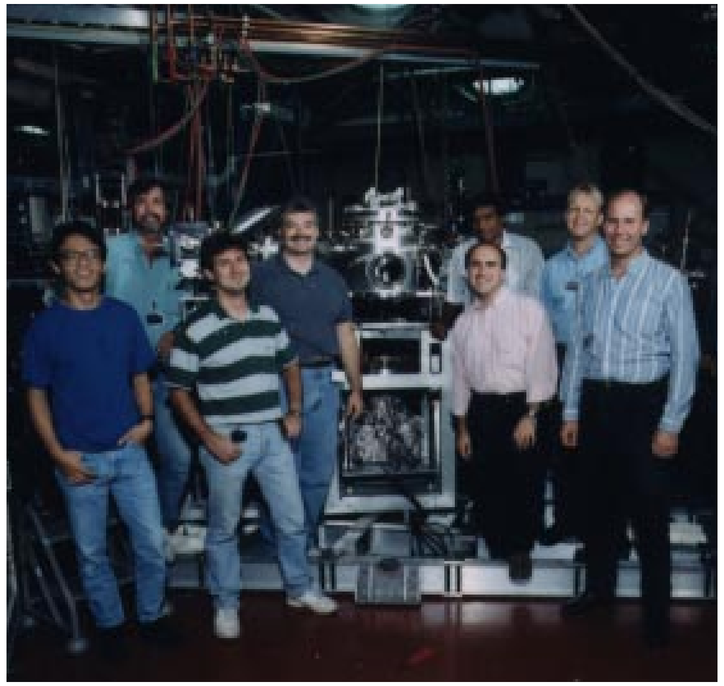
Probing with Synchrotron-Radiation-Based Spectroscopies

This Livermore team of researchers helped to build and begin operation of Beamline 8.0, a soft x-ray and vacuum ultraviolet beamline, at Lawrence Berkeley National Laboratory's Advanced Light Source.



MAKING things smaller isn't as easy as it looks! Using novel materials to manufacture atomic-scale microelectronic, electro-optic, and other devices requires a clear understanding of the materials' atomic, electronic, and bonding structures. Through studies they are conducting at the Advanced Light Source (ALS), a $100-million synchrotron-radiation user facility, researchers from Lawrence Livermore National Laboratory are helping to provide that understanding.

Headed by Lou Terminello of the Chemistry and Materials Science Directorate, the Livermore group is part of a large research team. It includes researchers from IBM, the University of Wisconsin, the University of Tennessee, Tulane University, and the Lawrence Berkeley National Laboratory, where the two-year-old ALS is housed. The team was formed to pool resources to build and operate a state-of-the-art, soft x-ray and vacuum ultraviolet beamline at the ALS. The 33-m-long beamline—called Beamline 8.0—was designed especially to provide the brightest and highest resolution photon flux in an energy range from 40 to 1,500 eV.

Using techniques such as photoemission, photoabsorption, soft x-ray fluorescence (SXF) spectroscopy, and photoelectron holography, the researchers conduct their experiments to essentially "capture" atomic-level images from the material sample they are probing.

Enhanced SXF

The initial experiments demonstrated the unique capability of the Advanced Light Source to enhance SXF spectroscopy in order to probe systems that are difficult if not impossible using other techniques. Last year, the Beamline 8.0 team became the first of the ALS users to publish its experimental results in refereed journals, with papers in *Physical Review Letters*,[1] *Review of Scientific Instruments*,[2] and *Applied Physics Letters*.[3] The reports focused on results using SXF spectroscopy to reach deep into the interior of materials to look at the atomic and electronic structures of graphite and titanium oxide. Resulting images showed dispersive features in fluorescence spectra.

While the collaborators share a technical affinity in advancing new characterization techniques, each affiliated organization has its own specific interest. For example, Tulane and the University of Tennessee are chiefly focused on SXF to examine the electronic structures of solids. On the other hand, IBM, which provided most of the funding for construction of the shared beamline, is interested in basic and applied research on microelectronic materials and on characterizing material interfaces.

Robust Interfaces

Interfaces are also a central thrust for the Livermore team's research. With funding from the Department of Energy's Office of Basic Energy Sciences, the team is studying the structure of heterogeneous interfaces, an important aspect of microelectronics or other advanced materials. Explains Terminello, "Because microelectronic devices are getting smaller and smaller, an interface is becoming a more important constituent of the overall device. Let's say you join dissimilar materials and want to traverse the interface with electrons for your electronic device. The interface very definitely has an impact on how, and whether, the device performs."

The team's materials science work at the ALS has involved making interfaces as well as characterizing them. In one experiment, the researchers grew oxides on silicon using nitrous oxide. "We found we could get a robust interface using that growth method because we are essentially growing a thin nitride film right at the interface," said Terminello. "That makes the interface less susceptible to breakdown when high-voltage fields are applied to very small devices."

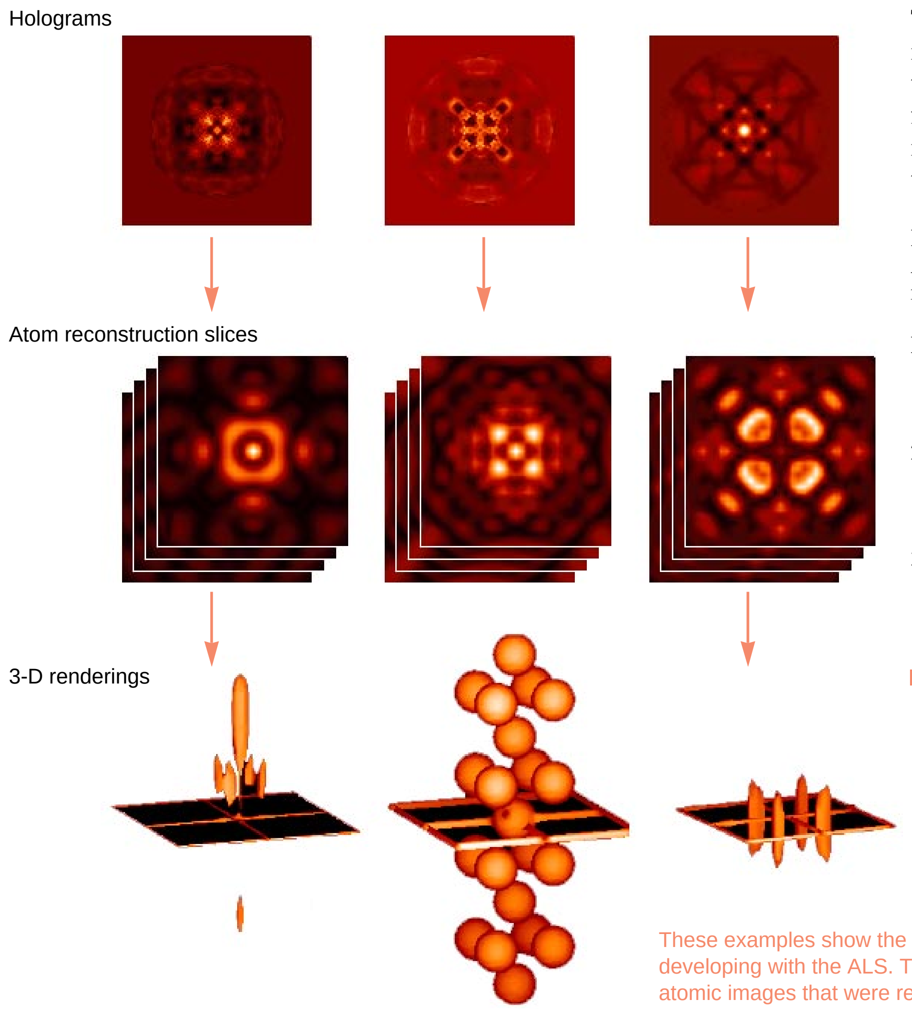
Livermore's ALS researchers are seeking to understand on an atomic scale the structure of materials such as thin films, multilayers, diamond films, novel semiconductors, and epitaxial overlays on single-crystal substrates, and then relate that knowledge to the properties that would govern the materials' performance in a variety of applications.

Seeing the Theory

The ALS experimentalists have been closely coupling their atomic-level measurements to work done by Livermore's theoretical scientists, who are forging new pathways in the computational study of novel materials and their interactions (see *Energy & Technology Review*, August–September 1994). Part of the structural information gathered by the ALS group, can be compared directly to elements of theoretical models that groups such as Livermore's H-Division have developed. Says Terminello, "What that comparison does is allow us to have greater confidence in the theoretical models for use in predicting the structure and behavior of new materials— so in the future we can achieve 'materials by design.'"

One of the Livermore team's principal tools to characterize interfaces is a specially developed electron spectrometer, based on a design originally created at IBM in the early 1980s. While an electron energy analyzer is a fairly common piece of research equipment, the device built for the ALS beamline permits more detailed and streamlined analysis of atomic and electronic structures. For example, it records how many electrons are being emitted from interface atoms in the sample under examination, and it simultaneously preserves the electron trajectories as they are emitted from the surface. Furthermore, the device collects all the angular information at one shot. The bottom line is that the unit allows researchers to efficiently do the angle mapping required to get the complete picture of the physics governing the emitted electrons.

The unit recorded its first photoemission in October 1994 and has been in use ever since. The device's angle-resolving capabilities became operational in July 1995. Terminello predicts that the analyzer will develop into a "workhorse" in the coming months as the team continues its nanoscale look at the fundamental properties of a variety of novel materials and observing the phenomena that are taking place within them.



These examples show the atom-imaging technique that the Livermore team is developing with the ALS. Top row: photoelectron holograms. Middle row: real-space atomic images that were recovered from holograms above. Bottom row: 3-D renderings made from above images (center one is an ideal model of the atoms).

Key Words: synchrotron radiation, spectroscopy, Advanced Light Source, Beamline 8.0, material interfaces.

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Operating a Tokamak from Across the Country

PHYSICISTS often share the use of large, expensive, experimental facilities to study the actions and reactions of minute particles. But demands upon existing facilities are high. Lawrence Livermore National Laboratory is pioneering the development of technology for remotely conducting magnetic fusion experiments as a way to maximize the use of experimental tokamak facilities. Fusion experts live all over the world, so their ability to conduct experiments from multiple locations will enable many new scientific collaborations.

Real-time data crosses the country within a tenth of a second via the Internet.

Split-second flash of light from inside the tokamak at MIT indicates a plasma has formed and the shot is successful.

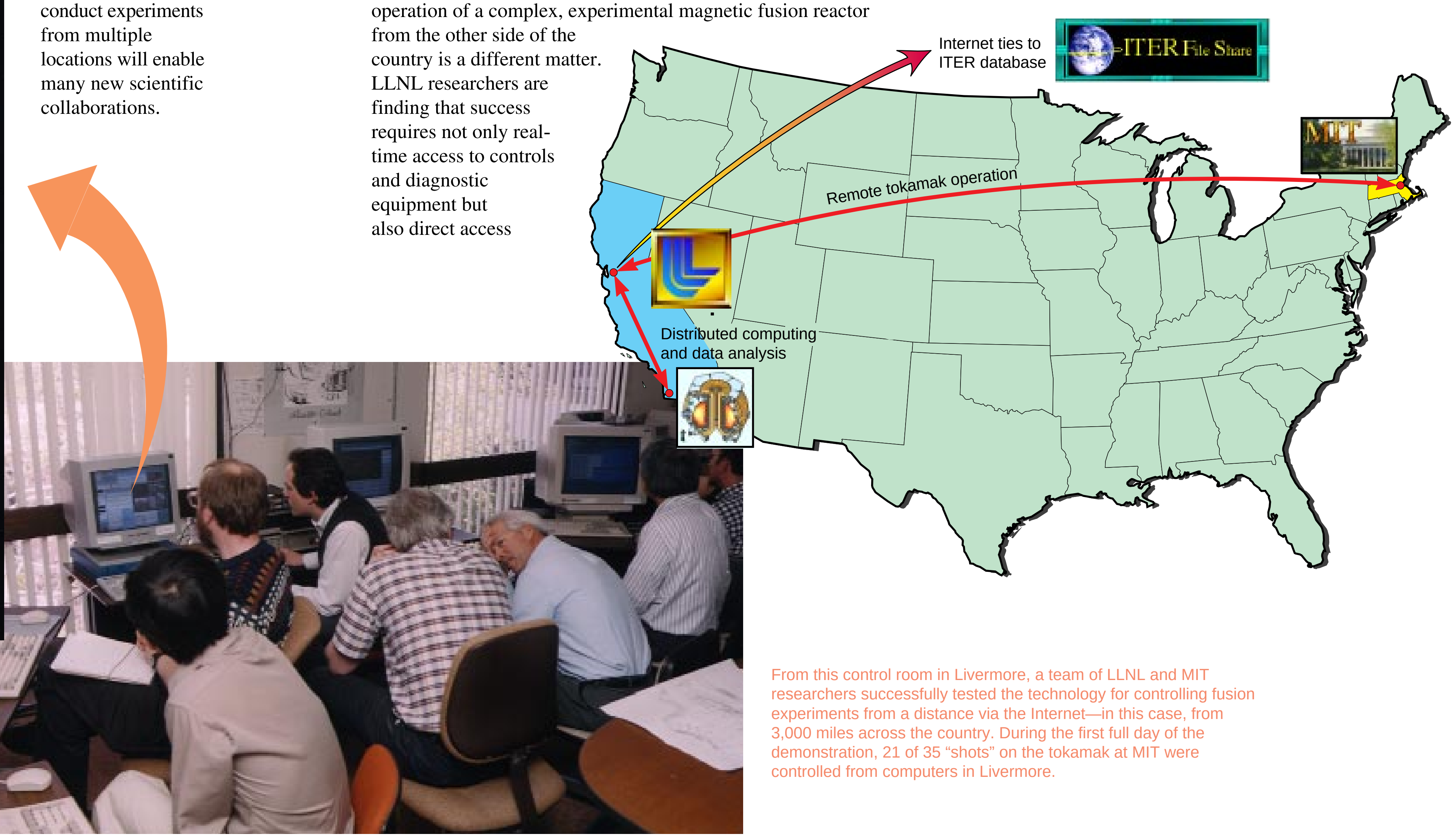
Real-time video of researchers in the control room at MIT

Greater demand also is being made for more efficient use of funds to construct and use such facilities. Like other electronic operations, remotely operating experiments will also significantly cut the time and cost of travel to these facilities as well. Scientists at one laboratory could control all phases of a physics experiment on a device at another location, while simultaneously conferring with colleagues at other laboratories and universities who are obtaining real-time data from the experiments in process.

While remote control of machines is nothing new, remote operation of a complex, experimental magnetic fusion reactor from the other side of the country is a different matter. LLNL researchers are finding that success requires not only real-time access to controls and diagnostic equipment but also direct access through sound and visuals to scientists and technicians resident at the experiment. The recent explosive growth of high-speed, wide-area computer networks like the Internet is making remote operation possible.

Working Toward Remote Operation

Since 1991, scientists at Livermore have been developing capabilities for remote operation of a tokamak. In a collaboration with General Atomics in San Diego, the Livermore project



From this control room in Livermore, a team of LLNL and MIT researchers successfully tested the technology for controlling fusion experiments from a distance via the Internet—in this case, from 3,000 miles across the country. During the first full day of the demonstration, 21 of 35 “shots” on the tokamak at MIT were controlled from computers in Livermore.

How Magnetic Fusion Works

Magnetic fusion scientists use a tokamak (the word is a Russian acronym) to duplicate the Sun's process of creating energy through fusion. The goal is to create a commercially viable energy source without contributing to global warming or acid rain and without producing toxic wastes.

In the doughnut-shaped tokamak, powerful magnets are used to confine plasma—a highly ionized gas like the material at the Sun's surface. Enough energy must be used to heat the plasma to a temperature sufficient to produce ion velocities high enough to react and fuse—at temperatures in the range of 20 million to 100 million degrees kelvin. Current tokamaks create plasma in bursts a few seconds long, but scientists are working toward steady-state operation, which is more advantageous for power generation and easier on the materials in the system.

Fusion energy has not found its way into our electrical sockets because confining and heating the plasma are very difficult. However, recent experiments give every indication that ignition for controlled fusion power applications will be achieved in the next 10 to 15 years.

staff has developed software to remotely access General Atomics' DIII-D tokamak. Today, when experiments are in process, researchers in Livermore can control diagnostic equipment, operate data acquisition systems, and obtain and view results. They have access to all computer-based information at the DIII-D. They also have created integrated, network-based, high-performance computing and data storage facilities. However, the main controls for actual remote operation of the DIII-D are not on the network.

Unlike the DIII-D, the Alcator C-Mod tokamak at Massachusetts Institute of Technology's Plasma Fusion Center, the newest tokamak in the U.S., was designed with network-based control and data acquisition systems. Although the Alcator C-Mod hardware was not designed specifically for remote operation, its systems are compatible with this option. Until recently, however, only a few instruments had been operated remotely.

In March 1995, scientists in Livermore conducted fusion experiments on the Alcator C-Mod device in Cambridge, Massachusetts, in the first transcontinental operation of a tokamak. The Livermore team and MIT researchers worked together to operate the tokamak using a part of the Internet called the Energy Sciences Network, or ESNet, which is managed by Livermore. The plasma shape, the particle fueling source, the radio frequency heating, and a reciprocating probe were all controlled in real time from Livermore over ESNet.

Scientists also exchanged a variety of data between Livermore and Cambridge: video images, experimental data from the diagnostic equipment inside the tokamak, and video and audio communications between researchers at each end (see figure pp. 32–33). Data and signals crossed the country in about 100 milliseconds. Multiple video cameras captured images of the control room in Cambridge, of the exterior and interior of the tokamak, and of researchers in Livermore. A flash of light inside the tokamak indicated each successful pulse, or shot. These real-time visuals of the people and equipment at Cambridge helped bring the experiment to the scientists in Livermore.

The ability to control the tokamak's systems from Livermore did not eliminate the need for a local staff at Cambridge. Engineers on site at the tokamak monitored all systems to assure the safety of the equipment and local personnel.

This demonstration was the definitive test for controlling a large, complex physics experiment from a remote location, and MIT and Livermore scientists learned much about the possibilities for remote collaboration. They also learned that work remains to be done to make the remote researcher more a part of the experiment.

Bringing Remote Operation Fully On Line

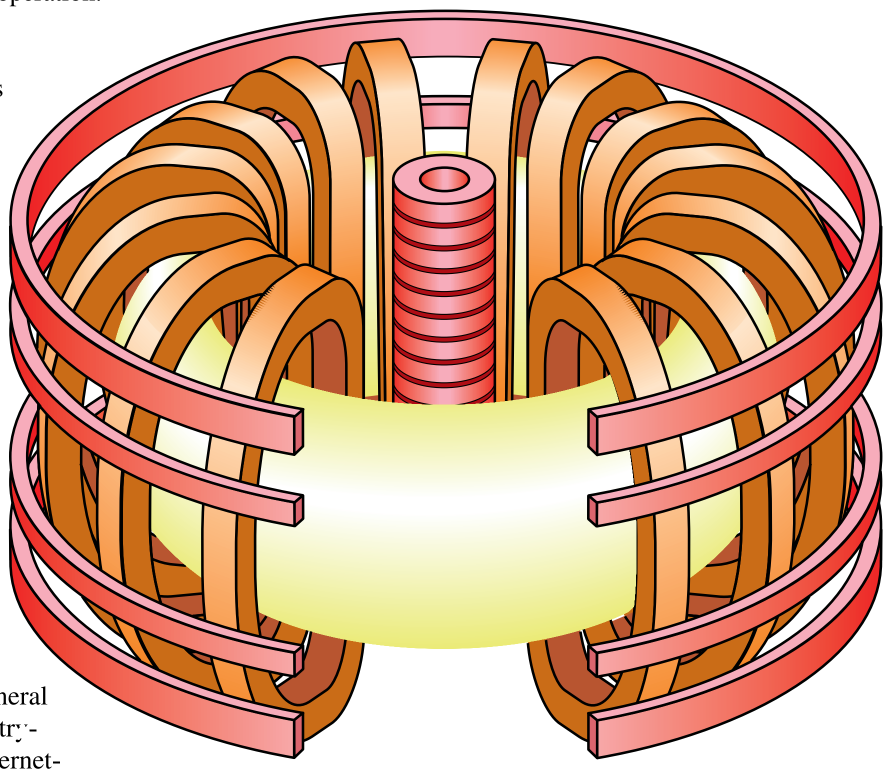
Remote operation is an integral part of the design of the huge International Thermonuclear Experimental Reactor (ITER), a magnetic fusion collaboration among the European Community, Japan, the Russian Federation, and the U.S. ITER is planned to operate in steady state with controlled ignition and steady burn. Design is under way at several international sites, although a location for the reactor itself has not yet been determined. Current planning includes a network of control room facilities in each of the partners' countries. ITER may be operating as early as 2007, by which time the participants expect to implement full remote operation.

With both a domestic tokamak and ITER in mind, Livermore recently began work on a DOE-funded Distributed, Collaboratory Experiment Environments Program to develop remote operation capabilities further. This two-year project involves eight national laboratories and universities working in four groups to develop testbeds for remote access to various kinds of expensive, hard-to-duplicate physics facilities—from an electron microscope to Lawrence Berkeley National Laboratory's Advanced Light Source to a tokamak. By building these testbeds and using them for real-world experiments, the groups are studying the technical and interactive aspects of controlling apparatus, taking data, and interacting with colleagues over wide-area networks. The goal is more than an incremental change in today's use of computers and local-area networks; rather, it is the introduction of a new realm.

Livermore is leading one of the four groups in a collaboration that includes Princeton Plasma Physics Laboratory, Oak Ridge National Laboratory, and General Atomics. This group is working to integrate an industry-standard distributed computing environment with Internet-based audio-visual communications to enhance remote collaborations on General Atomics' DIII-D tokamak. The project demands real-time synchronization and exchange of data among multiple computer networks, as well as the presentation of enough auditory and visual information associated with the control room environment so that remote staff are fully integrated in operations.

The vision is for a scientist thousands of kilometers away to get the same sense of presence and control as at the experiment site. The end result of this project should be distributed environments that provide location-independent access to instruments, data handling and analysis resources, and fellow collaborators. This merging of computers and electronic communications will bring substantially increased effectiveness to doing science and spur applications far beyond operating a physics experiment—to environmental monitoring, engineering design, medical triage, and remote diagnosis.

Tokamaks use magnetic fields from variously shaped magnets (orange, red) to contain a plasma (yellow) of hot gases.



Key Words: Magnetic fusion, remote operation, distributed computing.

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