Program Announcement To DOE National Laboratories

LAB 01-08

Scientific Discovery through Advanced Computing (SciDAC): Computational Chemistry

The Office of Basic Energy Sciences of the Office of Science (SC), U.S. Department of Energy (DOE), hereby announces its interest in receiving proposals for projects in theory, modeling, and simulation activities associated with the computational chemistry component of the Scientific Discovery through Advanced Computing (SciDAC) research program.

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, FAX: (301) 903-4110, E-mail: william.kirchhoff@science.doe.gov

DATES: Preproposals referencing Program Announcement 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 proposal will be communicated by electronic mail by February 27, 2000.

Formal proposals 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: Preproposals referencing Program Announcement 00-08 should be sent to Dr. William H. Kirchhoff, Office of Basic Energy Sciences, SC-14, Office of Science, U.S. Department of Energy, 19901 Germantown Road, Germantown, MD 20874-1290; e-mail is acceptable for submitting preproposals using the following address: sharon.bowser@science.doe.gov

Proposals referencing Program Announcement 01-08, should be forwarded to: U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, SC-14, 19901 Germantown Road, Germantown, MD 20874-1290, ATTN: Program Announcement 01-08. This address must be used when submitting proposals by U.S. Postal Service Express Mail or any commercial mail delivery service, or when hand-carried by the proposer.

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 extend dramatically 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 Number 2) 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 Program Announcement 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.

Proposals 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, proposals 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 proposals submitted in response to this notice will be for collaborative projects, possibly involving more than one institution. Proposals 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 proposals.

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 in 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 $1.5 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 proposals 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 $400,000 to $1,000,000 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 ($1.5 million) in the subsequent years should be separately identified for potential award increases if additional funds become available. The budget, if any, for proposed work in computer science and applied mathematics should be listed separately, as the Office of Advanced Scientific Computing Research may support this work (up to 20-25% of the total project cost).

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

The instructions and format described below should be followed. Reference Program Announcement LAB 00-08 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 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 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 applications 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)

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.

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)

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. As mentioned above, additional information is 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 25 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)

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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.

Posted at the Office of Science Grants and Contracts Web Site on January 11, 2001.