Program Announcement
To DOE National Laboratories

LAB 11-593

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

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

GENERAL INQUIRIES ABOUT THIS LAB ANNOUNCEMENT SHOULD BE DIRECTED TO:

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SUMMARY: The Office of Basic Energy Sciences (BES) and the Office of Advanced Scientific Computing Research (ASCR) of the Office of Science (SC), U.S. Department of Energy (DOE), hereby announce their interest in receiving DOE National Laboratory proposals from interdisciplinary teams to the Scientific Discovery through Advanced Computing (SciDAC) program, for Scientific Computation Application Partnerships (hereafter, Partnerships) in the area of Materials and Chemical Sciences.

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

The BES SciDAC Partnership portfolio will focus on the development of new algorithms and computational approaches which could dramatically accelerate the discovery of new materials and processes as well as provide fundamental understanding and improvement of current materials and processes. These elements are critical to the recently announced *Materials Genome Initiative for Global Competitiveness* www.whitehouse.gov/sites/default/files/microsites/ostp/materials_genome_initiative-final.pdf. Implementing these new algorithms on current and next generation massively parallel computers requires a team approach which includes materials and chemical scientists, applied mathematicians and computer scientists.

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

1. Capturing Solar Energy
2. Chemical Reactions
3. Magnetism and Superconductivity
4. Materials Under Extreme Environments
5. Separations
6. Energy Storage

Additional guidance may be found in BES Basic Research Needs Reports (*Basic Research Needs Reports* http://science.energy.gov/bes/besac/reports/) and the recently announced Materials Genome Initiative (www.whitehouse.gov/sites/default/files/microsites/ostp/materials_genome_initiative-final.pdf). While all of these areas are important to BES two overarching challenges that are especially relevant for SciDAC Partnership are: 1) the development of first-principles treatments of excited states and excited-state processes, and 2) electron correlation in finite and extended systems. It is expected that SciDAC Partnership projects will utilize the computational power available in DOE's Leadership Class machines. Projects may include requests to support software development. More specific information on each area of interest is included in the Description of Topical Areas section under SUPPLEMENTARY INFORMATION.

PRE-PROPOSAL: (Required)

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

Failure to submit a pre-proposal by an applicant will preclude the full proposal from due consideration. Only the Lead institution of a Partnership should submit the pre-proposal. Pre-proposals referencing Program Announcement LAB 11-593 should be submitted electronically by E-mail to james.davenport@science.doe.gov or mark.pederson@science.doe.gov . **No FAX or mail submission of pre-proposals will be accepted.**

The pre-proposal will be reviewed for conformance with the guidelines presented in this Announcement and suitability in the technical areas specified in this Announcement. A response to the pre-proposal encouraging or discouraging formal proposals will be communicated to the proposers by December 30, 2011. Proposers who have not received a response regarding the status of their pre-proposal by this date are responsible for contacting the program to confirm this status.

Only those pre-proposals that receive notification from DOE encouraging a formal proposal may submit full proposals. **No other formal proposals will be considered.**

The pre-proposals should consist of two to three pages of narrative describing the research objectives, the technical approach, the proposed team members, their expertise and their respective anticipated science program (BES or ASCR). The intent in requesting a pre-proposal is to save the time and effort of proposers in preparing and submitting a formal project proposal that may be inappropriate for the program. Pre-proposals will be reviewed relative to the scope and research needs as outlined in the summary paragraph and in the SUPPLEMENTARY INFORMATION. The pre-proposal should also include a cover sheet that identifies the title of the project, the institution or organization, principal investigator name, telephone number, fax number, e-mail address and the amount of funding requested for each year for the project for each funded institution. No biographical data need be included, nor is an institutional endorsement necessary. Since among the purposes of the pre-proposal is to facilitate BES and ASCR in planning the merit review and the selection of peer-reviewers without conflicts of interest, it is important that proposers ensure their list of supported or unsupported participants is as comprehensive as possible.

PROPOSAL DUE DATE:

Formal proposals submitted in response to this Program Announcement must be submitted from the DOE National Laboratory to the site office through Searchable FWP by **Monday, March 12, 2012, 11:59 p.m. Eastern Time**, to be accepted for merit review and to permit timely consideration for award in Fiscal Year 2012. **Each proposal should be in a single PDF file. The first few pages of the PDF should be the Field Work Proposal followed in the same PDF by the full technical proposal. You are encouraged to transmit your proposal well**

before the deadline. Only those proposers that receive notification from DOE encouraging a formal proposal may submit full proposals. PROPOSALS RECEIVED AFTER THE DEADLINE WILL NOT BE REVIEWED OR CONSIDERED FOR AWARD.

SUBMISSION INSTRUCTIONS:

LAB administrators should submit the entire LAB proposal and Field Work Proposal (FWP) via searchable FWP (https://www.osti.gov/fwp). Questions regarding the appropriate LAB administrator or other questions regarding submission procedures can be addressed to the Searchable FWP Support Center. All submission and inquiries about this Program Announcement must reference Program Announcement LAB 11-593.

SUPPLEMENTARY INFORMATION:

Scientific Discovery through Advanced Computing

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

- **FASTMath**: Frameworks, Algorithms, and Scalable Technologies for Mathematics (Director: Lori Diachin, Lawrence Livermore National Laboratory). Topics covered include structured and unstructured mesh tools and mesh-solver interfaces, particle methods, linear and nonlinear solvers, time integration, eigensolvers, and differential variational inequalities.

- **SUPER**: Sustained Performance, Energy and Resilience (Director: Robert Lucas, University of Southern California). Topics covered include performance engineering (including modeling and autotuning), energy efficiency, resilience, and optimization.

- **QUEST**: Quantification of Uncertainty in Extreme Scale Computations (Director: Habib Najm, Sandia National Laboratories). Topics covered include inverse problems, reduced

stochastic representations, forward uncertainty propagation, fault tolerance, and experimental design and model validation.

A successful Partnership will:

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

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

Reviewers of proposals submitted to this Announcement will be asked to comment upon the feasibility, benefits, and management of the proposed collaborations between the materials and chemical scientists supported by BES on the one hand, and the computational scientists (i.e., applied mathematicians and computer scientists/engineers) supported by ASCR on the other.

Description of Topical Areas

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

In order to enable future computational materials and chemical sciences approaches, automated excited-state methods: (1) incorporate potentially unforeseen and/or motivate improvements in mathematical approaches (2) provide controllable numerical precision (3) scale more favorably as a function of system size and (4) are computationally formulated in a manner that allows optimal use on current and next-generation HPC platforms will be required. Many BES reports in the Basic Research Needs Series (*Basic Research Needs Reports.* *http://science.energy.gov/bes/besac/reports/*) as well as joint BES ASCR workshop reports (*Discovery in Basic Energy Sciences: The Role of Computing at the Extreme Scale,* Edited by G. Galli and T. Dunning (2010) http://science.energy.gov/~/media/ascr/pdf/program-documents/docs/Bes_exascale_report.pdf and *Computational Materials Sciences and Chemistry: Accelerating Discovery and Innovation through Simulation-Based Engineering and Science,* Edited by G. Crabtree, S. Glotzer, B. McCurdy and J. Roberto (2011) http://science.energy.gov/~/media/bes/pdf/reports/files/cmsc_rpt.pdf) assert that accelerated predictive advances in excited-state properties and dynamics represent one of the highest-priority needs of the computational sciences community.

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

Additional Considerations

Verification and Validation and Data Sharing

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

Coordination with SciDAC Institutes and other Program Elements

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

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

Management Structure

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

- **Lead Principal Investigator -** The Lead Principal Investigator must be employed by the Lead institution and will serve as the primary contact responsible for communications

with the DOE Program Officers on behalf of all of the Principal Investigators in the Partnership.

- **Principal Investigator -** A Principal Investigator (PI) is the individual designated by the collaborating institution and empowered with the appropriate level of authority and responsibility for the proper conduct of the research within that organization. These authorities and responsibilities include the appropriate use of funds and administrative requirements such as the submission of scientific progress reports to DOE.
- **Senior/Key Personnel -** A senior/key person is an individual who contributes in a substantive, measurable way to the scientific or technical development or execution of the project.

Additional Guidance to Applicants

- Leadership class computation should accelerate scientific discovery in areas of strategic importance to DOE
    - Applicants must explain the benefits from leadership class computation
        - Impacts on Science (*how does it advance the BES mission?*)
        - Advancements in Computational Science (*how does it advance the ASCR mission?*)
        - Is the whole result larger than the sum of its parts?
    - Proposed research must employ state-of-the-art approaches enabling the effective use of the DOE leadership class computing resources
    - Applicants must identify metrics that will allow progress and contributions to be measured
- To that end, applicants must build and manage interdisciplinary, multi-institutional collaborations; in particular:
    - Applicants are encouraged to identify collaborations with researchers in the recently selected SciDAC Institutes, avoiding duplication of resources available at the Institutes; the goal is to build the functionality of a vertically integrated enterprise but with common resources found in the SciDAC Institutes
    - Alternatively, applicants may propose non-duplicative Applied Math/Computer Science expertise to supplement topics for which resources are provided by the Institutes, as well as expertise in topics for which no resources were provided by the Institutes.

Post-Award Process

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

Collaboration

Collaborative research projects with other institutions, such as universities, industry, non- profit organizations, and Federally Funded Research and Development Centers (FFRDCs), including the DOE National Laboratories, are encouraged under this Announcement. Collaborative proposals/applications submitted from different institutions, which are directed toward a single SciDAC Partnership, should clearly indicate they are part of a proposed collaboration and contain the Abstract for that SciDAC Partnership research project. In addition, such proposals/applications must describe the work and the associated budget for the research effort being performed under the leadership of the Principal Investigator at that participating institution.

Each collaborative proposal/application should have the same title as the Lead institution. The narrative should include a summary of the main contributions from each of the collaborating institutions and each proposal/application must have their own budget and budget justification.

Program Funding:

It is anticipated that up to $6,000,000 per year will be available for 5-12 awards to be made in Fiscal Year 2012 contingent on the availability of appropriated funds. Awards are expected to be made for a period of five years at a funding level appropriate for the proposed scope, with out-year support contingent on the availability of appropriated funds and satisfactory progress. Funding for the final two years is contingent upon satisfactory completion of a progress review during the third year of each project. DOE is under no obligation to pay for any costs associated with preparation or submission of proposals. DOE reserves the right to fund in whole or part, any, all or none of the proposals submitted to this Announcement.

Although a SciDAC Partnership may be supported by a single award, BES and ASCR expect each Partnership to be a collaboration comprised of several separate awards. BES and ASCR reserve the right to make fewer awards than would be possible at $6,000,000 per year, if an insufficient number of proposals are judged to be of suitable scientific quality or of sufficient relevance to the programs.

The instructions and format described below should be followed. You must reference Program Announcement LAB 11-593 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 DOE 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;**
   a. Does the proposed research address an important and relevant problem in basic energy science where breakthrough advances can be enabled by the use of leadership class computing resources?
   b. What science will become feasible with this collaboration that is not feasible now?
   c. Does the project demonstrate a functional partnership among the indicated domain scientists, applied mathematicians, and computer scientists?
   d. Does the research plan contain appropriate performance metrics that will allow progress and contributions to be measured?
   e. Does the project lead to new algorithms and/or software that will be made available to a broader community?

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

3. **Competency of Applicant's Personnel and Adequacy of Proposed Resources; and**
   a. How strong is the background, past performance, and potential of the lead principal investigators for successful execution of the proposed project?

b. Does the applicant have a proven record of success in managing diverse teams of scientific and technical experts and delivering results for advanced computational science research?
c. Has the applicant identified a credible and fruitful collaboration between domain scientists and applied mathematicians and computer scientists?
d. Is the work of any of the applied mathematicians and computer scientists identified in the proposal (regardless of their affiliation with the SciDAC Institutes) duplicative of work going on in the Institutes?
e. Are the roles and intellectual contributions of the Lead Principal Investigator and the BES/ASCR Principal Investigators and each senior/key personnel adequately described?

4. **Reasonableness and Appropriateness of the Proposed Budget.**
   a. Is the applicant's requested budget appropriate?
   b. Does the requested budget support the applicant's specified management structure in a meaningful way?

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

2. Summary of Proposal Contents

- Field Work Proposal (FWP) Format (Reference DOE Order 412.1A) (DOE ONLY)
- Proposal Cover Page
- 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 – 20-page limit
- Literature Cited
- Biographical Sketch(es)
- Description of Facilities and Resources
- Other Support of Investigator(s)
- Appendix (optional)

2.1 Submission Instructions

LAB administrators should submit the entire LAB proposal and Field Work Proposal (FWP) via searchable FWP (https://www.osti.gov/fwp). Questions regarding the appropriate LAB administrator or other questions regarding submission procedures can be addressed to the Searchable FWP Support Center. All submission and inquiries about this Program

Announcement must reference Program Announcement LAB 11-593. Full proposals submitted in response to this Announcement must be submitted to the searchable FWP database no later than 11:59 pm, Eastern Time, **March 12, 2012**. It is important that the entire peer reviewable proposal be submitted to the searchable FWP system as a single PDF file attachment.

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: Scientific Computation Application Partnerships in Materials and Chemical Sciences - LAB 11-593**
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 a **maximum of 20 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 20-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 20 pages may be reviewed without regard to the remainder.

The page count of 20 does not include the Cover Page and Budget Pages, the Title Page, the biographical material and publication information, or any Appendices. Letters of endorsement from unfunded collaborators should also be included, if applicable. Please do not submit general letters of support as these are not used in making funding decisions and can interfere with the selection of peer reviewers.

Background and Recent Accomplishments

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

Proposed Research and Tasks

In addition to the technical description of the proposed work and tasks, include a discussion of schedule, milestones, and deliverables.

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

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

Example budget table ($ in thousands)

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. For publications or collaborations with more than 10 authors or participants, only list those individuals in the core group with whom the Principal Investigator interacted on a regular basis while the research was being done. Also, 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.