

Center For Computational Sciences

Oak Ridge National Laboratory's Center for Computational Sciences (CCS), along with partners Argonne National Laboratory and Pacific Northwest National Laboratory, is poised to re-establish the United States' leadership in advanced scientific computing through a unique combination of people, facilities, programs, and partnerships. As one of the Department of Energy's leading unclassified scientific computing facilities, the CCS will pave the way for groundbreaking accomplishments through scientific simulation made possible by advances in ultrascale high-performance computing.

Solving the Future's Big Challenges

Through recent advances in supercomputing, simulation is rapidly becoming a peer to theory and experimentation in the pursuit of scientific discovery. Scientific simulation enabled by high-performance computing will underpin many of the future's scientific breakthroughs. Biology, climate, fusion and nanoscience represent some of the nation's important grand challenges targeted. Developing new energy sources, predicting climate change, and understanding how cells work, require the type of ultrascale computational capabilities that CCS plans to provide to the nation's top scientists and engineers.

Opening State-of-the-Art Facilities

Supported by the Department of Energy's Office of Advanced Scientific Computing Research, ORNL's Center for Computational Sciences is housed in the nation's largest unclassified computing facility. The new 170,000-square-foot facility, which includes 40,000 square feet of space for computer systems and data storage is part of the laboratory's \$300 million modernization program. The facility houses 400 multi-disciplinary staff and includes several unique assets such as the Science Exploratorium, a 35-million pixel, 30-foot wide display wall for high-resolution visualization of large scientific datasets. The facility has available 12 megawatts of power supplied by the Tennessee Valley Authority to run world-class supercomputers.



ORNL's Center for Computational Sciences

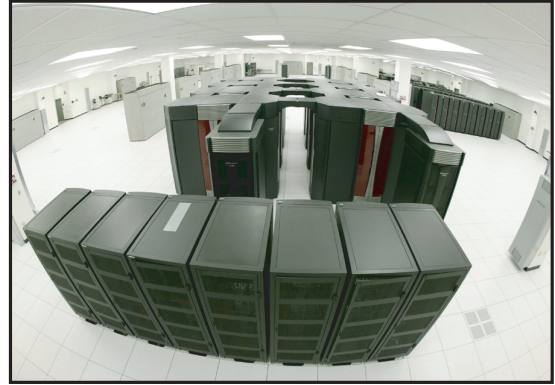
Pushing the Threshold of Human Comprehension

Working with the Department of Energy, ORNL's goal is to help the United States regain world leadership in high-performance computing. Japan has held this position since April 2002. Japan's Earth Simulator is capable of 40 teraflops (40 trillion calculations per second). ORNL seeks to achieve 100 teraflops by 2006 and 1,000 or more teraflops by the end of the decade. The CCS currently offers more than 10 teraflops of combined computing power for application to complex, scientific and engineering computing problems. The Center's present suite of supercomputers includes a Cray X1, an IBM Power4, a SGI Altix, and an IBM Power3.

Building High-Speed Networks

ORNL has several major networks in place or under construction, linking the CCS with Department of Energy laboratories, universities and other supercomputing centers. The Energy Sciences Network links ORNL with DOE laboratories at a data transfer speed of 622 megabits per second, with plans to upgrade to 2.5 gigabits per second. ORNL also connects to the academic community through the

Internet2 network, which has a data transfer speed of 10 gigabits per second. CCS is helping build two new networks, including the UltraScience Net, which will be used to carry large data streams needed for research in areas such as high-energy physics, climate modeling, nanotechnology, fusion and genomics and NSF's teragrid that connects CCS with other supercomputing centers.



Attracting World-Class Talent

New facilities and opportunities to work on grand challenges are drawing many of the world's brightest computational researchers to Oak Ridge. Recent additions include more than 40 science and technology staff members, 56 postdoctoral researchers, 55 graduate students and 12 joint appointees. The CCS is composed of staff from ORNL's Computing and Computational Sciences Directorate, guest and visiting researchers and collaborating researchers from ORNL's science and technology directorates. Many of the new researchers were attracted to ORNL by the opportunity to use the Laboratory's computational resources in addressing multidisciplinary challenges.

Establishing Partnerships

Teams from Argonne National Laboratory, Lawrence Livermore National Laboratory, Los Alamos National Laboratory, NASA, National Center for Atmospheric Research, Pacific Northwest National Laboratory, Princeton Plasma Physics Laboratory, and Sandia National Laboratories join ORNL researchers in addressing critical problems in climate change, biology, chemistry, materials, and fusion that require ultrascale computing capability. High performance computing centers—OSC, AHPCRC, ERDC, SDSC, and PSC—are working closely with CCS in the development of the Leadership Class facility.

ORNL works closely with the University of Tennessee, Oak Ridge Institute for Science Education, and Oak Ridge Associated Universities to develop academic partnerships with all interested parties through the Joint Institute for Computational Sciences, a new facility housed on the ORNL campus. Academic partners already expressing interest include Duke, Florida State, George Tech, Virginia Tech, the University of Virginia, North Carolina State University, and Vanderbilt University.

Three industry-leading vendors—Cray, IBM, and SGI are working closely with ORNL and its partners in the development of the Leadership Class facility. These collaborations will enable the exploration of different architectures and experimental approaches for high end computing for grand challenge science.

Computational Center for Industrial Innovation

Advances in high performance computing promise greater efficiencies in design, modeling and manufacturing that will impact the competitiveness of many sectors across the economy. The Computational Center for Industrial Innovation (CCII) is a designated national user facility within CCS, designed to promote beneficial interactions with industry, and making the most effective use of costly and, in many cases, unique equipment for national competitiveness. The Boeing Corporation and The Dow Chemical Company are among the first industries poised to take advantage of the leadership class computing through the CCII.

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