# Program Announcement
# To DOE National Laboratories

# LAB 11-505

# Office of Science
# Office of Advanced Scientific Computing Research

## *Scientific Discovery through Advanced Computing Institutes*

**GENERAL INQUIRES ABOUT THIS LAB ANNOUNCEMENT SHOULD BE DIRECTED TO:**

**Technical/Scientific Program Contact:**

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

**SUMMARY:**

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

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

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

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

One of the primary metrics for the success of the SciDAC Institutes is the extent to which its deliverables are used by application scientists. An equally important metric is the extent to which Institute researchers actively collaborate and leverage their expertise in achieving that success. This Announcement describes the process by which proposals for individual SciDAC Institutes are to be developed, submitted, and merit reviewed. The overall portfolio and management of Institute awards is expected to cover a significant portion of DOE computational science needs on current and emerging computational systems. Although the work of each proposed Institute is not science application-specific, it is likely – for the purposes of this Announcement – to be application-, architecture-, and Institutes-aware.

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

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

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

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

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

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

- **Institute Director -** The SciDAC Institute Director is the Lead Principal Investigator and must be employed by the Lead institution. The SciDAC Institute Director will serve as the primary contact responsible for communications with the DOE Program Officer on behalf of all of the Principal Investigators in the Institute.
- **Principal Investigator -** A Principal Investigator is the individual designated by the research organization and empowered with the appropriate level of authority and responsibility for the proper conduct of the research within that organization. These authorities and responsibilities include the appropriate use of funds and administrative requirements such as the submission of scientific progress reports to DOE. When an organization designates more than one Principal Investigator, it identifies them as individuals who share the authority and responsibility for leading and directing the research, intellectually and logistically.

- **Senior/Key Personnel -** A senior/key person is an individual who contributes in a substantive, measurable way to the scientific/technical development or execution of the project. This definition includes, but is not limited to, the SciDAC Institute Director and the Principal Investigator(s).

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

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

**Letter of Intent**

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

1. Cover sheet containing the name and mailing address of the applicant Lead institution; the planned title of the SciDAC Institute; the estimated annual cost and total cost of the project over the five-year project period; the name, institutional affiliation, e-mail address, and telephone number of the SciDAC Institute Director, Principal Investigator(s), and Senior/Key personnel expected to be involved in the planned application.
2. A one-page overview of the strategic plan for the proposed SciDAC Institute, including the vision, goals and key objectives.
3. A one-page overview of the research plan.

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

**DATES**

Full proposals submitted in response to this Announcement must be received by **May 2, 2011, 11:59 p.m. Eastern Time**, to be accepted for merit review and to permit timely consideration for award in Fiscal Year 2011.

Please see the SUBMISSION section below for further instructions on the method of submission for the proposal.

**SUBMISSION INSTRUCTIONS**

Have your LAB administrator submit the entire LAB proposal and Field Work Proposal (FWP) via Searchable FWP (https://www.osti.gov/fwp). If you have questions about who your LAB administrator is or how to use Searchable FWP, please contact the Searchable FWP Support Center. All submissions and inquiries about this Program Announcement must reference Program Announcement LAB 11-505.

**FOR FURTHER INFORMATION CONTACT:**

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

**SUPPLEMENTARY INFORMATION:**

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

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

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

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

**Basic Energy Sciences (BES)**

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

**Biological and Environmental Research (BER)**

Biological and Environmental Research (BER) supports fundamental, interdisciplinary research to achieve a predictive systems-level understanding of climate change, contaminant fate and transport in complex subsurface environments and systems biology, which requires the organization and integration of diverse interdisciplinary data and models in innovative ways. In particular, BER seeks to develop advanced computer models ranging from molecular to global scales and an ability to connect extremely large datasets from a wide variety of sources with models, which enables more holistic and robust predictions of complex system behavior. For example, both the Community Earth System Model (CESM; http://www.cesm.ucar.edu/) and BER's subsurface science modeling efforts will require the development of new model physics and numerical capabilities, manipulation and analysis of large and diverse data-sets, and frameworks for collaboration. Both also require conceptual and algorithmic frameworks for integrating the wide range of multi-physics over multi-scales that must be employed to provide understanding and prediction as well as innovative frameworks to quantify the uncertainty in prediction resulting from the model and observational uncertainties. Systems biology approaches facilitating genome-enabled, mechanistic descriptions of biological processes into

multidisciplinary, multiscale environmental process models is a unique, key point of the integration for BER programs. Potential SciDAC Institutes and BER science application partnership projects for systems biology should be aware of the Systems Biology Knowledgebase (http://www.sc.doe.gov/ober/kbase_plan.pdf ) efforts to address the enormous data storage, management, access, and utilization challenges for systems biology. Additional information about modeling challenges in the areas of climate, subsurface science, systems biology and BER programs in general can be found at:
http://www.sc.doe.gov/ober/BER_workshops.html and
http://www.sc.doe.gov/ober/ober_top.html

**Fusion Energy Sciences (FES)**

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

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

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

**Collaboration**

Collaborative research projects with other institutions, such as universities, industry, non- profit organizations, and Federally Funded Research and Development Centers (FFRDCs), which include the DOE National Laboratories, are strongly encouraged. Collaborative applications submitted from different institutions, which are directed toward a single SciDAC Institute, should clearly indicate they are part of a proposed collaboration and contain the Abstract for that SciDAC Institute research project. In addition, such proposals must describe the work and the associated budget for the research effort being performed under the leadership of the Principal Investigator at that participating institution. Further information on preparation of collaborative proposals may be accessed via the Internet at: http://www.sc.doe.gov/grants/colab.asp .

**Program Funding**

Awards are expected to be made for a period of five years at a funding level appropriate for the proposed scope, with out-year support contingent on the availability of funds and satisfactory progress. Five-year SC-total funding up to $13,000,000 per year is expected to be available to support the DOE-laboratory and non-DOE-laboratory portions of this FOA subject to appropriation of funds by the Congress. DOE is under no obligation to pay for any costs associated with the preparation or submission of an application. DOE reserves the right to fund, in whole or in part, any, all, or none of the applications submitted in response to this FOA.

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

**MAXIMUM AND MINIMUM AWARD SIZE.**
Proposals requesting less than $150,000 per year are unlikely to be successful collaborators in a SciDAC Institute.

**EXPECTED NUMBER OF AWARDS.**
Approximately 3 to 15 laboratory awards are expected.

**ANTICIPATED AWARD SIZE.**
Award sizes for each collaborating institution are anticipated to range from $150,000 to over $1,000,000 per year.

**PERIOD OF PERFORMANCE.**
Five years is standard. A nonstandard performance period requires additional justification.

**TYPE OF APPLICATION.**
DOE will accept new proposals under this Announcement.

**The instructions and format described should be followed. You must reference Program Announcement LAB 11-505 on all submissions and inquiries about this program.**

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

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 scientific merit review (peer review) and will be evaluated against the following evaluation criteria which are listed in descending order of importance. Included within each criterion are specific questions that the merit reviewers will be asked to consider:

**1)** Scientific and/or technical merit of the project

- Does the proposed research provide the capability to accelerate scientific discovery in areas of strategic importance to DOE?
- Does the research plan contain appropriate performance metrics that will allow progress and contributions to be measured?
- What is the likelihood that the applicant can overcome the key challenges and, as warranted, shift research directions in response to promising advances in basic research?

**2)** Appropriateness of the proposed method or approach

- Does the proposed research employ state-of-the-art approaches and lower the barriers to effectively use leadership-scale computing resources available to DOE researchers?
- Has the applicant identified commonalities in multiple (and different) scientific applications for addressing computational grand challenges and that will enable the Institute to structure its research plan in an efficient manner?

- Does the applicant have a process for leveraging basic research advances from Applied Mathematics and Computer Science?
- Does the applicant have appropriate plans for outreach to the broader computational science community?

**3)** Competency of the applicant's personnel and adequacy of the proposed resources

- Does the applicant have a proven record of success in managing diverse teams of scientific and technical experts and delivering results for advanced computational science research?
- Do the applicant's senior/key personnel have a proven record of research and development in the disciplines needed for success in projects of this complexity and magnitude?
- Are the roles and intellectual contributions of the SciDAC Institute Director, Principal Investigator(s), and each senior/key personnel adequately described?

**4)** Reasonableness and appropriateness of the proposed budget

- Is the applicant's requested budget appropriate?
- Does the requested budget support the applicant's specified management structure in a meaningful way?
- Does the applicant have a process for reallocating funds to address changing priorities?

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

- Potential impact of proposed research activities on SciDAC goals;
- Relation of the proposed research activities to other research efforts supported by ASCR;
- Potential for developing synergies with other SciDAC Institutes;
- Total amount of DOE funds available; and
- A management plan that addresses the organization, communications, and coordination of the Institutes. This plan should include mitigation strategies for foreseeable risks and explain how the Institute will have sufficient flexibility to adapt to changing priorities, challenges, and resources.

**2. Summary of Proposal Contents**

- Field Work Proposal (FWP) Format (Reference DOE Order 412.1A) (DOE ONLY)
- Proposal Cover Page – **Scientific Discovery through Advanced Computing Institutes (LAB 11-505)**
- Table of Contents
- Budget (DOE Form 4620.1) and Budget Explanation
- Abstract (one page)
- Narrative (main technical portion of the proposal, including background/introduction, proposed research and methods, timetable of activities, and responsibilities of key project personnel – 25-page limit
- Literature Cited
- Biographical Sketch(es)

- Description of Facilities and Resources
- Other Support of Investigator(s)
- Appendix (optional)

### 2.1 Submission Instructions

Have your LAB administrator submit the entire LAB proposal and FWP via Searchable FWP (https://www.osti.gov/fwp ). All submissions and inquiries about this Program Announcement must reference Program Announcement LAB 11-505. If you have questions about who your LAB administrator is or how to use Searchable FWP, please contact the Searchable FWP Support Center.

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

### 3. Detailed Contents of the Proposal

Adherence to type size and line spacing requirements is necessary for several reasons. No researcher should have the advantage, or by using small type, of providing more text in his or her proposal. Small type may also make it difficult for reviewers to read the proposal. Proposals must have 1-inch margins at the top, bottom, and on each side. Type sizes must be at least 11 point. Line spacing is at the discretion of the researcher but there must be no more than 6 lines per vertical inch of text. Pages should be standard 8 1/2" x 11" (or metric A4, i.e., 210 mm x 297 mm).

### 3.1 Field Work Proposal Format (Reference DOE Order 412.1A) (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.

### 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 and number: **Scientific Discovery through Advanced Computing Institutes (LAB 11-505)**
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 suffices, such as 5a, 5b.

**3.4 Budget and Budget Explanation**

A detailed budget is required for the entire project period 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/budgetform.pdf

**3.5 Abstract**

Summarize the proposal in one page. Give the project objectives (in broad scientific terms), the approach to be used, and what the research is intended to accomplish. State the hypotheses to be tested (if any). At the top of the abstract give the lead DOE national Laboratory, project title, names of all the investigators and their institutions, and contact information for the principal investigator, including e-mail address.

**3.6 Narrative** (main technical portion of the proposal, including background/introduction, proposed research and methods, timetable of activities, and responsibilities of key project personnel).

The narrative comprises the research plan for the project and is limited to **maximum 25 pages**. It should contain enough background material in the Introduction, including review of the relevant literature, to demonstrate sufficient knowledge of the state of the science. The major part of the narrative should be devoted to a description and justification of the proposed project, including details of the 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. It is important that the 25-page technical information section provide a complete description of the proposed work, because reviewers are not obliged to read the Appendices. Proposals exceeding these page limits may be rejected without review or the first 25 pages may be reviewed without regard to the remainder.

The page count of 25 does not include the Face Page and Budget Pages, the Title Page, the biographical material and publication information, or any Appendices. However, it is important that the 25-page technical information section provide a complete description of the proposed work, since reviewers are not obliged to read the Appendices.

<u>Background and Recent Accomplishments</u>

0 Background – explanation of the importance and relevance of the proposed work.

0 Recent Accomplishments – this subsection is mandatory for renewal proposals and should summarize the proposed work and the actual progress made during the previous funding period.

<u>Proposed Research and Tasks</u>

In addition to the technical description of the proposed work and tasks, include a discussion of the following:

0 Impact of the proposed research on other fields of science, if appropriate.

0 Project schedule, milestones, and deliverables.

If any portion of the project is to be done in **collaboration** with another institution (or institutions), provide information on the institution(s) and what part of the project it will carry out. 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."

However, if you are submitting as a Lead Institution, in addition to meeting all criteria for submitting a peer reviewable proposal, please provide a one-page project narrative for the SciDAC Institute as well as the following information about the SciDAC Institute in the form of a table as shown below:

- Name of the SciDAC Institute and the Institute Director
- Identify the collaborating Institutions and the Principal Investigators at each Institution
- Proposed annual budget for the SciDAC Institute and for each collaborating Institution

**Sample Table for the Lead Institution**

| **SciDAC Institute** | **Year 1** | **Year 2** | **Year 3** | **Year 4** | **Year 5** | **Total** |
|---|---|---|---|---|---|---|
| Name of the SciDAC Institute and the Institute Director | $ | $ | $ | $ | $ | $ |
| **Collaborating Institutions** | | | | | | **Total** |
| (Start by the Lead Institution)<br>Name of the Institution and the Principal Investigator | $ | $ | $ | $ | $ | $ |
| Name of the Institution and the Principal Investigator | $ | $ | $ | $ | $ | $ |
| Name of the Institution and the Principal Investigator | $ | $ | $ | $ | $ | $ |
| **TOTAL** | $ | $ | $ | $ | $ | $ |

If you are submitting a proposal as a collaborator within a SciDAC Institute, please include the name of the SciDAC Institute in the title of your proposal, and identify the Lead Institution and Institute Director in your project summary.

### 3.7 Literature Cited

Give full bibliographic entries for each publication cited in the narrative. Each reference must include the names of all authors (in the same sequence in which they appear in the publication), the article and journal title, book title, volume number, page numbers, and year of publication. Include only bibliographic citations. Principal investigators should be especially careful to follow scholarly practices in providing citations for source materials relied upon when preparing any section of the proposal.

### 3.8 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 and must include:

*Education and Training.* Undergraduate, graduate and postdoctoral training, provide institution, major/area, degree and year.

*Research and Professional Experience.* Beginning with the current position list, in chronological order, professional/academic positions with a brief description.

*Publications.* Provide a list of up to 10 publications most closely related to the proposed project. For each publication, identify the names of all authors (in the same sequence in which they appear in the publication), the article title, book or journal title, volume number, page numbers, year of publication, and website address if available electronically. Patents, copyrights and software systems developed may be provided in addition to or substituted for publications.

*Synergistic Activities.* List no more than five professional and scholarly activities related to the effort proposed.

To assist in the identification of potential conflicts of interest or bias in the selection of reviewers, the following information must also be provided in each biographical sketch.

> *Collaborators and Co-editors:* A list of all persons in alphabetical order (including their current organizational affiliations) who are currently, or who have been, collaborators or co-authors with the investigator on a research project, book or book article, report, abstract, or paper during the 48 months preceding the submission of the proposal. Also, include those individuals who are currently or have been co-editors of a special issue of a journal, compendium, or conference proceedings during the 24 months preceding the submission of the proposal. Finally, list any individuals who are not listed in the previous categories with whom you are discussing future collaborations. If there are no collaborators or co-editors to report, this should be so indicated.
>
> *Graduate and Postdoctoral Advisors and Advisees:* A list of the names of the individual's own graduate advisor(s) and principal postdoctoral sponsor(s), and their current organizational affiliations. A list of the names of the individual's graduate students and postdoctoral associates during the past five years, and their current organizational affiliations.

### 3.9 Description of Facilities and Resources

Facilities to be used for the conduct of the proposed research should be briefly described. Indicate the pertinent capabilities of the institution, 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).

### 3.10 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 (months per year or percentage of the year) devoted to the project.

### 3.11 Appendix

Information not easily accessible to a reviewer may be included in an appendix, but **do not use the appendix to circumvent the page limitations of the proposal.** Reviewers are not required to consider information in an appendix, and reviewers may not have time to read extensive appendix materials with the same care they would use with 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 $50,000 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.