

Office of Energy Research

Notice 97-14

Advanced Computational Testing and Simulation Software Activities

Department of Energy
Office of Energy Research

Energy Research Financial Assistance Program Notice 97-14; Advanced Computational Testing and Simulation Software Activities

AGENCY: U.S. Department of Energy

ACTION: Notice inviting grant applications

SUMMARY: The Mathematical, Information, and Computational Sciences (MICS) Division of the Office of Computational and Technology Research (OCTR), Office of Energy Research (ER), U.S. Department of Energy (DOE) announces its interest in receiving applications for research grants in Advanced Computational Testing and Simulation Software Activities.

DATES: Formal applications submitted in response to this notice must be received not later than 4:30 p.m. E.D.T., July 16, 1997, to permit timely consideration for award early in fiscal year 1998.

ADDRESSES: Formal applications, referencing Program Notice 97-14, should be forwarded to: U.S. Department of Energy, Office of Energy Research, Grants and Contracts Division, ER-64, 19901 Germantown Road, Germantown, Maryland 20874-1290, Attn: Program Notice 97-14. The above address also must be used when submitting formal applications by U.S. Postal Service Express Mail, any commercial mail delivery service, or when hand-carried by the applicant.

FOR FURTHER INFORMATION CONTACT: Dr. Mary Anne Scott, Office of Energy Research, U.S. Department of Energy, OCTR/MICS, ER-31, 19901 Germantown Road, Germantown, MD 20874-1290. Tel: (301) 903-6368; E-mail: scott@er.doe.gov.

SUPPLEMENTARY INFORMATION: The vision of the DOE 2000 Initiative is to accelerate DOE mission accomplishments through advanced collaboration and simulation. Objectives include improved ability to solve DOE's scientific problems, an increased R & D productivity and efficiency, and enhanced access to DOE resources by R & D partners.

One of the two major thrusts for addressing these objectives is the Advanced Computational Testing and Simulation (ACTS) Toolkit. This toolkit will provide an integrated set of software tools, algorithms, and environments that accelerate the adoption and use of advanced computing by DOE programs for mission-critical problems. The toolkit will include capabilities for representing complex geometries, solving diverse numerical equations, simplifying multi-

language parallel execution, evaluating and enhancing code performance, and dynamically steering calculations during execution. The strategy for building this toolkit is to select a base set of existing successful tools, provide support to make them interoperable, and then add new tools and interfaces to make the entire toolkit robust for diverse application needs.

In FY 1997, the founding efforts for the ACTS Toolkit were begun -- the Scientific Template Library (SciTL). SciTL concentrates on three areas of tool development: interoperable numeric libraries, object-oriented libraries and capabilities for modular code development, and runtime libraries for efficient parallel execution (including dynamic load-balancing). All portions of the SciTL work are tied to specific DOE applications (Accelerated Strategic Computing Initiative (ASCI) codes and ER Grand Challenges) and initially targeted to specific computing platforms (ASCI machines). The FY 1997 SciTL project description, including detailed plans, deliverables, and participants, can be found via the Internet at the following URL:
<http://www.acl.lanl.gov/SciTL>

In FY 1998, the ACTS Toolkit efforts will begin to expand. Applications are solicited to build on the SciTL to further advance the strategies of the ACTS Toolkit. Technical areas of interest include, but are not limited to: additional application-specific data structures required for scientific codes, additional numerical solvers, parallel and distributed data structures to support numerical techniques; high-performance parallel input/output components, language interoperability (primarily Fortran, C, and C++), tools for enhancing fault tolerance, tools for easily saving and restoring complex pointer-based structures and objects, tools for debugging and performance analysis/tuning; and toolkit components required for new domains of use. Applications are also encouraged for expanding the use of the ACTS Toolkit to a wider range of DOE applications and for expanding the types of computing platforms on which the Toolkit can be used.

Successful applications will relate to the current SciTL structure by one or more of the following:

- * Building new ACTS Toolkit capabilities by using the current functionality provided by the SciTL interface,
- * Expanding capabilities of the SciTL interface by developing complementary libraries that interoperate with relevant portions of the existing SciTL components,
- * Evaluating the current capabilities of the SciTL components for their functionality, performance, and portability in the context of new application and/or computing systems domains,
- * Restructuring portions of the existing SciTL components to enhance functionality, improve performance, and/or expand portability,
- * Linking the ACTS Toolkit with components in the other DOE 2000 thrust: National Collaboratories (see the Internet web page at URL: <http://www.mcs.anl.gov/DOE2000/>).

Applications may be for up to three years in duration, with second and third year funding subject to progress demonstrated in annual reviews. Based on anticipated available funding and sufficient applications of high merit, approximately 4-6 applications averaging \$250K/year could be supported.

Applications will be subjected to formal merit review (peer review) and will be evaluated against the following criteria listed in descending order of importance as codified for review of applications from the academic and industrial sectors in 10 CFR part 605:

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

Within the Scientific and/or Technical Merit criterion above, the following subcriteria will be used for evaluation purposes (relative to the current SciTL), and will be evaluated equally:

- i. Increased functionality
- ii. Enhanced performance
- iii. Improved usability
- iv. Widened scope of applicability

Within the Appropriateness of Method criterion above, applicants are encouraged to identify opportunities for collaboration with ongoing DOE 2000 projects and other applications important to DOE missions.

External peer reviewers will be selected with regard to both their scientific expertise and the absence of conflict-of-interest issues. Non-federal reviewers will be used, and submission of an application constitutes agreement that this is acceptable to the investigator(s).

Information about the development and submission of applications, eligibility, limitations, evaluation, selection processes, and other policies and procedures may be found in the Application Guide for the Office of Energy Research Financial Assistance Program and 10 CFR Part 605. The Application Guide is available from the U.S. Department of Energy, Office of Energy Research, OCTR/MICS, ER-31, 19901 Germantown Road, Germantown, MD 20874-1290. Telephone requests may be made by calling (301)903-5800. Electronic access to ER's Application Guide is possible via the Internet at the following URL:
<http://www.er.doe.gov/production/grants/grants.html>.

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
for Resource Management
Office of Energy Research

Published in the Federal Register April 28, 1997, Vol. 62, No. 81,
pages 22917-22918.