Office of Science
Notice 03-17

Theory, Modeling and Simulation in Nanoscience

Department of Energy

Office of Science Financial Assistance Program Notice 03-17: Theory, Modeling and Simulation in Nanoscience

AGENCY: U.S. Department of Energy

ACTION: Notice inviting grant applications.

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. The full text of Program Notice 03-17 is available via the Internet using the following web site address: http://www.science.doe.gov/production/grants/grants.html.

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

Formal applications in response to this notice 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: Preapplications referencing Program Notice 03-17 should be sent via e-mail using the following address: nanoscience.preposal@science.doe.gov.

Formal applications referencing Program Notice 03-17 must be sent electronically by an authorized institutional business official through DOE's Industry Interactive Procurement System (IIPS) at: http://e-center.doe.gov (see also http://www.science.doe.gov/production/grants/grants.html.) IIPS provides for the posting of solicitations and receipt of applications in a paperless environment via the Internet. In order to submit applications through IIPS your business official will need to register at the IIPS website. The Office of Science will include attachments as part of this notice that provide the appropriate forms in PDF fillable format that are to be submitted through IIPS. Color images should be submitted in IIPS as a separate file in PDF format and identified as such. These images should be kept to a minimum due to the limitations of reproducing them. They should be numbered and referred to in the body of the technical scientific application as Color image 1, Color image 2, etc. Questions regarding the operation of IIPS may be E-mailed to the IIPS Help Desk at: HelpDesk@pr.doe.gov or you may call the help desk at: (800) 683-0751. Further information on the use of IIPS by the Office of Science is available at: http://www.science.doe.gov/production/grants/grants.html.

If you are unable to submit the application through IIPS, please contact the Grants and Contracts Division, Office of Science at: (301) 903-5212, in order to gain assistance for submission through IIPS or to receive special approval and instruction on how to submit printed applications.

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 applications 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. Applications are sought which seek to establish new capabilities in nanoscience that incorporate, and thereby elucidate, its special features. Applications 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.

Applications to the BES and ASCR base programs through the Continuing Solicitation for all Office of Science Programs Notice 03-01, found at: http://www.science.doe.gov/production/grants/grants.html, which may have the potential for contributing to the nanoscience theory, modeling and simulation activities, should so indicate.

Collaboration

Applicants 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 applications 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.

Preapplications

Preapplications are strongly encouraged but not required prior to submission of a full application. However, notification of a successful preapplication is not an indication that an award will be made in response to the formal application. The preapplication 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 preapplication 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

Applications will be subjected to scientific merit review (peer review) and will be evaluated against the following evaluation criteria listed in descending order of importance as codified at 10 CFR 605.10(d):

1. Scientific and/or Technical Merit of the Project,
2. Appropriateness of the Proposed Method or Approach,
3. Competency of Applicant's Personnel and Adequacy of Proposed Resources,
4. Reasonableness and Appropriateness of the Proposed Budget.

The evaluation of applications 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 applicants to perform basic research related to nanoscience and transform these research results into software that can be widely deployed;
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;
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 an application constitutes agreement that this is acceptable to the investigator(s) and the submitting institution. Reviewers will be selected to represent expertise in the 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.

Information about the development and submission of applications, eligibility, limitations, evaluation, selection process, and other policies and procedures including detailed procedures for submitting applications from multi-institution partnerships may be found in 10 CFR Part 605, and in the Application Guide for the Office of Science Financial Assistance Program. Electronic access to the Guide and required forms is made available via the World Wide Web at: http://www.science.doe.gov/production/grants/grants.html. The Project Description must be 20 pages or less, including tables and figures, but exclusive of attachments. The application must contain an abstract or project summary, letters of intent from collaborators, and short vitae. DOE is under no obligation to pay for any costs associated with the preparation or submission of applications if an award is not made.

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

John Rodney Clark
Associate Director of Science
for Resource Management

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