Computational Science at Argonne National Laboratory

We are America's *first* national laboratory. We are one of the U.S. Department of Energy's largest research centers. We're a *multidisciplinary* laboratory, with more than two hundred research projects ranging from studies of the atomic nucleus to climate change research. Our research is *world class*. And the atmosphere is *diverse*, *friendly*, and *productive*. All these are reasons for choosing Argonne for computational science.

Conducting World-Class Research

Argonne conducts basic and applied scientific research across a wide spectrum of disciplines, ranging from high-energy physics, chemistry, and molecular biology to climatology, energy transmission, and transportation. Argonne's renowned research facilities include the Advanced Photon Source, the Intense Pulsed Neutron Source, and the Superconducting Heavy Ion Linac. Argonne is also a world leader in computer software and hardware development.

New Technology for the New Millennium

At Argonne, world-class computational resources and technology are enabling diverse and powerful innovations in information technology. Computer scientists and mathematicians in the Mathematics and Computer Science (MCS) Division are teaming with computational chemists, biologists, materials scientists, and other experts to advance the frontiers of science and engineering in many different areas.

Scalable Computing Research Systems

Peta-scale computing systems promise to open new frontiers for research and computing applications. Our driving goal is to carry out the research that will enable us to deliver petaflop performance for as many application regimes as possible as soon as hardware is available. Argonne currently operates BGL, a 2048-processor IBM BlueGene/L system, for use in both systems and applications research, as well as Chiba City, a large computing cluster devoted to developing scalable open software. In addition, the Laboratory has deployed a terascale cluster called Jazz, with proven performance of one trillion floating point operations per second, to support and expand computational science research at Argonne.

Advanced Networking

Argonne leads the TeraGrid Grid Infrastructure Group, which provides extraordinarily large and fast distributed infrastructure for open scientific research, spanning eight resource partner sites, which together provide more than 40 teraflops of computing capability and mass storage capability in the petabytes, linked by networks operating at tens of Gigabit/sec.

Collaborative Technologies

Advances in communications, collaboration, and visualization technologies are providing new ways for scientists and engineers to share and analyze complex data. Argonne's Globus Alliance is devising fundamental mechanisms for integrating geographically distributed computers, scientific instruments, and data. The Globus Toolkit is the backbone for numerous computational science projects, such as the GriPhyN project. Our multimedia display, presentation, and interaction environment – the Access Grid – supports large-scale distributed meetings, collaborative work sessions, seminars, lectures, tutorials, and training. Wall-sized display technology with 10 million pixels allows visualization of simulations and other digital information in great detail.

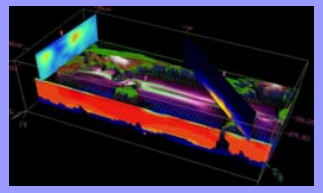
Office of Science
U.S. DEPARTMENT OF ENERGY

mcs

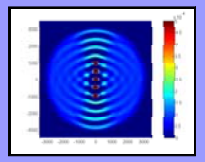
"The field of computational science constitutes one of the great frontiers - and opportunities - of science, from its growing use in 'numerical laboratories' in the context of direct numerical simulations to providing quantitative tools for systems-level analyses of complex phenomena, from the biological to the astrophysical, from basic sciences to engineering. In addition, simulations provide a powerful tool for bridging theory and experimentation, complementing classical analytical tools for problems in which nonlinearities and complexity challenge our understanding." — *Bob Rosner, Director, Argonne National Laboratory*

At the Forefront of Computational Research

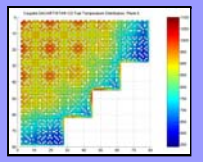
Sophisticated new computer models are simulating a wide range of complex phenomena, including climate modeling, nanosciences, and nuclear physics. Argonne is a world leader in the development of software tools that make these simulations possible on the most advanced computer hardware.



Climate Modeling: Argonne's Model Coupling Toolkit enables high-performance global climate models with oceanic and terrestrial cycles.



Nanosciences: Argonne's 3-dimensional finite-difference time-domain approach allows the simulation of near-field effects in nanophotonics systems.



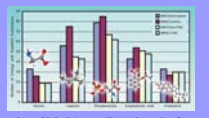
Nuclear Physics: Argonne is developing 3-dimensional multiphysics simulations of the full core of a nuclear reactor.

Astrophysics: The University of Chicago's ASCI Flash Center simulates a stellar flame front as it burns through fuel in full gravity.

Scientific Discovery through Advanced Computing (SciDAC)

The DOE's Scientific Discovery through Advanced Computing (SciDAC) program offers exciting opportunities for attacking cutting edge computational problems. Argonne participates in more than a dozen SciDAC projects.

- ***Numerical algorithms and software***: optimal PDE solvers, component technology, mesh and discretization techniques, optimization algorithms
- ***Parallel programming tools***: programming models, message-passing models, scientific data management
- ***Middleware***: security and group-to-group display technology
- ***Collaborative environments***: collaboratories for particle physics, plasma physics, earth science, and data grids



State of the art algorithms in the Toolkit for Advanced Optimization (ANL) provide up to 40% improvement in the time for optimizing molecular structures with MPQC (SNL) and NWChem (PNNL). Data management employs Global Arrays (PNNL), and software integration uses the Common Component Architecture (CCA).

For further information about Argonne computational science research, see http://www.mcs.anl.gov/LANS/computational-science.html. To discuss CSGF practicum opportunities, contact Ray Bair (bair@mcs.anl.gov).