Program Announcement
To DOE National Laboratories
LAB 06-04

Scientific Discovery through Advanced Computing

SUMMARY: The Office of Science (SC), U.S. Department of Energy (DOE), hereby announces interest in receiving peer-reviewable Field Work Proposals (FWPs) for projects in the Scientific Discovery through Advanced Computing (SciDAC) research program. 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 the emerging petaascale 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 Announcement is seeking proposals 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.

Proposals 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 researchers should observe that the program is structured to be interdisciplinary and multi-institutional in nature.

Synergistic collaborations are encouraged. Collaborative proposals involving multiple institutions, that may include universities, laboratories, and/or private institutions, are anticipated for the majority of submissions. Researchers may request a period of performance of up to five (5) years.

DATES: Potential researchers 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 proposals, 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 proposals will be communicated to the researchers by January 30, 2006.

Full proposals submitted in response to this Annoucement must be submitted to the DOE Electronic Proposals Management Applications (e PMA) system (https://epma.doe.gov) no later than 8:00 pm, Eastern Time, **March 6, 2006**, to be accepted for merit review and to permit timely consideration for award in Fiscal Year 2006. It is important that the entire peer reviewable proposal be submitted to the ePMA system as a single PDF file attachment.

Please see the "Addresses" section below for futher instructions on the methods of submission for the full proposal.

ADDRESSES: Letters-of-Intent should be submitted electronically as an email attachment (not pdf) to scidac-2_lab@mics.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.

Peer-reviewable Field Work Proposals submitted to the Office of Science must be submitted electronically as a pdf file by March 6, 2006 to be considered for award. The email submission to scidac-2_lab@mics.doe.gov should use the phrase "SciDAC Science Application" or "SciDAC Enabling Technology," as appropriate, in the subject line.

A complete formal FWP in a single Portable Document Format (PDF) file must be submitted through the DOE ePMA system (https://epma.doe.gov) as an attachment. To identify that the FWP is responding to this program announcement, please fill in the following fields in the "ePMA Create Proposal Admin Information" screen as shown:

> **Proposal Short Name:**
> **Fiscal Year:**
> **Proposal Reason:**
> **Program Announcement Number:** Lab 06-04 *
> **Program announcement Title:** Scientific Discovery through Advanced Computing *
> **Proposal Purpose:**

Estimated Proposal Begin Date:
HQ Program Manager Organization:

* Please use the wording shown when filling in these fields to identify that the FWP is responding to this program announcement.

FOR FURTHER INFORMATION CONTACT: Walt Polansky, Mary Anne Scott, or Dave Goodwin, Office of Advanced Scientific Computing Research, Telephone (301) 903-5800; e-mail: 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 proposals 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 to a hybrid of packet switched services and high bandwidth circuit switched services, perhaps directly over wavelengths. It is anticipated that some proposals 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 Proposals

This announcement requests proposals in the Science Application areas discussed in Section 2 and in the Enabling Technologies areas discussed in Section 3.

Successful researchers 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 researchers 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 $31,000,000 will be available for 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 a proposal. DOE reserves the right to fund, in whole or in part,

any, all, or none of the proposals submitted in response to this announcement.

The following two sections are offered to provide background in-depth information on areas that are of interest to the Office of Science 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 US 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. *Proposals 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. Proposals 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 Quadrapole (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.

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Astrophysics: Computational astrophysics encompasses many research areas of interest and relevance to high-energy physics, nuclear physics, and Advanced Simulation and Computing. SciDAC proposals 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 proposals 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.

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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 SciDAC 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 are accelerating improved representation of key processes in the current version of high-end climate models; accelerating development of frameworks that will test the above representations in the fully coupled system; and running the fully coupled climate model efficiently on high- performance scientific supercomputers that are either available for DOE researchers, or being envisaged under the Leadership Computing Facility at ORNL.

Themes in this call include:

1. Construction of innovative model integration and evaluation frameworks to more rapidly introduce and test ideas and approaches proposed to improve existing state-of-the-science climate models. There are emerging representations and parameterizations of processes to be considered for potential inclusion in the next generation of models, *e.g.* aerosol indirect effect, cloud microphysics, dynamic vegetation, ocean biogeochemistry and atmospheric chemistry. Testing these in an efficient framework is crucial in determining which schemes are viable for inclusion in next-generation coupled earth system models. The intent is to increase dramatically the accuracy of computer model-based projections of future climate system response to the increased atmospheric concentrations of greenhouse gases.

2. Development and testing of approaches to advance global carbon cycle models and to couple the physical climate system with the global carbon cycle. The purpose of adding the carbon cycle is to progress beyond the specification of atmospheric carbon dioxide concentrations - such as e.g. in the ongoing Intergovernmental Panel for Climate Change Fourth Assessment (IPCC AR4) - to the specification of actual anthropogenic emissions, and modeling the fate of emissions through feedbacks between the carbon cycle and the climate. A fully coupled carbon-climate model is an essential tool that would help answer strategic questions related to DOE's climate change research mission objectives (

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3. Effort aimed at computational performance and adaptation to new computer architectures of climate models; improved formulations and algorithms for all component models; and coupled model integration, testing and evaluation. As the science advances and new knowledge is gained, there is a demand to include more process representations into the models and to improve acknowledged shortcomings in existing process descriptions. This demand is likely to overwhelm even the most optimistic projections of computer power increases. Accordingly, there is a need to evaluate the costs, benefits and trade-offs required to allocate scarce computer and human resources to determine which improvements to include in the next generation of climate models. The intent is to increase dramatically the throughput of computer model-based predictions of future climate system response to the increased atmospheric concentrations of greenhouse gases.

DOE laboratory researchers are strongly encouraged to collaborate with researchers in other DOE laboratories and institutions, where appropriate, and to include cost sharing wherever feasible.

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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.

Proposals 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.

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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.

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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 face 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.

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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 proposals 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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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 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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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 proposals must include a plan for supporting their software over the long term. All proposals 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. Proposals 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.

<u>Centers for Enabling Technologies</u>: 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; and
- 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 proposals.*

In order to foster broad availability and use of CET-developed code, all CET proposals 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. Proposals 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.

Proposals 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.

Proposals 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 offers 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 proposals 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 or the collocation of domain scientists with teams of mathematicians and computer scientists. Such 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 proposal, 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, <u>applications/proposals should also provide the requested computer science and applied mathematics costs separately in an appendix</u> in order to be considered for support by the Office of Advanced Scientific Computing Research under a partnership agreement.

ASCR POCs: Anil Deane (301) 903-1465 deane@mics.doe.gov; Thomas Ndousse (301) 903- 9960 tndousse@er.doe.gov; Fred Johnson (301) 903-3601 fjohnson@er.doe.gov; Gary Johnson (301) 903- 4361 garyj@er.doe.gov; Mary Anne Scott (301) 903-6368 scott@er.doe.gov; Yukiko Sekine (301) 903-5997 yukiko.sekine@science.doe.gov

Collaborative Proposals

It is expected that the majority of proposals 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 proposals focused on a single research activity submitted in response to this notice (i.e. proposals involving more than one institution) should be submitted as described below:

- 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. Each laboratory must submit a peer-reviewable field work proposal (as described below) in PDF format to scidac-2_lab@mics.doe.gov . Each application or FWP must include a common technical description of the overall research activity.
- The research activity should be given one common title and that title should be used by all submitting institutions.
- 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 FWP must include a separate Field Work Proposal (FWP) Format Cover Page (Reference DOE Order 5700.7C), Budget Page (DOE F 4620.1). Each proposal must also contain an appendix with a 1-2 page summary of the tasks and milestones to be completed by the institution submitting the proposal. 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.
- The lead institution must separately submit a complete proposal in a single PDF file that identifies and contains the common technical description of the overall project and a summary budget for the entire project, including the annual funding proposed for each institution. In addition, this proposal must contain the Cover Pages (SF 424 R&R) and Budget Pages (DOE F 4620.1) for each institution involved in the project. The cover page and budget pages for the lead institution should be included in the front of the proposal, and the cover pages and budget pages of the other institutions should be included in the first appendix. Finally, this complete proposal must include a 1-2 page summary of the tasks and milestones for each collaborating institution in the second appendix.

Synergistic collaborations with researchers in federal laboratories and Federally Funded Research and Development Centers (FFRDCs), including the DOE National Laboratories are encouraged. 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 $31,000,000 available to support new SciDAC projects. The number of awards will be determined by the number of excellent proposals, the total funds available for this program and the availability of appropriated funds. These funds provided by participating offices may be up to the following: ASCR, $20,000,000; BER, $6,000,000; FES, $1,000,000; NP, $1,000,000; and HEP, $5,000,000.

Awards are anticipated to fall in four categories-Science Applications, Centers for Enabling Technologies, Institutes, and Scientific Application Partnerships *(Note: The funding ranges provided below are for guidance only. Meritorious proposals 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. Science 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. These funding levels are provided as guidance.

Merit Review

After an initial screening for eligibility and responsiveness to the solicitation, proposals 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:

1. Scientific and/or Technical Merit of the Project,
2. Appropriateness of the Proposed Method or Approach,
3. Competency of the 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 researchers 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 proposal 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 proopsal 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.

The instructions and format described below should be followed. Reference Program Announcement LAB 06-04 on all submissions and inquiries about this program.

<div align="center">

OFFICE OF SCIENCE
GUIDE FOR PREPARATION OF SCIENTIFIC/TECHNICAL PROPOSALS
TO BE SUBMITTED BY NATIONAL LABORATORIES

</div>

Proposals from National Laboratories submitted to the Office of Science (SC) as a result of this program announcement will follow the Department of Energy Field Work Proposal process with additional information requested to allow for scientific/technical merit review. The following guidelines for content and format are intended to facilitate an understanding of the requirements necessary for SC to conduct a merit review of a proposal. Please follow the guidelines carefully, as deviations could be cause for declination of a proposal without merit review.

1. Evaluation Criteria

Proposals will be subjected to formal merit review (peer review) and will be evaluated against the following criteria which are listed in descending order of importance:

Scientific and/or technical merit of the project;
Appropriateness of the proposed method or approach;
Competency of the personnel and adequacy of the proposed resources; and
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 researchers 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 proposal 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, the uniqueness of the proposer's capabilities, and demonstrated usefulness of the research for proposals in other DOE Program Offices as evidenced by a history of programmatic support directly related to the proposed work.

2. Summary of Proposal Contents

- Field Work Proposal (FWP) Format (Reference DOE Order 5700.7C) (DOE ONLY)
- Proposal Cover Page
- Table of Contents
- Abstract
- Narrative
- Literature Cited
- Budget (DOE Form 4620.1) and Budget Explanation
- Other Support of Investigator(s)
- Biographical Sketch(es)
- Description of Facilities and Resources
- Appendix

If a collaboration is proposed, please list ALL Collaborating Institutions/PIs and indicate which ones will also be submitting applications or proposals. Also indicate the PI who will be the point of contact and coordinator for the combined research activity. ***The work scope explanation for each participating institution should be included in the appendix***.

2.1 Number of Copies to Submit

A complete formal FWP in a single Portable Document Format (PDF) file must be submitted through the DOE ePMA system (https://epma.doe.gov) as an attachment. To identify that the FWP is responding to this program announcement, please fill in the following fields in the "ePMA Create Proposal Admin Information" screen as shown:

Proposal Short Name:
Fiscal Year:
Proposal Reason:
Program Announcement Number: Lab 06-04 *
Program announcement Title: Scientific Discovery through Advanced Computing *
Proposal Purpose:
Estimated Proposal Begin Date:
HQ Program Manager Organization:
* Please use the wording shown when filling in these fields to identify that the FWP is responding to this program announcement.

A completed formal FWP in a single Portable Document Format (PDF) file referencing Program Announcement LAB 06-04 must be submitted via email to scidac-2_lab@mics.doe.gov.

3. Detailed Contents of the Proposal

Proposals must be readily legible, when photocopied, and must conform to the following three requirements: the height of the letters must be no smaller than 10 point with at least 2 points of spacing between lines (leading); the type density must average no more than 17 characters per inch; the margins must be at least one-half inch on all sides. Figures, charts, tables, figure legends, etc., may include type smaller than these requirements so long as they are still fully legible.

3.1 Field Work Proposal Format (Reference DOE Order 5700.7C) (DOE ONLY)

The Field Work Proposal (FWP) is to be prepared and submitted consistent with policies of the investigator's laboratory and the local DOE Operations Office. Additional information is also requested to allow for scientific/technical merit review. Laboratories may submit proposals directly to the SC Program office listed above. A copy should also be provided to the appropriate DOE operations office.

3.2 Proposal Cover Page

The following proposal cover page information may be placed on plain paper. No form is required.

Title of proposed project
SC Program announcement title
Name of laboratory
Name of principal investigator (PI)
Position title of PI
Mailing address of PI
Telephone of PI
Fax number of PI
Electronic mail address of PI
Name of official signing for laboratory*
Title of official

Fax number of official
Telephone of official
Electronic mail address of official
Requested funding for each year; total request
Use of human subjects in proposed project:
> If activities involving human subjects are not planned at any time during the proposed project period, state "No"; otherwise state "Yes", provide the IRB Approval date and Assurance of Compliance Number and include all necessary information with the proposal should human subjects be involved.

Use of vertebrate animals in proposed project:
> If activities involving vertebrate animals are not planned at any time during this project, state "No"; otherwise state "Yes" and provide the IACUC Approval date and Animal Welfare Assurance number from NIH and include all necessary information with the proposal.

Signature of PI, date of signature
Signature of official, date of signature*

*The signature certifies that personnel and facilities are available as stated in the proposal, if the project is funded.

3.3 Table of Contents

Provide the initial page number for each of the sections of the proposal. Number pages consecutively at the bottom of each page throughout the proposal. Start each major section at the top of a new page. Do not use unnumbered pages and do not use suffixes, such as 5a, 5b.

3.4 Abstract

Provide an abstract of no more than 250 words. Give the broad, long-term objectives and what the specific research proposed is intended to accomplish. State the hypotheses to be tested. Indicate how the proposed research addresses the SC scientific/technical area specifically described in this announcement.

3.5 Narrative

The narrative comprises the research plan for the project and is limited to 5 pages per task. It should contain the following subsections:

Background and Significance: Briefly sketch the background leading to the present proposal, critically evaluate existing knowledge, and specifically identify the gaps which the project is intended to fill. State concisely the importance of the research described in the proposal. Explain the relevance of the project to the research needs identified by the Office of Science. Include references to relevant published literature, both to work of the investigators and to work done by other researchers.

Preliminary Studies: Use this section to provide an account of any preliminary studies that may be pertinent to the proposal. Include any other information that will help to establish the experience and competence of the investigators to pursue the proposed project. References to appropriate publications and manuscripts submitted or accepted for publication may be included.

Research Design and Methods: Describe the research design and the procedures to be used to accomplish the specific aims of the project. Describe new techniques and methodologies and explain the advantages over existing techniques and methodologies. As part of this section, provide a tentative sequence or timetable for the project.

Subcontract or Consortium Arrangements: If any portion of the project described under "Research Design and Methods" is to be done in collaboration with another institution, provide information on the institution and why it is to do the specific component of the project. Further information on any such arrangements is to be given in the sections "Budget and Budget Explanation", "Biographical Sketches", and "Description of Facilities and Resources".

3.6 Literature Cited

List all references cited in the narrative. Limit citations to current literature relevant to the proposed research. Information about each reference should be sufficient for it to be located by a reviewer of the proposal.

3.7 Budget and Budget Explanation

A detailed budget is required for the entire project period, which normally will be three years, and for each fiscal year. It is preferred that DOE's budget page, Form 4620.1 be used for providing budget information*. Modifications of categories are permissible to comply with institutional practices, for example with regard to overhead costs.

A written justification of each budget item is to follow the budget pages. For personnel this should take the form of a one-sentence statement of the role of the person in the project. Provide a detailed justification of the need for each item of permanent equipment. Explain each of the other direct costs in sufficient detail for reviewers to be able to judge the appropriateness of the amount requested.

Further instructions regarding the budget are given in section 4 of this guide.

* Form 4620.1 is available at web site: http://www.science.doe.gov/grants/Forms-E.html.

3.8 Other Support of Investigators

Other support is defined as all financial resources, whether Federal, non-Federal, commercial or institutional, available in direct support of an individual's research endeavors. Information on active and pending other support is required for all senior personnel, including investigators at collaborating institutions to be funded by a subcontract. For each item of other support, give the organization or agency, inclusive dates of the project or proposed project, annual funding, and level of effort devoted

to the project.

3.9 Biographical Sketches

This information is required for senior personnel at the institution submitting the proposal and at all subcontracting institutions (if any). The biographical sketch is limited to a maximum of **two pages** for each investigator.

3.10 Description of Facilities and Resources

Describe briefly the facilities to be used for the conduct of the proposed research. Indicate the performance sites and describe pertinent capabilities, including support facilities (such as machine shops) that will be used during the project. List the most important equipment items already available for the project and their pertinent capabilities. Include this information for each subcontracting institution, if any.

3.11 Appendix

Include collated sets of all appendix materials with each copy of the proposal. Do not use the appendix to circumvent the page limitations of the proposal. Information should be included that may not be easily accessible to a reviewer.

Reviewers are not required to consider information in the Appendix, only that in the body of the proposal. Reviewers may not have time to read extensive appendix materials with the same care as they will read the proposal proper.

The appendix may contain the following items: up to five publications, manuscripts (accepted for publication), abstracts, patents, or other printed materials directly relevant to this project, but not generally available to the scientific community; and letters from investigators at other institutions stating their agreement to participate in the project (do not include letters of endorsement of the project).

4. Detailed Instructions for the Budget
(DOE Form 4620.1 "Budget Page" may be used)

4.1 Salaries and Wages

List the names of the principal investigator and other key personnel and the estimated number of person-months for which DOE funding is requested. Proposers should list the number of postdoctoral associates and other professional positions included in the proposal and indicate the number of full-time-equivalent (FTE) person-months and rate of pay (hourly, monthly or annually). For graduate and undergraduate students and all other personnel categories such as secretarial, clerical, technical, etc., show the total number of people needed in each job title and total salaries needed. Salaries requested must be consistent with the institution's regular practices. The budget explanation should

define concisely the role of each position in the overall project.

4.2 Equipment

DOE defines equipment as "an item of tangible personal property that has a useful life of more than two years and an acquisition cost of $25,000 or more." Special purpose equipment means equipment which is used only for research, scientific or other technical activities. Items of needed equipment should be individually listed by description and estimated cost, including tax, and adequately justified. Allowable items ordinarily will be limited to scientific equipment that is not already available for the conduct of the work. General purpose office equipment normally will not be considered eligible for support.

4.3 Domestic Travel

The type and extent of travel and its relation to the research should be specified. Funds may be requested for attendance at meetings and conferences, other travel associated with the work and subsistence. In order to qualify for support, attendance at meetings or conferences must enhance the investigator's capability to perform the research, plan extensions of it, or disseminate its results. Consultant's travel costs also may be requested.

4.4 Foreign Travel

Foreign travel is any travel outside Canada and the United States and its territories and possessions. Foreign travel may be approved only if it is directly related to project objectives.

4.5 Other Direct Costs

The budget should itemize other anticipated direct costs not included under the headings above, including materials and supplies, publication costs, computer services, and consultant services (which are discussed below). Other examples are: aircraft rental, space rental at research establishments away from the institution, minor building alterations, service charges, and fabrication of equipment or systems not available off- the-shelf. Reference books and periodicals may be charged to the project only if they are specifically related to the research.

a. Materials and Supplies

The budget should indicate in general terms the type of required expendable materials and supplies with their estimated costs. The breakdown should be more detailed when the cost is substantial.

b. Publication Costs/Page Charges

The budget may request funds for the costs of preparing and publishing the results of research, including costs of reports, reprints page charges, or other journal costs (except costs for prior or early publication), and necessary illustrations.

c. Consultant Services

Anticipated consultant services should be justified and information furnished on each individual's expertise, primary organizational affiliation, daily compensation rate and number of days expected service. Consultant's travel costs should be listed separately under travel in the budget.

d. Computer Services

The cost of computer services, including computer-based retrieval of scientific and technical information, may be requested. A justification based on the established computer service rates should be included.

e. Subcontracts

Subcontracts should be listed so that they can be properly evaluated. There should be an anticipated cost and an explanation of that cost for each subcontract. The total amount of each subcontract should also appear as a budget item.

4.6 Indirect Costs

Explain the basis for each overhead and indirect cost. Include the current rates.

_____
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/.

1