

Office of Science
Notice DE-FG02-06ER06-04

*Scientific Discovery through
Advanced Computing*

U.S. Department of Energy

Office of Science Financial Assistance Program - Notice DE-FG02-06ER06-04: Scientific Discovery through Advanced Computing

AGENCY: U.S. Department of Energy
Office of Science

ACTION: Notice inviting grant applications.

SUMMARY: The Office of Science (SC) and the National Nuclear Security Administration (NNSA), U.S. Department of Energy (DOE), hereby announce interest in receiving applications for projects in the Scientific Discovery through Advanced Computing (SciDAC) research program. (Note: NSF will participate in the following Science Applications - Climate Modeling and Simulation and High Energy and Nuclear Physics with Petabytes.) The SciDAC program was initiated in 2001 as a partnership involving all SC program offices-Advanced Scientific Computing Research, Basic Energy Sciences, Biological and Environmental Research, Fusion Energy Sciences, High-Energy Physics and Nuclear Physics-to fully realize the potential of emerging petascale computers at that time for advancing scientific discovery. Researchers have achieved key scientific insights in a number of areas of National importance, yet many challenges of multi-scale, multi-disciplinary problems now facing science programs in DOE require advanced modeling and simulation capabilities on petascale computers. A second challenge is driven by the need for capture, storage, transmission, sharing and analysis of large-scale experimental and observational data, as well as data from simulations. This Notice is seeking applications that contribute to:

- The creation of a comprehensive, scientific computing software infrastructure that fully integrates applied mathematics, computer science, and computational science in the physical, biological, and environmental sciences for scientific discovery at the petascale level, and
- A new generation of data management and knowledge discovery tools for the large data sets obtained from large experimental facilities and from high end simulations.

Applications are sought that:

- Address obtaining significant insight into, or actually solve, a challenging problem of National scientific or engineering significance clearly related to DOE missions through computational science,

- Create scientific simulation codes that: achieve high single node performance; scale to thousands of nodes and tens-of-thousands of processors; and can be readily ported to other computer architectures,
- Develop applied mathematics and computer science methodology focused on computational science at the petascale and work with application teams to apply innovations,
- Integrate computational science with discipline-driven applications through teaming and partnerships with computer scientists and applied mathematicians,
- Engage experimental and observational data-intensive science, and/or
- Empower new scientific communities to achieve scientific discovery through computational science.

Prospective applicants should observe that the program is structured to be interdisciplinary and multi-institutional in nature. The Department's National Nuclear Security Administration is a partner in this program.

Synergistic collaborations with researchers in Federal Laboratories and Federally Funded Research and Development Centers (FFRDCs), including the DOE National Laboratories are encouraged, though no funds will be provided to these organizations under this Notice. Laboratories should respond to the LAB 06-04 Announcement posted at: <http://www.science.doe.gov/grants/grants.html>. Partnerships among multiple institutions, that may include universities, laboratories, and/or private institutions, are anticipated for the majority of submissions. Applicants may request a period of performance of up to five (5) years.

Teams funded by the current SciDAC program that apply under this Notice must clearly delineate the new challenges they are facing.

DATES: Potential applicants are **required** to submit a one (1) to two (2) page Letter-of-Intent by January 23, 2006, which includes the title of the proposed effort, the program area addressed, the names of the principal investigator and all senior personnel, participating institutions, organizational approach, projected funding request (if possible) and summary/abstract. For multi-institution applications, a single Letter-of-Intent should be submitted by the PI of the lead institution. Letters of Intent will be reviewed for conformance with the guidelines presented in this Notice and suitability in the technical areas specified in this Notice. A response to the Letters of Intent encouraging or discouraging formal applications will be communicated to the applicants by January 30, 2006.

Formal applications in response to this Notice should be received by March 6, 2006, to be accepted for merit review and funding in Fiscal Year 2006.

ADDRESSES: Letters-of-Intent should be submitted electronically as an email attachment (not pdf) to scidac-2@mcs.doe.gov. Please use the phrase "SciDAC Science Application-PI_Lastname-Institution" or "SciDAC Enabling Technology-PI_Lastname-Institution" in the subject line (where PI Lastname is the surname of the lead PI and Institution is the lead institution). A copy to the appropriate POC is also encouraged. Applications submitted to the Office of Science must be submitted electronically through Grants.Gov by **March 6, 2006**, to be

considered for award. In addition, a copy of the full application should also be submitted electronically as a single pdf file to scidac-2@mics.doe.gov. The email should use the phrase "SciDAC Science Application" or "SciDAC Enabling Technology," as appropriate, in the subject line.

Formal Applications

Applications submitted to the Office of Science must be submitted electronically through [Grants.gov](https://grants.gov) to be considered for award. The Funding Opportunity Number is: DE-FG02-06ER06-04 and the CFDA Number for the Office of Science is: 81.049. Instructions and forms are available on the [Grants.gov](https://grants.gov) website. Please see the information below and also refer to the "Funding Opportunity Announcement", Part IV - Application and Submission Information; H. Other Submission and Registration Requirements for more specific guidance on "Where to Submit" and "Registration Requirements." If you experience problems when submitting your application to [Grants.gov](https://grants.gov), please visit their customer support website: <http://www.grants.gov/CustomerSupport>; email: support@grants.gov; or call 1-800-518-4726.

The Research & Related Other Project Information form of the grants.gov template should be completed in the following manner. Project Narrative is Field 7 on the form. The first page of your narrative must include the following information:

Applicant/Institution:

Street Address/City/State/Zip:

Principal Investigator:

Address:

Telephone Number:

Email:

DOE/Office of Science Program Office:

DOE/Office of Science Program Office Technical Contact:

DOE Grant Number (if Renewal or Supplemental Application): Is this a Collaboration? If yes, please list ALL Collaborating Institutions/PIs

- and indicate which ones will also be submitting applications. Also indicate the PI who will be the point of contact and coordinator for the combined research activity.

* Note that collaborating applications must be submitted separately.

The narrative comprises the research plan for the project and must be 20 pages or less, including tables and figures, but excluding forms and certifications, when printed using standard 8.5" by 11" paper with 1 inch margins (top, bottom, left, and right) and font not smaller than 11 point. EVALUATORS WILL ONLY REVIEW THE NUMBER OF PAGES SPECIFIED IN THE PRECEDING SENTENCE. Letters of commitment for collaboration of non-funded collaborators and short curriculum vitae of all senior personnel must be included in the application. Applications not meeting these requirements will be deemed ineligible during the initial screening process. The major part of the narrative should be devoted to a description and justification of the proposed project, including details of the methods to be used. It should also

include a timeline for the major activities of the proposed project, and should indicate which project personnel will be responsible for which activities. 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."

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](http://www.grants.gov)). See <http://www.grants.gov/GetStarted>. Use the Grants.gov Organization Registration Checklist 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 14 days** to complete these requirements. It is suggested that the process be started as soon as possible.

VERY IMPORTANT - Download PureEdge Viewer: In order to download the application package, you will need to install PureEdge Viewer. This small, free program will allow you to access, complete, and submit applications electronically and securely. For a free version of the software, visit the following Web site: <http://www.grants.gov/DownloadViewer>.

FOR FURTHER INFORMATION CONTACT: Walt Polansky, Mary Anne Scott, or Dave Goodwin, Office of Advanced Scientific Computing Research, Telephone (301) 903-5800; ascr-scidac_coordination@mics.doe.gov

SUPPLEMENTARY INFORMATION:

Background:

1. Scientific Discovery through Advanced Computing

Advanced scientific computing will be a key contributor to scientific research in the 21st Century. Within the Office of Science (SC), scientific computing programs and facilities are already essential to progress in many areas of research critical to the Nation. Major scientific challenges exist in all SC research programs that can best be addressed through advances in scientific supercomputing, e.g., designing materials with selected properties, elucidating the structure and function of proteins, understanding and controlling plasma turbulence, and designing new particle accelerators. To help ensure its missions are met, SC is bringing together advanced scientific computing and scientific research in an integrated program entitled "Scientific Discovery Through Advanced Computing."

The Opportunity and the Challenge

During the past five years, the SciDAC program has clearly shown the benefits of teaming computational scientists, computer scientists and applied mathematicians in tackling challenging

scientific problems. It has demonstrated that important scientific accomplishments are possible through simulation and modeling with focused collaboration and active partnership of domain scientists, applied mathematicians, and computer scientists. Successes have been documented in such areas as accelerator design, chemistry, combustion, climate modeling, and fusion. The program has also demonstrated that large scale simulation offers some of the most cost-effective opportunities for answering a number of scientific questions in areas, such as the fundamental structure of matter and the production of heavy elements in supernovae.

Extraordinary advances in computing technology in the past decade have set the stage for a major advance in scientific computing. . Within the next five to ten years, computers 1,000 times faster than today's terascale computers will become available. These advances herald a new era in scientific computing. In FY 2004 DOE's Office of Science launched an aggressive program to develop and deploy leadership-class computing facilities and announced a twenty-year scientific facilities roadmap that will provide a rich scientific infrastructure for the next two decades. A copy of the plan may be found at: http://www.science.doe.gov/Sub/Facilities_for_future/20-Year-Outlook-screen.pdf.

To exploit this opportunity, these computing advances must be translated into corresponding increases in the productivity of the scientific codes used to model physical, chemical, and biological systems. *This is a daunting problem.* Current advances in computing and networking technologies are being driven by market forces in the commercial sector, not by scientific computing. Harnessing commercial computing technology for scientific research poses problems unlike those encountered in previous supercomputers, in magnitude, as well as in kind. A comparable challenge applies to harnessing commercial network technology for the integration of scientific applications through networks to achieve required end-to-end performance. Towards the end of this decade new systems are expected to emerge which will offer new architectures for scientific computation. New advances in mathematics, algorithms, computer science, and an ever-changing array of new computer architectures make the field of computational science one of continuing challenges.

The Investment Plan of the Office of Science

To take advantage of the opportunity offered by petascale computers, SC will fund a set of coordinated investments as outlined in its long-range plan for scientific computing, *Scientific Discovery through Advanced Computing*, (See Footnote Number 1) submitted to Congress on March 30, 2000. First, it will create a *Scientific Computing Software Infrastructure* that bridges the gap between the advanced computing technologies being developed by the computer industry and the scientific research programs sponsored by the Office of Science. Specifically, SC plans to:

- Create a new generation of *Scientific Simulation Codes* that take full advantage of the extraordinary computing capabilities of terascale computers.
- Create the *Mathematical and Computing Systems Software* to enable the Scientific Simulation Codes to effectively and efficiently use terascale computers.

- Create a *Distributed Science Software Environment* to enable management, dissemination, and analysis of large data sets from simulation-intensive and experimental/observational-intensive science.

These activities are supported by a *Scientific Computing Hardware Infrastructure* that will evolve to meet the needs of its research programs. The *Hardware Infrastructure* provides the stable computing resources needed by the scientific applications; responds to innovative advances in computer technology that impact scientific computing; and allows the most appropriate and economical resources to be used to solve each class of problems. Specifically, SC plans to support:

- A *Flagship Computing Facility*, the National Energy Research Scientific Computing Center (NERSC), to provide robust, high-end computing resources needed by a broad range of scientific research programs.
- *Leadership Computing Facilities*, at Oak Ridge National Laboratory to provide very large scale computing resources tailored for specific scientific applications.
- *Capability resources* to support code development, scalability testing and other development activities to prepare application codes for terascale and petascale computations.
- *Early access to new emerging systems architectures*, e.g., BlueGene/L, to port and tune codes that may benefit from such systems.

These systems will evolve over the course of the next five years into petascale systems with hundreds of thousands of processors representing a variety of computer architectures to meet the needs of the SciDAC computational applications, as well as other computational science needs of the Office of Science.

The allocation of computing resources available to individual projects will be not be part of this solicitation but will be contingent on review and award through the process as described at: <http://hpc.science.doe.gov>. Within the available computational resources, every effort will be made to ensure that successful applications will have the resources needed to support their efforts.

The systems that are part of the *Hardware Infrastructure* are embedded in a networking environment for science, the Energy Sciences Network (ESnet), that delivers the end-to-end capabilities needed to support scientific applications, and is evolving into a hybrid of packet switched services and high bandwidth circuit switched services, perhaps directly over wavelengths. It is anticipated that some applications may need to negotiate services across multiple, independent networks to achieve end-to-end performance.

The Benefits

The *Scientific Computing Software Infrastructure*, along with the upgrades to the hardware infrastructure, will enable laboratory and university researchers to solve the most challenging scientific problems faced by the Office of Science at a level of accuracy and detail never before achieved. These developments will have significant benefit to all of the government agencies

who rely on high-performance scientific computing to achieve their mission goals, as well as to the U.S. high-performance computing industry.

Request for Cooperative Agreement Applications

This notice requests applications for cooperative agreements in the Science Application areas discussed in Section 2 and in the Enabling Technologies areas discussed in Section 3, with the exception of sub-sections specifically requesting grant applications. Cooperative Agreements differ from grants in that there is continuing substantial involvement by DOE in the conduct of the research.

Successful applicants of Science Applications must devise a multi-disciplinary research strategy that addresses both the domain science and computational science challenges facing their simulation or data management issue.

Successful applicants of Enabling Technologies must ensure that source code is fully and freely available for use and modification throughout the scientific computing community via a preapproved open source process.

To ensure that the SciDAC program meets the broadest needs of the research community, the successful applications are expected to participate in the annual SciDAC meeting, develop and maintain a project web site, and interact with other program participants on cross-cutting issues. It is anticipated that up to approximately \$36,000,000 will be available for grants and cooperative agreement awards in FY 2006, subject to the availability of funds. The DOE is under no obligation to pay for any costs associated with the preparation or submission of an application. DOE reserves the right to fund, in whole or in part, any, all, or none of the applications submitted in response to this Notice. The following two sections are offered to provide background in-depth information on areas that are of interest to the Office of Science along with NNSA and NSF for: 1) *the scientific and technical applications for a number of science domains of importance to the DOE mission, and 2) the enabling technology dimensions needed to achieve the SciDAC vision.*

2. Science Applications

The SciDAC program is structured as a set of coordinated investments across all SC mission areas with the goal of achieving breakthrough scientific advances via computer simulation that are impossible using theoretical or laboratory studies alone. In addition, the use of advanced computing technologies to accelerate scientific discovery is not limited to simulation-based science. It can also be applied to improving experimental science. Over the five years of the SciDAC program, researchers have achieved key scientific insights in a number of areas of National importance, including fusion, combustion, climate modeling, high energy and nuclear physics, and astrophysics. These advances have been accomplished through the development of state-of-the-art-simulation codes. The results of these simulations, together with associated theory and experiment, help ensure that the U.S. maintains a leadership role in science and technology.

The major source of acceleration in simulation-based science has been the strength and depth of partnerships among application domains, computer science, and applied mathematics.

Applications for research in the scientific domains must include a plan for partnerships that integrate advanced applied mathematics and computer science technologies with the proposed domain-specific efforts. In addition, the plan may request additional resources for closely related computer science and applied mathematics research to ensure adequate integration. Work proposed in computer science or applied mathematics should be clearly identified. Additional information on the approach for partnerships is outlined in Section 3.

Challenges and opportunities remain in a number of scientific domains. Applications are sought for the following domains.

Accelerator Science and Simulation: A comprehensive, coherent petascale simulation capability for the U.S. particle and nuclear accelerator community is critical for the near and long-term priorities of DOE's Office of Science. High Energy Physics priorities are driven by optimization needs of existing HEP accelerators, such as the B-Factory and Tevatron, design of possible future accelerators, such as ILC other next-generation facilities, and maintaining a vital DOE accelerator R&D program. Near-term Nuclear Physics facility priorities are the Rare Isotope Accelerator (RIA) and the Continuous Electron Beam Accelerator Facility (CEBAF) Upgrade. In the longer term the Office of Nuclear Physics will explore the development of an electron-nucleus collider that would allow the gluon saturation of nuclear matter to be seen. Topic areas for modeling needs therefore include: high-accuracy computation of modes for superconducting RF cavities; realistic simulation of wakefield effects; parallelization of Radio Frequency Quadrupole (RFQ) simulations; self-consistent 3D calculations of Coherent Synchrotron Radiation; (CSR) forces and their effects on the beam; electron cooling of heavy-ion beams; optimization of Particle In Cell (PIC) codes; and adaptive mesh techniques for intense beams. Accelerator simulation codes which run on a variety of platforms, scale to petaflops and many thousands of processors, which are robust, documented, and can be easily used by accelerator researchers at all DOE HEP and NP facilities, and are well integrated with visualization capacities will have the greatest impact on the field.

BES POC: Roger Klaffky, (301)-903-1873, Roger.Klaffky@science.doe.gov HEP POC: Craig Tull, (301)-903-0468 Craig.Tull@science.doe.gov NP POC: Sidney A. Coon, (301)-903-7878 Sidney.A.Coon@science.doe.gov

Astrophysics: Computational astrophysics encompasses many research areas of interest and relevance to high-energy physics, nuclear physics, and Advanced Simulation and Computing. SciDAC applications for work in astrophysical and cosmological simulations are invited and will be judged in part based on their relevance to these program missions. While some examples of topical research areas are given below, successful SciDAC applications need not be limited to these areas.

Modeling of explosive astrophysical events, including Type Ia supernovae, gamma-ray bursts, X-ray bursts and core collapse supernovae is needed, not only for the quantitative understanding of the mechanics of supernovae, but also because all of these type of events produce unique nucleosynthesis products responsible for nearly all of the elements in the solar system and in

living creatures. In addition, detailed simulations of these objects, in conjunction with astrophysical data, can shed new light on the physics of particle interactions and the properties of fundamental particles.

In particular, Type Ia supernovae are significant scientifically because of their use as standard candles in determining the expansion rate of the universe for measurements of dark energy, a technique which can be improved by a quantitative understanding of the transition from white dwarf stars to supernovae. Simulations of other types of supernovae and astrophysical objects also need to be performed to determine whether they can be used as standard candles, and what systematic variations limit their utility. A detailed simulation of core collapse supernovae brings together nuclear physics including neutrino physics, fluid dynamics, radiation transport of neutrinos, and general relativity and successful simulations could advance knowledge of nucleosynthesis and the properties of fundamental particles.

Unknown particles and forces (so-called dark matter and dark energy) make up 95% of the universe. DOE and NASA have both identified dark energy as a priority in their science programs. The two agencies have laid out a plan for a space-based, competed Joint Dark Energy Mission (JDEM) to determine the nature of dark energy. In addition, DOE supports several current experiments which are aimed at directly detecting cosmic dark matter or producing it in high-energy collisions. Computational techniques, which couple 2- and 3-dimensional simulations of complex astrophysical phenomena and structures with ground and space-based observations of dark matter and dark energy will be necessary to shed light on the properties of these unknown agents and perhaps interpret possible discoveries.

Other topics of interest include, but are not limited to: simulations of celestial objects, such as gamma ray bursts, to study the astrophysical acceleration mechanisms that produce the highest energy cosmic rays; simulations of dynamical processes which can explain and predict the intergalactic magnetic fields which affect the propagation of these particles; cosmic microwave background (CMB) simulations required to understand the CMB data from the very early universe; and simulations which can predict the imprint of gravitational waves on the CMB to directly see inflation in the early universe.

HEP POC: Craig Tull, (301)-903-0468 Craig.Tull@science.doe.gov NP POC: Sidney A. Coon, (301)-903-7878 Sidney.A.Coon@science.doe.gov NNSA POC: Dr. Njema Frazier, 202-586-5789 Njema.Frazier@nnsa.doe.gov

Climate Modeling and Simulation: SciDAC climate modeling applications program continues to lead the evolution of DOE's long-standing climate modeling and simulation research agenda. The program, focused on developing, testing and applying climate simulation and prediction models that stay at the leading edge of scientific knowledge and computational technology, is tightly integrated with the goals of the Climate Change Prediction Program (CCPP; <http://www.science.doe.gov/ober/CCRD/model.html>) to advance climate change science and improve climate change projections using state-of-the-science coupled climate models, on time scales of decades to centuries and space scales of regional to global.

DOE is currently funding the testing, development, evaluation of high-end climate models and their use to answer strategic questions related to DOE's mission. Thus, the high priority areas: continued improvement in the representation of key processes in the current version of high-end climate models; continued development of frameworks that will test the above representations in the fully coupled system; and issues associated with running the fully coupled climate model efficiently on high-performance scientific supercomputers that are either available, or being envisaged under the Leadership Computing Facility at ORNL and other high-end computing resources available for DOE researchers.

The program will continue the development of climate models of the future based on theoretical foundations and improved computational methods that have the potential to run efficiently on current and future generations of high-performance scientific supercomputers. The intent is to increase dramatically both the accuracy and throughput of computer model-based predictions of future climate system response to the increased atmospheric concentrations of greenhouse gases. This notice requests applications in the following two areas:

- 1.** Renewal applications for cooperative agreements for continued successful development of prototype climate models of the future including new formulations, numerical methods, algorithms and computational techniques, that will underpin the construction of production-quality coupled climate general circulation models in the next five-year time frame. The requests must clearly demonstrate progress under past support, e.g., model formulations that accurately simulate critical climate processes, efficient algorithms that execute on high-end computer architectures, such as multi-threaded and processor-in-memory designs. Renewal application requests should be roughly at previous level of funding or less. Multiple-year funding of awards is expected, with out-year funding contingent upon the availability of appropriated funds, progress of the research, and programmatic needs.

- 2.** The DOE CCPP and NSF Climate and Large Scale Dynamics (CLD) programs are jointly sponsoring Small Grants for Exploratory Research (SGER) applications for exploratory research related to model development of the Community Climate System Model (CCSM). Information on the CCSM, including the CCSM Scientific Steering Committee may be found at: <http://www.cesm.ucar.edu/>. These grants are intended for focused research on a particular aspect of CCSM that has received inadequate attention or that has been identified as a gap in understanding/simulation by the relevant CCSM working groups. SGER applications must include a statement about how the research proposed will benefit near-term, high priority CCSM development, being as explicit as possible about the issue(s) that will be addressed by the intended research.

Examples of near-term high priorities are: improving tropical variability simulations including El Niño Southern Oscillation (ENSO); improving the representation of the Arctic Ocean hydrological cycle; testing of aerosol-cloud parameterizations to address the indirect effect of aerosols; and incorporation of terrestrial carbon cycle processes. The research should be designed to ultimately lead to testing of parameterization schemes for potential inclusion in the next version of the CCSM. The request should not exceed \$25,000 and the duration is typically

12-18 months. Larger requests will be considered provided there is strong justification. Contingent on availability of funds, a maximum of 10 awards will be made.

NSF POC: Jay Fein, (703) 292 8527 jfein@nsf.gov BER POC: Anjuli Bamzai, (301) 903 0294 Anjuli.Bamzai@science.doe.gov

Computational Biology: GTL encompasses many types of data, each with algorithm research and development challenges in analyzing data for a broad range of purposes. Examples of objectives include:

- New generation of high-throughput, automated, annotation pipeline tools that keep pace with the exponentially increasing output of current and next-generation sequencing technologies. These tools should conform to current accuracy requirements and be compatible with existing downstream proteomic, expression and systems data formats.
 - New algorithms with improved comparative approaches to annotate organism and community sequences, identifying, for example, promoter and ribosome-binding sites, repressor and activator sites, and operon and regulon sequences.
 - Protein-function inference from sequence homology, fold type, protein interactions, and expression.
 - Automated linkage of gene, protein, and function catalog to phylogenetic, regulatory, structural, and metabolic relationships.
- Identify peptides, proteins, and their post-translational modifications of target proteins in mass spectrometry (MS) data.
 - New MS identification algorithms for tandem MS.
- Quantitate changes in cluster expression data from arrays or MS.
 - New expression data-analysis algorithms.
- Automatically identify interacting protein events in fluorescence resonance energy transfer (FRET) confocal microscopy.
 - New automated processing of images and video to interpret protein localization in the cell and to achieve high-throughput analysis.
- Reconstruct protein machines from 3D cryoelectron microscopy.
 - New automated multi-image convolution and reconstruction algorithms.
- Compare metabolite levels under different cell conditions.
 - Algorithms for metabolite method analysis, both global and with spatial resolution.

Modeling complex biological systems will require new methods to treat the vastly disparate length and time scales of individual molecules, molecular complexes, metabolic and signaling pathways, functional subsystems, individual cells, and, ultimately, interacting organisms and ecosystems. Such systems act on time scales ranging from microseconds to thousands of years. The systems must couple to huge databases created by an ever-increasing number of high-throughput experiments. Challenges include determining the right calculus to describe regulation, metabolism, protein interaction networks, and signaling in a way that allows quantitative prediction. Possible solutions include use of differential equations, stochastic or deterministic methods, control theory or ad hoc mathematical network solutions, binary or discrete value networks, Chaos theory, and emerging and future new abstractions.

BER POC: John Houghton, (301) 903 8288 John.Houghton@science.doe.gov

Fusion Science: Improved simulation and modeling of fusion systems is essential for achieving the predictive scientific understanding needed to make fusion energy practical. The success of the ITER project strongly depends on the development of such validated predictive capability. Current large scale simulations in fusion plasma science include integrated modeling of electromagnetic wave interactions with plasmas described in the MHD approximation as well as work on understanding the plasma edge. Efforts are also underway in modeling plasma turbulence and macroscopic stability using two-fluid or extended MHD models.

Integrated simulation of magnetic fusion systems involves the simultaneous modeling of the core and edge plasma regions, as well as the interaction of the plasma with material surfaces. In each of these plasma regions, there is transport of heat, particles and momentum driven by plasma turbulence, abrupt rearrangements of the plasma caused by large-scale instabilities, and interactions with neutral atoms and electromagnetic waves. Many of these processes must be computed on short time and spatial scales, while the predictions of integrated modeling are needed for the entire device on longer time scales. This mix of physical complexity and widely differing spatial and temporal scales in integrated modeling, results in a unique computational challenge.

In addition, the further development of collaborative technologies is critical to the success of the Fusion Energy Sciences program. Such fusion collaboratories will be essential to fully exploit present and future facilities, especially since the international fusion community is moving toward fewer and larger machines, such as ITER, and large scale integrated simulations.

Applications to be funded under this announcement should focus on:

- Efforts to further develop and facilitate international fusion collaboratories since international cooperation is of increasing importance for Fusion Energy Sciences.
- The development of an integrated software environment for multi-physics, multi-scale simulations of fusion systems, including the algorithms, software methodology, and framework for designing, building, and validating the software components needed for comprehensive plasma simulations.

OFES POC: Rostom Dagazian (301)-903-4926 Rostom.Dagazian@science.doe.gov

Groundwater Reactive Transport Modeling and Simulation: Scientifically rigorous models of subsurface reactive transport that accurately simulate contaminant mobility across multiple length scales remain elusive. The Department of Energy has long-term clean-up and management responsibility for its Cold War era production facilities, and the responsibility for monitoring the behavior of contaminants in ground waters around existing and future waste disposal and storage areas. Conceptual model development and computer simulation of contaminant transport are important elements of the decision-making process for environmental remediation and monitoring. Innovative, new approaches to performing multi-physics, multi-phase, multi-component, multi-dimensional subsurface reactive flow and transport simulations

that take advantage of high performance, " leadership class" computing capabilities are sought. Specific areas of potential interest include:

- Computational methods exploring efficient means of solving very large systems of equations, inherent in subsurface reactive transport modeling, on high performance computers.
- Incorporation of methods of model abstraction, parameter sensitivity and uncertainty analyses into high performance computer simulations of subsurface reactive transport.
- Incorporation of characterization data from field measurement techniques such as seismic geophysical analyses or, at a smaller scale, high resolution laboratory measurement techniques into computational models.
- Methods exploring optimal hardware architecture and, optimal conceptual and computational model complexity for subsurface reactive transport simulation.
- Computational methods examining the scalability ("upscaling"), spatial variability and temporal variability of biogeochemical reactions occurring at the molecular level to the field scale.
- Development of parallel programming and output visualization tools enabling subsurface scientists to more easily access and utilize the high performance computing assets within DOE.

Simulation of subsurface reactive transport processes on high performance, "leadership class" computers has not been widely utilized by subsurface scientists or environmental managers responsible for remediation decision-making. The intent of this call is to explore what options "leadership class" computing can bring to the understanding of subsurface reactive transport of fluids and contaminants and to foster collaborations among subsurface scientists and computational scientists in order to facilitate use of these high performance computing assets for environmental applications.

BER POC: Robert T. Anderson, (301) 903 5549 Todd.Anderson@science.doe.gov

High-Energy Physics: SciDAC supports cross-disciplinary research into cutting-edge problems in scientific computing. As pioneers in the computing sciences since their inception, HEP researchers are fully committed to continuing to advance the state of the art of scientific computing and applying the most modern techniques and tools to our work.

The HEP mission has three research thrusts The Energy Frontier (i.e., testing and refining our understanding of the standard model), The Dark Universe (i.e., investigating the nature of dark energy, dark matter, and the origins of the cosmos), and Neutrinos (i.e., measuring the properties and behavior of this unique family of particles). Each of these domains faces different computational and data management challenges, many of which are ideally suited to the SciDAC program of work.

To fully realize our scientific goals and make the most effective use of the large facilities and collaborations which characterize the current generation of HEP research, we will need simulation, data management, and data analysis and visualization applications which run on a wide variety of computer architectures, from commodity clusters to specialized machines to

supercomputers and which are easily accessible to researchers at small universities, as well as large National Laboratories

HEP POC: Craig Tull, (301)-903-0468 Craig.Tull@science.doe.gov

High Energy and Nuclear Physics with Petabytes: High energy physics and nuclear physics experiments stand at the threshold of revolutionary challenges and opportunities. Experiments at colliding beams and the next generation of fixed targets are key to the advancing the understanding of the physics or the universe on the smallest length and time scales, and at the level at which the fundamental particles transition into matter.

With the next generation of physics accelerators and detectors, instruments with an analog data rate of a petabyte a second will yield petabytes per year after data selection and compression. Even with this high degree of selectivity, revolutionary new approaches to data management and data analysis are needed to allow scientific intuition and intellect deal with the daunting volume of data. This notice seeks applications that address the data intensive research challenges of high energy physics and nuclear physics, including the production environment for distributed data-intensive science, and provide innovative approaches to data analysis environments characterized by having tens to hundreds of scientists simultaneously accessing refined datasets of tens of terabytes.

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Materials Science & Chemistry: Materials science and chemistry remain key research areas for the National Nuclear Security Administration. Understanding and accurately modeling material properties, reactions, and interactions, and doing so on length scales that range in excess of 10 orders of magnitude, is integral to the program. This includes the development of improved simulation methods for complex quantum systems enabled by developing supercomputer technology. The Advanced Simulation and Computing (ASC) program is interested in research in this area that can be applied to the computer modeling of materials.

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Nuclear Physics: Increased computational resources, algorithmic development and a coherent petascale effort spanning all of nuclear structure and reactions are important for the advancement of nuclear physics, including nuclear astrophysics, neutrino physics and fundamental symmetries. Nuclear structure and reactions play an essential role in the science to be investigated at the Rare Isotope Accelerator (RIA) and in nuclear physics applications to the Science-Based Stockpile Stewardship (SBSS) program and other DOE mission needs, such as energy research and threat reduction. Future theory progress on the equation of state of the quark-gluon plasma and the evaluation of the dynamics of the reaction observed at the Relativistic Heavy Ion Collider (RHIC) can be advanced through significant increase of the computational and algorithmic development needed to solve relativistic radiative transport and covariant second order dissipative hydrodynamics equations on this terascale level.

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Quantum Chromodynamics (QCD): The goal of the SciDAC program in QCD is to create opportunities for major scientific advances through highly accurate simulations of the lattice gauge theory. The physics issues to be addressed include calculations of matrix elements needed for precise tests of the standard model, determination of the properties of strongly interacting matter under extreme conditions of temperature and density, the internal structure of nucleons and other strongly interacting particles, and QCD calculations of hard-to-measure baryon-baryon interactions needed for low energy nuclear and hypernuclear physics. Major improvements in lattice calculations will be driven by improvements in computer hardware, software environments, algorithms, and theoretical formulations of QCD. As well, the regular structure of lattice calculations has made them amenable to efficient execution on specially designed computers whose design echoes that regularity. The enormous amount of computation needed to achieve meaningful physics results has made the cost effectiveness of such computers a necessity.

A major accomplishment of the SciDAC 1 QCD program was the development of a unified programming environment that has enabled the U.S. lattice gauge community to achieve high efficiency on a wide variety of terascale computers. The platform exploits the special features of QCD calculations which made them particularly well suited to massively parallel computers. This interface now underpins QCD calculations on MPP machines, such as Seaborg at NERSC, specialized machines such as the QCDOC at BNL, and the commodity clusters being built at FNAL and JLab. The software infrastructure includes tools to archive and retrieve files annotated with XML metadata consistent with the newly created International Lattice Data Grid.

There are many possible directions for further progress. One immediate need, to advance these important calculations in High Energy and Nuclear Physics, is adapting the current simulation environment to additional hardware architectures, such as cluster computers based on multi-core chips or the IBM Blue Gene/L. Another is enhancing the simulation environment both to execute the best existing codes with higher performance and to facilitate the rapid development and evaluation of new algorithms and methods.

The data sets generated by realistic lattice simulations are large enough so that new software tools are needed to manage them and access to them to ensure that their physics potential is most effectively exploited. As well, new tools are needed to visualize the increasingly complex data analyses being applied to the results of these calculations.

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Radiation Transport: Determining the processes and interactions of radiation transport is an extremely complex proposition. To date we have been limited both in our scientific understanding and our computational resources. Without the compute power to move beyond diffusion methods to Monte Carlo or discrete ordinate multi-particle, multi-group transport

methods, those using as few approximations as possible, we cannot fully investigate transport, or resulting energy deposition, of radiation.

In weapons, as in other complex systems, such as engines and reactors, transport is a key element of the coupled, multi-physics present. The development of models and codes capable of realistically dealing with radiation in 2 and 3D is critical to the predictive capability of the codes and therefore the confidence we place in the computational results upon which decisions are based.

The Advanced Simulation and Computing (ASC) program and the Office of Science are interested in research in this area that can be applied to the computer modeling of transport.

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Turbulence: The development of models and codes that can incorporate the exact equations governing the Reynolds stresses, and which predict dynamic instabilities are still sought. Presently, Large Eddy Simulation (LES) methods, viscosity modeling methods, and fluid approximation model methods stand at the forefront of our ability to model turbulent flow. However, the physics of turbulence, and the mathematical and computational representation of that physics are still open research areas that require ongoing effort. The Advanced Simulation and Computing (ASC) program is interested in research in this area that can be applied to the computer modeling of turbulence.

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3. Enabling Computational Technologies

The key to the success of the SciDAC program has been the power of multidisciplinary teams that bring together experts in the scientific discipline, computer science, and applied mathematics. Multidisciplinary teams have achieved progress that could not have been made in any other way. It is increasingly hard for a small team of experts in a single area to develop a state-of-the-art simulation code that uses the latest mathematical algorithms and runs effectively on today's complex computer architectures. Successes to-date have relied on new infrastructure in applied mathematics, computer science, and distributed computing technology. This program element has several dimensions. It must provide the following:

- Comprehensive, integrated, scalable, and robust high performance computing software infrastructure to enable effective use of leadership class computing resources.
- Comprehensive, integrated, scalable, and robust distributed computing technologies for experimental facilities and science.
- Targeted efforts to integrate advanced applied mathematics and computer science technologies into selected applications projects.

All applications must include a plan for supporting their software over the long term. All applications must also include a plan for developing partnerships with science applications.

The framework for accomplishing these objectives includes, but is not limited to, Centers for Enabling Technologies (CET), Science Institutes, and Partnerships. Centers for Enabling Technologies are large teams centered around developing software infrastructure with a specific focus, such as performance analysis or advanced tools for differential equations. SciDAC Institutes are university-led and are complementary to the CETs, addressing additional dimensions as discussed below. For example, there could be an Institute centered around large scale optimization for engineering problems. Finally, Partnerships provide support to integrate computational science with discipline-driven applications. Applications to this notice can request funding for any one of these three elements, however, requests for Partnerships must be included with requests for support under science domain topics.

Centers for Enabling Technologies: Centers for Enabling Technologies (CET) address the Mathematical and Computing Systems Software Environment element of the SciDAC Scientific Computing Software Infrastructure. This infrastructure envisions a comprehensive, integrated, scalable, and robust high performance software environment, which overcomes difficult technical challenges to enable the effective use of terascale and petascale systems by SciDAC applications. CETs address needs for: new algorithms which scale to parallel systems having hundreds-of-thousands of processors; methodology for achieving portability and interoperability of complex high performance scientific software packages; operating systems and runtime tools and support for application execution performance and system management; and effective tools for feature identification, data management and visualization of petabyte-scale scientific data sets.

CETs also address the Distributed Science Software Environment element of the SciDAC Scientific Computing Software Infrastructure. This infrastructure recognizes the use of advanced computing technologies to improve experimental science, as well as accelerate scientific discovery through modeling and simulation. This can be accomplished through the development and application of advanced data and analysis capabilities, computation in support of experiment, and technologies for the automation of experiments.

CETs provide the essential computing and communications infrastructure for support of SciDAC applications. The CET effort encompasses a multi-discipline approach with activities in:

- Algorithms, methods, and libraries -- Algorithms, methods and libraries that are fully scalable to many thousands of processors with full performance portability.
- Program development environments and tools -- Component-based, fully integrated, terascale and petascale program development and tools, which scale effectively and provide maximum utility and ease-of-use to developers and scientific end users.
- Operating system and runtime software and tools -- Systems software that scales to hundreds-of-thousands of processors, supports high performance application-level communication, I/O, performance analysis and optimization, and provides the highest levels of fault tolerance, reliability, manageability, and ease of use for end users, tool developers and system administrators.
- Visualization and data management systems -- Scalable, intuitive systems fully supportive of SciDAC application requirements for moving, storing, analyzing, querying, manipulating and visualizing multi-petabytes of scientific data and objects.

- Distributed data management and computing tools - Scalable and secure systems for the analysis of large volumes of data produced at experimental facilities, often through complex workflows, and consumed by a large and distributed user community, as well as end-to-end network tools and services to support high-end applications.
- Real-time computing at experimental facilities

The complexity of these challenges and the strong emphasis on scalability, interoperability and portability requires novel approaches in the proposed technical research and the research management structure. CETs emphasize working directly with applications and the support of application partnerships to enable:

- Development and application of mathematical and/or computing systems software that allows scientific simulation codes to take full advantage of the extraordinary capabilities of terascale and petascale computers.
- Close working relationships with application teams and other SciDAC teams to ensure that the most critical computer science and applied mathematics issues are addressed in a timely and comprehensive fashion.
- Addressing all aspects of the successful research software lifecycle including transition of a research code into a robust production code and long term software evolution and maintenance and end user support. *The software lifecycle must be addressed in all CET applications.*

In order to foster broad availability and use of CET-developed code, all CET applications must specify the type of open source license that will be used and the mechanisms, including web sites, workshops, and other community-based activities that will be used to disseminate information about CET software.

SciDAC Institutes: Science and engineering are critically dependent on the existence of robust and reliable high-performance computing applications codes. These application codes are in turn critically dependent on the algorithms and software developed by the high-performance computer science community. The SciDAC Institutes are university-led centers of excellence intended to complement the efforts of the Centers for Enabling Technologies, as well as centers formed under-specific science domains. This will be achieved by focusing on major software issues through a range of collaborative research interactions. Applications are sought on software methods or techniques that are important to a number of specific science problems.

Characteristics of a SciDAC Institute are that it may:

- Concentrate efforts to develop, test, maintain, and support optimal algorithms, programming environments, systems software and tools, and applications software.
- Focus on a single general method or technique(for example, large scale optimization for engineering problems).
- Be a focal point for bringing together a critical mass of leading experts from multiple disciplines to focus on key problems in a particular area of enabling technologies.
- Forge relationships between experts in software development, scientific application domains, high performance computing, and industrial partners (e.g., a "Computational

End Station" allowing computational scientists to improve and utilize community codes where coordination around integrated modeling strategies, algorithms and specialized suites of software tools is important for success).

- Reach out to engage a broader community of scientists in the activities of scientific discovery through advanced computation and collaboration.
- Have a dimension of training and outreach in high performance computing topics, including for graduate students and postdocs.
- Scientific applications that sufficiently integrate the above will be considered for award.

Applications may include scope to ensure that SciDAC tools are robust and widely available on diverse platforms through building and supporting test environments, coordination of software releases, and implementation of mechanisms to facilitate porting and tuning.

Applications should describe the organizational model which might be: 1) part of a university, 2) a separate organization, like a non-profit corporation, or 3) a university-led distributed center involving multiple institutions, that may include other universities, industry, non-profit organizations, Federal Laboratories and Federally Funded Research and Development Centers (FFRDCs), which include the DOE National Laboratories.

Partnerships: The major source of progress in simulation-based science depends upon the strength and depth of partnerships among application domains, computer science, and applied mathematics. Scientific Application Partnerships offer support for this type of multidisciplinary interaction.

Science Application Partnerships (SAP or Partnerships) are a broad activity of the Office of Advanced Scientific Computing Research (ASCR) formed when applied mathematics and computer science research can significantly enhance a targeted science area of importance to SC. Funding for these Partnerships is shared between ASCR and the other SC offices along with oversight responsibilities. Thus SAP projects must have components relevant to each office that is involved. This SciDAC program element seeks to fund activities that form a partnership between computational mathematics and computer science with a science domain.

Thus applications submitted under Section 2. Science Applications may identify specific, targeted activities to be considered for funding as Scientific Application Partnerships. The SAP projects are to be managed by a single lead PI and Institution and should identify the other Investigators as "Application Science (S)", "Applied Mathematics (M)" or "Computer Science (CS)". It is envisioned that SAP projects will demonstrate a balance between S and M/CS personnel.

The key elements and characteristics expected for science applications projects are:

- Focus on a targeted application science area that lies within the scope of topics listed in Section 2 under Science Applications.
- Leverage for inserting existing or new applied mathematics and computer science research into an identified science area to enable or otherwise significantly enhance the

field. It may provide the insertion of new technologies directly into application codes or explore new programming and/or modeling methodology for petascale applications.

- It may involve collocation of computational mathematicians and computer scientists with application teams. These individuals may also act as liaisons to foster interactions with CETs.
- A cohesive project with a shared goal. Each institution and investigator must clearly identify their contribution towards this goal. Projects that appear disjoint in this regard are discouraged.

Potential partnership activities should be clearly identified in a Science Application submission, and the requested funding for partnership efforts in computer science and applied mathematics should be included with the other project costs on the Budget Page. However, applications should also provide the requested computer science and applied mathematics costs separately in an appendix in order to be considered for support by the Office of Advanced Scientific Computing Research under a partnership agreement.

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Collaborative Applications

It is expected that the majority of applications submitted in response to this notice will be for scientific simulation teams involving more than one institution. Other institutions may be universities, industry, non-profit organizations, Federal Laboratories and Federally Funded Research and Development Centers (FFRDCs), which include the DOE National Laboratories. Collaborative applications focused on a single research activity submitted in response to this notice (i.e., applications involving more than one institution) should be submitted as described below. The research activity should be given a title that is used by all submitting institutions.

- Each university, industrial organization, and non-profit organization involved in a proposed collaborative research project must submit a separate application in PDF format to grants.gov, and each application must include a common technical description of the overall research activity.
- A lead Principal Investigator (PI) must be identified who has overall coordination responsibility for the integrated research activity--the lead PI's institution is referred to as the lead institution. The applications from the collaborating institutions must each identify a Co-PI who is responsible for the part of the research to be carried out at his/her institution.
- In addition to the common technical description of the overall project, each application must include a separate set of application forms for the institution. Each application must also contain an appendix with a 1-2 page summary of the tasks and milestones to be completed by the institution submitting the application. The description of these tasks and milestones must be sufficiently clear that it is obvious how they relate to the common technical description of the overall research project.

Synergistic collaborations with researchers in Federal Laboratories and Federally Funded Research and Development Centers (FFRDCs), including the DOE National Laboratories are encouraged, though no funds will be provided to these organizations under this Notice. A separate Laboratory solicitation will be posted. Additional information regarding the submission of a collaborative application can be accessed via the web at:

<http://www.science.doe.gov/grants/Colab.html>.

Program Funding

It is anticipated that in Fiscal Year 2006 SciDAC partners will have up to approximately \$36,000,000 available to support new SciDAC projects. The number of awards will be determined by the number of excellent applications and the total funds available for this program, and subject to the availability of funds. These funds provided by participating offices may be up to the following: ASCR, \$25,000,000; BER, \$2,250,000; FES, \$1,000,000; NNSA, \$4,000,000; NP; \$1,000,000; and HEP, \$2,000,000.

Awards are anticipated to fall in four categories-science applications, Centers for Enabling Technologies, Institutes, and Scientific Application Partnerships. (Note: The funding range provided below are for guidance only. Meritorious applications requesting funding outside the suggested range will receive full consideration). Science Applications may be funded from \$200,000 up to \$800,000 per year for two to five years. Most of these are expected to be teams with two or more institutions participating, each receiving from \$50,000 up to \$300,000 per year. Centers for Enabling Technologies are expected to be large distributed teams and may be funded at \$1,500,000 to \$3,000,000 per year for up to five years. SciDAC Institutes are expected to be funded at \$1,000,000 to \$2,500,000 per year for up to five years. In both cases, participating institutions may be funded at from \$50,000 to \$300,000 per year. Scientific Application Partnerships are expected to be funded at \$50,000 to \$500,000 per year for one to three years.

Merit Review

After an initial screening for eligibility and responsiveness to the solicitation, 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,
- 4) Reasonableness and Appropriateness of the Proposed Budget.

In considering item 1 particular attention will be paid to:

- a) The potential of the proposed project to make a major scientific advance in a specific domain or to have a significant impact in the effectiveness of SciDAC applications researchers;
- b) The demonstrated capabilities of the applicants to perform basic research and transform these research results into software that can be widely deployed;
- c) Knowledge of and coupling to previous efforts in scientific simulation;

- d) For enabling technology applications, the likelihood that the algorithms, methods, mathematical libraries, and software components that result from this effort will have impact on or is extensible to science disciplines outside of the SciDAC applications projects;
- e) Identification and approach to software integration and long term support issues, including component technology, documentation, test cases, tutorials, end user training, and quality maintenance and evolution; and
- f) Extent to which the application incorporates broad community (industry/academia/other federal programs) interaction;

In considering item 2, particular attention will be paid to

- a) Quality of the plan for effective coupling to emerging advances in enabling technology or to applications researchers;
- b) Quality and clarity of the proposed work schedule and deliverables;
- c) Quality of the proposed approach to intellectual property management and open source licensing;
- d) Quality of the plan for effective collaboration among participants; and
- e) Quality of the plan for ensuring communication with other advanced computation and simulation efforts or enabling technology efforts.

The evaluation 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.

External peer reviewers are selected with regard to both their scientific expertise and the absence of conflict-of-interest issues. Non-federal reviewers will often be used, and submission of an application constitutes agreement that this is acceptable to the investigator(s) and the submitting institution. Reviewers will be selected to represent expertise in the science and technology areas proposed, applications groups that are potential users of the technology, and related programs in other Federal Agencies or parts of DOE.

Submission Information

Information about the development and submission of applications, eligibility, limitations, evaluation, selection process, and other policies and procedures including detailed procedures for submitting applications from multi-institution partnerships may be found in 10 CFR Part 605, and in the Application Guide for the Office of Science Financial Assistance Program. Electronic access to the Guide and required forms is made available via the World Wide Web at: <http://www.science.doe.gov/grants/grants.html>. The research plan for the project must be 20 pages or less, including tables and figures, but exclusive of attachments. The application must contain an abstract or project summary, letters of intent from collaborators, current and pending support, and short vitae.

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

Martin Rubinstein
Director

Grants and Contracts Division
Office of Science

Posted on the Office of Science Grants and Contracts Web Site
December 23, 2005.

1 -- Copies of the SC computing plan, Scientific Discovery through Advanced Computing, can be downloaded from the SC website at: <http://www.osti.gov/scidac/>.