Office of Science
Notice 01-08

Scientific Discovery through Advanced Computing: Computational Chemistry

Department of Energy
Office of Science

Office of Science Financial Assistance Program Notice 01-08; Scientific Discovery through Advanced Computing: Computational Chemistry

AGENCY: U.S. Department of Energy

ACTION: Notice inviting research grant applications.

SUMMARY: The Office of Basic Energy Sciences of the Office of Science (SC), U.S. Department of Energy (DOE), hereby announces its interest in receiving applications for projects in theory, modeling, and simulation activities associated with the computational chemistry component of the Scientific Discovery through Advanced Computing (SciDAC) research program. The full text of Program Notice 01-08 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 01-08, should be received by 4:30 p.m., E.S.T., February 7, 2001. A response encouraging or discouraging the submission of a formal application will be communicated by electronic mail by February 27, 2000. Formal applications in response to this notice should be received by 4:30 p.m., E.S.T., March 15, 2001, to be accepted for merit review and funding in FY 2001.

ADDRESSES: Preapplications referencing Program Notice 01-08 should be sent via e-mail using the following address: sharon.bowser@science.doe.gov.

Formal applications referencing Program Notice 01-08, should be forwarded to: U.S. Department of Energy, Office of Science, Grants and Contracts Division, SC-64, 19901 Germantown Road, Germantown, MD 20874-1290, ATTN: Program Notice 01-08. This address must be used when submitting applications by U.S. Postal Service Express Mail or any commercial mail delivery service, or when hand-carried by the applicant.

FOR FURTHER INFORMATION CONTACT: Dr. William H. Kirchhoff, Office of Science, U.S. Department of Energy, 19901 Germantown Road, Germantown, MD 20874-1290, telephone: (301) 903-5809, E-mail: william.kirchhoff@science.doe.gov, fax: (301) 903-4110.

SUPPLEMENTARY INFORMATION:

Background: Scientific Discovery through Advanced Computing

Advanced scientific computing will be a key contributor to scientific research in the 21st Century. Within the Office of Science (SC), scientific computing programs and facilities are already essential to progress in many areas of research critical to the nation. Major scientific challenges exist in all SC research programs that can best be addressed through advances in scientific supercomputing, e.g., designing materials with selected properties, elucidating the structure and function of proteins, understanding and controlling plasma turbulence, and designing new particle accelerators. To help ensure its missions are met, SC is bringing together advanced scientific computing and scientific research in an integrated program entitled "Scientific Discovery Through Advanced Computing."

The Opportunity and the Challenge

Extraordinary advances in computing technology in the past decade have set the stage for a major advance in scientific computing. Within the next five to ten years, computers 1,000 times faster than today's computers will become available. These advances herald a new era in scientific computing. Using such computers, it will be possible to dramatically extend our exploration of the fundamental processes of nature (e.g., the structure of matter from the most elementary particles to the building blocks of life) as well as advance our ability to predict the behavior of a broad range of complex natural and engineered systems (e.g., the earth's climate or an automobile engine).

To exploit this opportunity, these computing advances must be translated into corresponding increases in the performance of the scientific codes used to model physical, chemical, and biological systems. This is a daunting problem. Current advances in computing technology are being driven by market forces in the commercial sector, not by scientific computing. Harnessing commercial computing technology for scientific research poses problems unlike those encountered in previous supercomputers, in magnitude as well as in kind. As noted in the 1998 report (See Footnote Number 1) from the NSF/DOE "National Workshop on Advanced Scientific Computing" and the 1999 report (See Footnote Number2) from the President's Information Technology Advisory Committee, this problem will only be solved by increased investments in computer software-in research and development

on scientific simulation codes as well as on the mathematical and computing systems software that underlie these codes.

Investment Plan of the Office of Science

To meet the challenge posed by the new generation of terascale computers, SC will fund a set of coordinated investments as outlined in its long-range plan for scientific computing, Scientific Discovery through Advanced Computing (See Footnote Number 3) submitted to Congress on March 30, 2000. First, it will create a Scientific Computing Software Infrastructure that bridges the gap between the advanced computing technologies being developed by the computer industry and the scientific research programs sponsored by the Office of Science. Specifically, the SC effort proposes to:

- Create a new generation of Scientific Simulation Codes that take full advantage of the extraordinary computing capabilities of terascale computers.
- Create the Mathematical and Computing Systems Software to enable the Scientific Simulation Codes to effectively and efficiently use terascale computers.
- Create a Collaboratory Software Environment to enable geographically separated scientists to effectively work together as a team and to facilitate remote access to both facilities and data.

These activities are supported by a Scientific Computing Hardware Infrastructure that will be tailored to meet the needs of its research programs. The Hardware Infrastructure is robust, to provide the stable computing resources needed by the scientific applications; agile, to respond to innovative advances in computer technology that impact scientific computing; and flexible, to allow the most appropriate and economical resources to be used to solve each class of problems. Specifically, the SC proposes to support:

- A Flagship Computing Facility, the National Energy Research Scientific Computing Center (NERSC), to provide the robust, high-end computing resources needed by a broad range of scientific research programs.
- Topical Computing Facilities to provide computing resources tailored for specific scientific applications and to serve as the focal point for an application community as it strives to optimize its use of terascale computers.
- Experimental Computing Facilities to assess the promise of new computing technologies being developed by the computer industry for scientific applications.

Both sets of investments will create exciting opportunities for teams of researchers from laboratories and universities to create new revolutionary computing capabilities for scientific discovery.

Background: Theory, Modeling, and Simulation for Chemistry
This solicitation addresses the Scientific Simulation Codes element of the SciDAC program and in particular, theory, modeling, and simulation for chemistry.

Great progress has been made in the past half century in bringing molecular theory and modeling from a purely qualitative aid to an exact predictive tool for describing the chemical reactions of three and four atom systems, most notably for atoms in the first two rows of the periodic table. Predictive tools for many processes of importance to the Department of Energy's mission such as, but not limited to, combustion and catalysis occur between more complex molecules and between molecules and extended structures such as clusters or surfaces. Moreover, processes such as combustion and catalysis involve a complex interaction of chemistry with fluid dynamics. Predictive modeling of such processes is currently beyond the capabilities of existing computational resources and computational methods. Applications are solicited for the development of computational approaches to solving problems in the modeling of chemical processes that exceed current computational capabilities. Of particular interest are long-standing problems in computational approaches to predicting chemistry such as:

- reduction of the power law scaling of current quantum chemistry algorithms for systems with large numbers of atoms and electrons, i.e., alternative approaches to handling the electron correlation problem for many electron systems.
- calculation with chemical accuracy of the properties of open shell systems such as free radicals and excited electronic states appropriate to many areas of chemistry.
- calculation of the significant properties of complex systems consisting of hundreds of reactions coupled with fluid dynamics and turbulence.

Advances in computational chemistry in recent years in providing accurate descriptions of increasingly complex systems have come as much from improvements in theory and software as from improved computational hardware. Consequently, applications submitted under this announcement may address fundamental aspects of chemical theory so long as they promise to break through the barriers that currently exist in computational models. That is, while it is anticipated that successful applicants to this announcement will be primarily concerned with taking advantage of the computational resources being developed under SciDAC, it is not necessarily a requirement.

Collaboration

It is expected that all applications submitted in response to this notice will be for collaborative projects, possibly involving more than one institution. Applications submitted from different institutions, which are directed at a common research activity, may include a common technical description of the overall research project. However, each must have a qualified principal investigator, who is responsible for the part of the effort at each institution, and separate face pages and budget pages for each institution. The budget for the proposed work in computer science and applied mathematics should be clearly identified and described, as the Office of Advanced Scientific Computing Research may support this work (up to 20-25% of the total project cost). In addition, if the distinct scope of work proposed for each institution is not specified in the common technical description, it must be clearly stated in the individual applications. Applicants should include cost sharing whenever feasible. Collaborations with researchers in federal laboratories and Federally Funded Research and Development Centers (FFRDCs), including the DOE National Laboratories are encouraged.

Since each project will be developing new computational tools and physics models that could be useful in other projects, it is important that there be good communication between the different projects. Greater collaboration than usual is anticipated to be required for the research projects likely to be funded under this notice. The investigators involved should anticipate regularly scheduled meetings, not to exceed three per year, during the start up of the SciDAC program in order to assure the necessary coordination of efforts between physical scientists, mathematicians, and computer scientists.

Program Funding

It is anticipated that up to $1 million annually will be available for multiple awards for research in the areas described in this notice. Initial awards will be made in FY 2001 in the categories described above, and applications may request project support for up to three years. All awards are contingent on the availability of funds, research progress, and programmatic needs. Annual budgets for successful, individual projects submitted under this notice are expected to range from $100,000 to $500,000 per project in FY 2001, depending on the number of investigators and institutions involved. Annual budgets may increase in subsequent years but will be subject to the overall annual maximum guidance and availability of funds. Any proposed effort that exceeds the annual maximum ($1 million) in the subsequent years should be separately identified for potential award increases if additional funds become available.

As required by the SC Grant Application Guide, applicants must submit their budgets using the Budget Page (DOE Form 4620.1) with one Budget Page for each year of requested funding. The requested funding for the proposed work in computer science and applied mathematics should be included with the other projects costs on the Budget Page. However, applicants are also requested to list the proposed computer science and applied mathematics costs separately in an appendix, as the Office of Advanced Scientific Computing Research may support this work (up to 20-25% of the total project cost).

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), title of the project, and the field of scientific research. 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. Preapplications will be reviewed by DOE relative to the scope and research needs of the computational chemistry program.

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 under item 2, Appropriateness of the Proposed Method or Approach, will also consider the quality of the plan for effective coupling to emerging advances in supercomputing.

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.

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

Ralph H. De Lorenzo
Acting Associate Director of Science
for Resource Management

FOOTNOTES:
1. This workshop was sponsored by the National Science Foundation and the Department of Energy and hosted by the National Academy of Sciences on July 30-31, 1998. Copies of the report may be obtained from: http://www.er.doe.gov/production/octr/mics/index.html
2. Copies of the PITAC report may be obtained from: http://www.ccic.gov/ac/report/.
3. Copies of the SC computing plan, Scientific Discovery through Advanced Computing, can be downloaded from the SC website at: http://www.sc.doe.gov/production/octr/index.html.

Published in the Federal Register January 11, 2001, Volume 66, Number 8, Pages 2413-2416.