

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 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 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 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 projects 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