

chemical, and biological systems such as fluids, materials, magnetized plasmas, or protein molecules. This includes, but is not limited to, methods for solving large systems of partial differential equations (PDEs) on parallel computers, techniques for choosing optimal values for parameters in large systems with hundreds to hundreds of thousands of parameters, improving our understanding of fluid turbulence, and developing techniques for reliably estimating the errors in simulations of complex physical phenomena.

In addition to the existing research topics described, MICS plans to invest in new areas of applied mathematics research to support DOE's mission. Such investments may include research in multiscale algorithms, the mathematics of feature identification in large datasets, asymptotically optimal algorithms for solving PDEs, fast multipole and related hybrid methods, and algorithms for handling complex systems with constraints. The MICS research portfolio in Applied Mathematics emphasizes investment in long-term research that will result in the next generation of computational tools for scientific discovery.

Collaboratory Research

Collaboratories link geographically dispersed researchers, data, and tools via high performance networks to enable remote access to facilities, access to large datasets, shared environments, and ease of collaboration. The objective of the collaboratory component of the MICS portfolio is to support research for developing the software infrastructure that will enable universal, ubiquitous, easy access to remote resources or that will contribute to the ease with which distributed teams work together. Enabling high performance for distributed scientific applications is an important consideration. The middleware component for collaboratories encompasses activities in:

- Building the application frameworks that allow discipline scientists to express and manage the simulation, analysis, and data management aspects of overall problem solving.
- Supporting construction, management, and use of widely distributed application systems.
- Facilitating human collaboration through common security services, and resource and data sharing.
- Providing remote access to, and operation of, scientific and engineering instrumentation systems.

- Managing and securing the computing and data infrastructure as a persistent service.

This announcement also calls for grant applications to address the fundamental issues involved in providing uniform software services that manage and provide access to heterogeneous, distributed resources, that is, high-performance middleware services that support DOE's science mission. The emphasis is on investment in long-term research that will result in the next generation of high-performance software infrastructure for scientific discovery.

Computer Science Research

The objective of the computer science component of the MICS research portfolio is to support research that results in a comprehensive, scalable, and robust high performance software infrastructure that translates the promise and potential of high peak performance to real performance improvements in DOE scientific applications. This software infrastructure must address needs for: Portability and interoperability of complex high performance scientific software packages; operating systems tools and support for the effective management of terascale and beyond systems; and effective tools for feature identification, data management, and visualization of petabyte-scale scientific data sets. The Computer Science component encompasses a multi-discipline approach with activities in:

- Program development environments and tools—Component-based, fully integrated, terascale program development and runtime tools, which scale effectively and provide maximum performance, functionality, and ease-of-use to developers and scientific end users.
- Operating system software and tools—Systems software that scales to tens of thousands of processors, supports high performance application-level communication, and provides the highest levels of performance, fault tolerance, reliability, manageability, and ease of use for system administrators, tool developers, and end users.
- Visualization and data management systems—Scalable, intuitive systems fully supportive of DOE application requirements for moving, storing, analyzing, querying, manipulating, and visualizing multi-petabytes of scientific data and objects.
- Problem Solving Environments—Unified systems focused on the needs of specific scientific applications, which enable radically improved ease-of-use of

complex systems software and tools by domain application scientists.

The MICS research portfolio in Computer Science emphasizes investment in long-term research that will result in the next generation of high performance tools for scientific discovery.

High-Performance Networks Research

In the next few years, complex science experiments in DOE are expected to generate several petabytes of data that will be transferred to geographically distributed terascale computing facilities for analysis and visualization by thousands of scientists across the world. In addition, many emerging energy research problems require coordinated access to distributed resources—people, data, computers, and facilities. This emerging, distributed terascale-science environment calls for ultra-high-speed networks—networks that can deliver multi-gigabits/sec throughput to scientific applications securely. Grant applications in network research must therefore address the issues of ultra high-speed networks by focusing on:

- Ultra high-speed network protocols—innovative, new approaches to transport protocols and dynamic provisioning technologies for ultra-high-speed networks that will enable large-scale distributed science applications to efficiently harness the abundant bandwidth made possible by Dense Wave Division Multiplexing (DWDM) optical technologies. For ultra-high-speed transport protocols, this may include, but is not limited to, significant modifications to existing transport protocols, such as UDP, TCP, TCP variants, and TCP alternatives that can deliver multi-gigabit throughput to high-end scientific applications. For dynamic provisioning, the focus is on advanced network technologies for agile DWDM networking that offer bandwidth on-demand, scheduled end-to-end bandwidth, differentiated DWDM services, and DWDM traffic engineering. Respondents must address the theoretical foundations of the proposed work with rigorous mathematical and algorithm principles.

- Performance evaluation of cyber security systems—formal techniques for modeling and evaluating the performance and effectiveness of cyber security systems and policies. This may include techniques for formal specification of cyber security requirements and implementation.

- Ultra-high-speed network services—advanced network-aware services that enable the efficient, effective, and secure utilization of ultra-