Institute will be a collaboration comprised of several separate awards. ASCR reserves the right to make fewer awards than would be possible at $13,000,000 per year. If an insufficient number of applications are judged to be of suitable scientific quality or of sufficient relevance to the programs.

Merit Review

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

1. Scientific and/or Technical Merit of the Project;
2. Appropriateness of the Proposed Method or Approach;
3. Competency of Applicant's Personnel and Adequacy of Proposed Resources; and
4. Reasonableness and Appropriateness of the Proposed Budget.

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

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

Posted on the Office of Science Grants and Contracts Web Site
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