Advanced Scientific Computing Research
FY 2006 Accomplishments
Applied Mathematics Research
Argonne National Laboratory
Mathematics and Computer Science Division

Multiscale Analysis Reveals New Insights into Pattern Formation in Biological Systems. How do random mixtures of molecular components organize themselves into large-scale cellular structures? To answer this question, Argonne researchers are developing a multiscale mathematical framework to simulate the process of self-organization in biological systems. The focus is on microtubules, the building blocks of cellular structure. A major accomplishment has been the discovery of a previously unidentified cluster state. In addition to providing insights into biological systems, this work has potential application to the formation of transient patterns in populations of mobile bacteria.

Simulations on Massively Parallel (32,000 Processors) Architectures Provide New Insights into Galaxies. Argonne applied mathematicians have developed a state-of-the-art code, Nek5000, that features high-order numerical discretizations and multigrid solvers capable of scaling to thousands of processors. Such extreme scalability is needed to simulate magnetohydrodynamics in complex domains. A major advance this year was the port of Nek5000 to the 32,000- processor Blue Gene platform at IBM Watson (BGW), where the researchers were able to identify an unexpected linear angular vector profile during their study of angular momentum transport in galaxies.

Spectral Element Techniques Remove the Memory Bottleneck in Accelerator Simulations. The performance of accelerators is often limited by the Wavefield effect, which depends on the intensity and distribution of the electron bunch. Traditional finite-difference time-domain methods require about 10^{12} grids and 80 TB of memory for simulating the accelerator chamber. Argonne computer scientists have developed a spectral element discontinuous Galerkin code that now makes the Wakefield problem completely tractable. Only 6×10^{9} grids are needed to resolve a 500 GHz wavelength, with a reasonable memory requirement of only 400 GB.

Toolkit Poised to Play Major Role in the Global Nuclear Energy Partnership. Solvers from Argonne's PETSc (Portable, Extensible Toolkit for Scientific Computing) system have been integrated into a neutronics code, allowing much larger simulations than previously possible. The neutronics code will be coupled with other codes by using a framework being developed for GNEP (Global Nuclear Energy Partnership). The results will enable accurate, fully coupled, high-resolution simulations of fission reactors for the first time.

Awards

Lagrange Prize in Continuous Optimization. Sven Leyffer of Argonne National Laboratory (jointly with Roger Fletcher, University of Dundee, and Philippe Toint, University of Namur) has won the Lagrange Prize in Continuous Optimization for seminal work on filter methods. The prize is awarded by the Mathematical Programming Society and the Society for Industrial and Applied Mathematics only once every three years for original work published in the past six years. Leyffer and his colleagues designed a mathematical filter algorithm that solves a problem of nonlinear programming and may have use in a range of engineering and design applications.

DOE INCITE Award. Argonne researchers Paul Fischer, Fausto Cattaneo, and Aleksandr Obabko received a DOE INCITE award of 2 million hours of supercomputing time to study how stars and solar systems form. The award, which was announced by DOE Secretary of Energy Spencer Abraham in December 2005, was one of only three INCITE awards granted that year. Recently, the researchers also received an extended allocation of 64 "rack days" on the IBM Blue Gene Watson system to continue this work, which is providing new insights into plasma and fusion science.