Computational Science Center

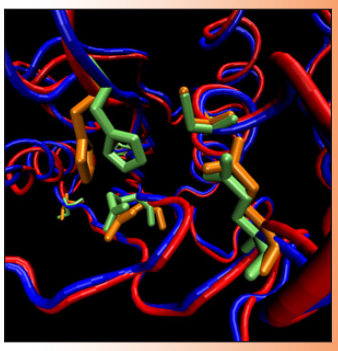
At Brookhaven National Laboratory

Purpose:
To provide computational science capabilities through the use of powerful, state-of-the-art computers for researchers in biology, chemistry, physics, applied mathematics, medicine, and nanoscience

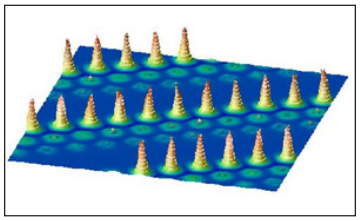
Sponsor:
U.S. Department of Energy's Office of Science

Features:
Large Linux clusters and two QCDOC computers with 12,288 processors each

www.bnl.gov/csc



Computer simulation of the structure of adenovirus proteinase



Calculated spin density of cobalt nanowires on platinum

The Computational Science Center (CSC) at Brookhaven National Laboratory brings together researchers in biology, chemistry, physics, applied mathematics, medicine, and nanoscience to take advantage of the vast opportunities for scientific discovery that the powerful computers of the 21st century have made possible.

Science has become increasingly dependent on computers. Many of Brookhaven's major facilities, such as its premiere physics facility — the Relativistic Heavy Ion Collider — require extremely sophisticated computing power to capture, store and analyze data. Indeed, the functioning of the Laboratory requires a huge network of data storage and distribution. Altogether, Brookhaven invests about $22 million per year in computing hardware and services.

With a staff of 15, the CSC has replaced Brookhaven's Center for Data Intensive Computing and incorporates the staff of the Laboratory's Scientific Computing Services Group.

New Kind of Science

While calculations a century ago were performed with paper and pencil, computers are the indispensable tools of science today. With the huge amount of data involved in many experiments, powerful computers that can solve data-intensive problems must be employed.

Initially, the CSC plans to accommodate research in computational biology, a growing field at Brookhaven and throughout the U.S. In this field, scientists use computers to create interactive models of the complex biological systems they study. Computational analysis of large biological databases, computer modeling of protein-folding, and determining protein structure are some of the investigations that are undertaken with the aid of computers.

New Tools for Science

A typical desktop PC contains one processor. At the CSC, computer clusters running the Linux operating system — typically containing from 100 to 200 processors — are currently available for performing scientific calculations for Brookhaven scientists and their collaborators.

In 2005, Brookhaven Lab will acquire two massively parallel computers for nuclear and high-energy physics. Known as QCDOC, for quantum chromodynamics (the basic theory of elementary particles) on a chip, they will share a similar architecture with IBM's Blue Gene/L, one of the world's fastest computers. Each of these computers, designed by a team from Columbia University, IBM, and the RIKEN BNL Research Center, contains more than 12,000 IBM processors, each with its own memory and an extremely fast interprocessor communication network. Each processor is connected by 24 wires to its neighbors – the equivalent of a 24-lane superhighway for data sharing.

Physicists will use QCDOC computers for calculations in quantum chromodynamics 75 percent of the time, while CSC staff and researchers pursuing other scientific projects will use them the remaining 25 percent of the time.

10/04