Program Announcement
To DOE National Laboratories
LAB 03-17

Theory, Modeling
and
Simulation in Nanoscience

SUMMARY: The Office of Advanced Scientific Computing Research (ASCR) and the Office of Basic Energy Sciences (BES) of the Office of Science (SC), U.S. Department of Energy (DOE), hereby announce their interest in receiving applications for projects in the area of theory and modeling in nanoscience. Partnerships among universities, National Laboratories, and industry are encouraged.

NOTE: Each FFRDC is limited to only two proposals as leading institution. FFRDC investigators may appear as lead or co-investigator on only one university or FFRDC led proposal.

DATES: Preapplications referencing Program Announcement LAB 03-17 should be received by February 18, 2003.

Formal proposals in response to this announcement should be received by 4:30 p.m., E.S.T., April 9, 2003, to be accepted for merit review and funding in Fiscal Year 2003.

ADDRESSES: Preproposals referencing Program Announcement LAB 03-17 should be sent via e-mail using the following address: nanoscience.preposal@science.doe.gov.

Formal proposals, referencing Program Announcement LAB 03-17, must be submitted as PDF files on a CD accompanying a printed original of the proposal and seven copies and sent to: U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Materials Sciences, and Engineering Sciences Division, SC-13/Germantown Building, 1000 Independence Avenue, SW, Washington, D.C. 20585-1290, ATTN: Program Announcement LAB 03-17.

When submitting proposals by U.S. Postal Service Express Mail, any commercial mail delivery service, or when hand carried by the researcher, the following address must be used: U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Materials Sciences, and Engineering Sciences Division, SC-13, 19901 Germantown Road, Germantown, MD 20874-1290, ATTN: Program Announcement LAB 03-17.

FOR FURTHER INFORMATION CONTACT: Dr. William Kirchhoff, U.S. Department of Energy, Office of Science, SC-14/Germantown Building, 1000 Independence Avenue, S.W., Washington, DC 20585-1290, telephone: (301) 903-5809, E-mail: William.Kirchhoff@Science.doe.gov; Dr. Dale Koelling, U.S. Department of Energy, Office of

Science, SC-13/Germantown Building, 1000 Independence Avenue, S.W., Washington, DC 20585-1290, telephone: (301) 903-2187, E-mail: Dale.Koelling@Science.doe.gov; or Dr. Charles H. Romine, U.S. Department of Energy, Office of Science, SC-31/Germantown Building, 1000 Independence Avenue, S.W., Washington, DC 20585-1290, telephone: (301) 903-5800, E-mail: Chuck.Romine@Science.doe.gov, fax: (301) 903-7774.

SUPPLEMENTARY INFORMATION:

In May of 2002, a workshop on Theory and Modeling in Nanoscience was held in San Francisco, sponsored by the Basic Energy Sciences and Advanced Scientific Computing Research Advisory Committees to the Office of Science of the U.S. Department of Energy. The charge to the workshop was to identify challenges and opportunities for theory, modeling and simulation in nanoscience and nanotechnology, and to investigate the growing and promising role of applied mathematics and computer science in meeting those challenges. The final report of the workshop can be found at http://www.sc.doe.gov/bes/Theory_and_Modeling_in_Nanoscience.pdf.

Background: The Revolution in Theory, Modeling and Simulation

The past two decades have seen the fundamental techniques of theory, modeling and simulation undergo a revolution that parallels the experimental advances on which the new field of nanoscience is based. This period has seen the development of density functional algorithms, quantum Monte Carlo techniques, *ab initio* molecular dynamics, advances in classical Monte Carlo methods and mesoscale methods for soft matter and fast-multipole and multigrid algorithms. The application of these and other new theoretical capabilities are providing quantitative understanding of the novel behavior of nanoscale systems. The same two decades have also seen dramatic advances in computing hardware, which have increased raw computing power by four orders of magnitude. The combination of new theoretical and computational methods with increased computing power has made it now possible to simulate systems with millions of degrees of freedom.

The application of new experimental tools to nanosystems has created a concurrent need for a quantitative, predictive understanding of matter at the nanoscale. The absence of quantitative models that describe newly observed phenomena increasingly limits progress in the field. Without reliable, robust predictive tools and models for the quantitative description of structure and dynamics at the nanoscale, the research community will miss important scientific opportunities in nanoscience. The lack of such tools inhibits widespread applications in fields of nanotechnology ranging from molecular electronics to biomolecular materials. New investments in both human and computational resources are required to maintain the creative pace of nanoscience and nanotechnology.

The Opportunity and the Challenge

The nanoscale is not just another step towards miniaturization. It is a qualitatively new scale where materials properties depend on size and shape, as well as composition, and differ significantly from the same properties in the bulk or in isolated molecules. It is at this scale where one crosses over from the smallest scales, where a quantum mechanical description is

required, to the larger scales, where a classical description is often adequate. All approximations and assumptions used previously are suspect for systems at this scale and must be reexamined. Fundamental methods for theory, modeling and simulation developed for larger or smaller scales will need to be modified, extended, and sometimes combined into a more complete description. Completely new methods may be required. Synergism created within a team of researchers from nanoscience, computational science and applied mathematics can accelerate progress and broaden insight. Thus, the current solicitation for proposals allows for and encourages the building of teams of theorists, computational scientists, applied mathematicians, and experts in high-performance computing. There are many theory, modeling and simulation challenges in the broad topical areas of: (1) nano building blocks (nanotubes, quantum dots, clusters and nanoparticles); (2) complex structures and interfaces involving such building blocks; and (3) the assembly and growth of nanostructures, including (but not limited to):

- Determining the essential science of transport mechanisms at the nanoscale.
- Devising theoretical and simulation approaches to study nanointerfaces, which dominate many nanoscale systems and are highly complex and heterogeneous.
- Simulating, with reasonable accuracy, the optical properties of nanoscale structures and modeling nanoscale opto-electronic devices.
- Simulating complex nanostructures involving "soft" biological or organic structures, and "hard" inorganic ones, as well as nanointerfaces between hard and soft matter.
- Simulating self-assembly and directed self-assembly.
- Bridging from length- and time-scales appropriate for electronic motion to those needed for larger scale phenomena --- all the way up to macroscopic properties.
- Devising theoretical and simulation approaches to quantum coherence, decoherence, and spintronics.
- Developing self-validating and benchmarking methods.

Each of these challenges represents an opportunity for theory, modeling and simulation to provide new insights into the dynamic behavior of nanoscale systems.

Investment Plan of the Office of Science

A new investment in theory, modeling and simulation in nanoscience will have a major impact on the national nanoscience initiative, by stimulating the formation of alliances and teams of experimentalists, theorists, applied mathematicians, and computer and computational scientists to meet the challenge of developing a broad quantitative understanding of structure and dynamics at the nanoscale. The Department of Energy is uniquely situated to build such a program in theory, modeling and simulation in nanoscience. First, DOE currently supports much of the nation's experimental work in nanoscience, and new facilities dedicated to nanoscience research are currently being built at the DOE national laboratories. Second, the Department maintains an internationally renowned program in applied mathematical sciences research, a program that has been responsible for much of the fundamental research that forms the foundation of mathematical modeling and computational science. Third, the Department provides unique resources and more than two decades of experience in high performance computing and algorithms. The combination of these three capabilities makes the Department a natural home for nanoscience theory, modeling and simulation. This solicitation provides the mechanism for

beginning to capitalize on this unique combination of strengths by stimulating new research efforts in theory, modeling and simulation in nanoscience, built around strong teams of interdisciplinary researchers.

Solicitation Emphasis

This solicitation is to accelerate computational nanoscience. Nanoscience is considered to be the study of the properties and processes unique to the nanoscale and of the larger systems that incorporate nanoscale objects, so long as one or more nanoscale-driven properties remain significant. A nanoscale object is one in which at least two dimensions are in the range between a few and a few hundred nanometers. Proposals are sought which seek to establish new capabilities in nanoscience that incorporate, and thereby elucidate, its special features. Proposals may involve any of the broad topical areas or any combination thereof:

(1) nano building blocks (nanotubes, quantum dots, clusters and nanoparticles)
(2) complex structures and interfaces involving such building blocks
(3) assembly and growth of nanostructures

addressing prediction of properties and dynamical behavior. Nanotechnology, which is the design of specific devices, is not directly a part of this solicitation.

It is expected that a responsive project will progress beyond current limitations and will require serious development. This joint solicitation anticipates the necessity of a closely interacting team of researchers composed of people from the nanoscience field(s), computer experts, and applied mathematicians. Applied mathematics research applicable to theory, modeling and simulation in nanoscience includes (but is not limited to):

- Fast algorithms - new algorithms or variants of algorithms that lower the asymptotic computational complexity of a computation. Examples include fast multipole methods, fast Poisson solvers in complex geometries, fast eigensolvers, fast linear solvers, Monte Carlo (including improvements in variants such as Quantum Monte Carlo and Kinetic Monte Carlo), fast data exploration techniques, and fast computational geometry.
- Optimization and Predictability - energy minimization problems of unprecedented size and complexity, optimization methods that incorporate domain knowledge, optimization methods for understanding self-assembly processes, optimal control methods for design of nanosystems, predictability analysis and uncertainty quantification.
- Multiscale mathematics - that is, new mathematical techniques for effectively transferring quantitative information across a wide range of length- and time-scales, for merging atomistic and continuum modeling, new adaptive methods, separation of scales, and for coping with models where complex interactions between scales makes separation impossible. Here, it should be pointed out that nanoscience offers two separate opportunities. In the individual building blocks, the number of interacting scales is significantly reduced permitting addressing fundamental issues. The composites, on the other hand, exhibit greater interactions between different scales but with special constraints.

Proposals to the BES and ASCR base programs which may have the potential for contributing to the nanoscience theory, modeling and simulation activities, should so indicate.

Collaboration

Researchers are encouraged to collaborate with researchers in other institutions, such as: universities, industry, non-profit organizations, federal laboratories and Federally Funded Research and Development Centers (FFRDCs), including the DOE National Laboratories, where appropriate, and to include cost sharing wherever feasible. Additional information on collaboration is available in the Application Guide for the Office of Science Financial Assistance Program that is available via the Internet at: http://www.sc.doe.gov/production/grants/Colab.html.

Program Funding

It is anticipated that up to $4 million annually will be available for multiple awards for this program. Initial awards will be made late in Fiscal Year 2003 or early Fiscal Year 2004, in the categories described above, and proposals may request project support for up to five years. All awards are contingent on the availability of funds and programmatic needs. Annual budgets for successful projects are expected to range from $1,000,000 to $2,000,000 per project although smaller projects of exceptional merit may be considered. Annual budgets may increase in the out-years but should remain within the overall annual maximum guidance. Any proposed effort that exceeds the annual maximum in the out-years should be separately identified for potential award increases if additional funds become available.

Preproposals

Preproposals are strongly encouraged but not required prior to submission of a full proposal. However, notification of a successful preproposal is not an indication that an award will be made in response to the formal proposal. The preproposal should identify on the cover sheet the institution, Principal Investigator name(s), address(s), telephone, and fax number(s) and E-mail address(es), and the title of the project. A brief (one-page) vitae should be provided for each Principal Investigator. The preproposal should consist of a two to three page narrative describing the research project objectives, the approach to be taken, and a description of any research partnerships.

Merit Review

Proposals will be subjected to scientific merit review (peer review) and will be evaluated against the following evaluation criteria 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 Applicant's Personnel and Adequacy of Proposed Resources,
4. Reasonableness and Appropriateness of the Proposed Budget.

The evaluation of a proposal under item 1, Scientific and Technical Merit, will pay particular attention to:

a) The potential of the proposed project to make a significant impact in nanoscience research;
b) The demonstrated capabilities of the researchers to perform basic research related to nanoscience and transform these research results into software that can be widely deployed; and
c) The likelihood that the algorithms, methods, mathematical libraries, and software components that result from this effort will have a substantial impact on the nanoscience research community outside of the projects.

The evaluation under item 2, Appropriateness of the Proposed Method or Approach, will also consider the following elements related to Quality of Planning:

a) Quality of the plan for effective coupling of nanoscience researchers, computational scientists and applied mathematicians; and
b) Quality and clarity of proposed work schedule and deliverables.

Note that external peer reviewers are selected with regard to both their scientific expertise and the absence of conflict-of-interest issues. 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. Reviewers will be selected to represent expertise in the technology areas proposed, applications groups that are potential users of the technology, and related programs in other Federal Agencies or parts of DOE, such as the Advanced Strategic Computing Initiative (ASCI) within DOE's National Nuclear Security Administration.

The Project Description must be 20 pages or less, including tables and figures, but exclusive of attachments. The proposal must contain an abstract or project summary, letters of intent from collaborators, and short vitae. DOE is under no obligation to pay for any costs associated with the preparation or submission of proposals if an award is not made.

The instructions and format described below should be followed. Reference Program Announcement LAB 03-17 on all submissions and inquiries about this program.

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

NOTE: Each FFRDC is limited to only two proposals as leading institution. FFRDC investigators may appear as lead or co-investigator on only one university or FFRDC led proposal.

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

Reasonableness and appropriateness of the proposed budget

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 and Budget Explanation
Other support of investigators
Biographical Sketches
Description of facilities and resources
Appendix

2.1 Number of Copies to Submit

An original and seven copies of the formal proposal/FWP must be submitted. (Unless otherwise instructed in this Program Announcement.)

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 suffices, 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 20 pages. 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.sc.doe.gov/production/grants/Forms.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 laboratory submitting the proposal and at all subcontracting institutions. 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.