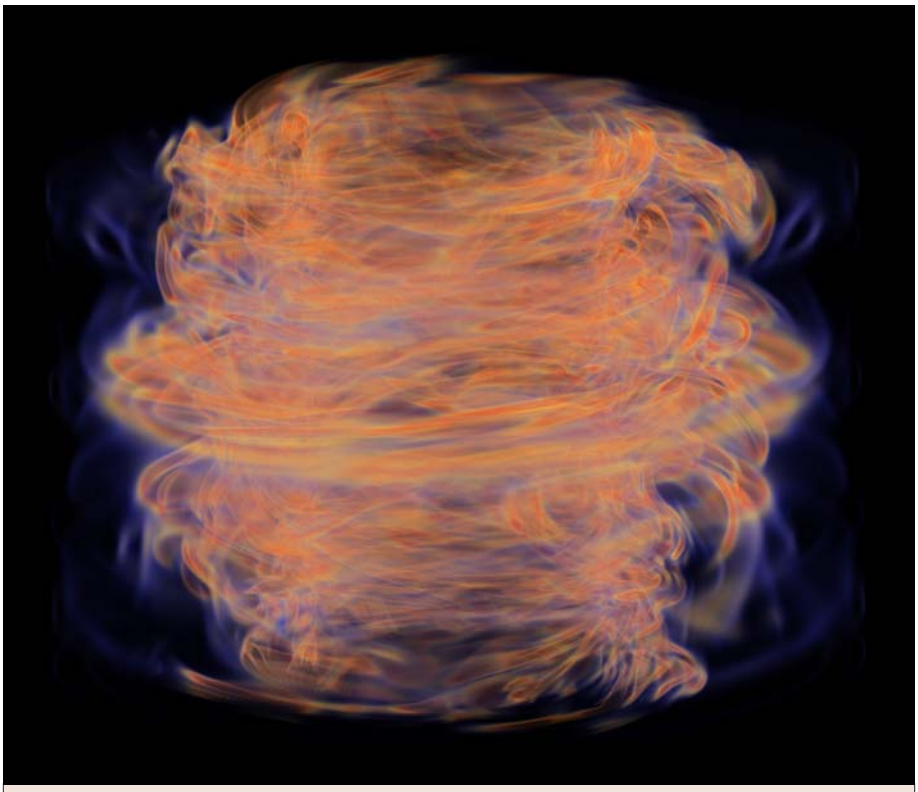
Argonne NATIONAL LABORATORY

Mathematics and Computer Science

Visionary projects receive time on Blue Gene/L supercomputers at Argonne, IBM

Computing projects ranging from understanding Parkinson's disease to modeling climate change have been awarded large amounts of joint time on Blue Gene/L computer systems at Argonne National Laboratory and IBM's T.J. Watson Research Center in Yorktown Heights, N.Y. The computer time is available to researchers through the Department of Energy Office of Science's INCITE program — Innovative and Novel Computational Impact on Theory and Experiment.

"It's good to see the Department of Energy fostering the big ideas, the visionary projects that wouldn't happen otherwise," said Ray Bair, director of the Laboratory Computing Resource Center and Senior Computational Scientist in Argonne's Mathematics and Computer Science Division. "These projects are ones you couldn't approach on a lesser facility. Some of them might even be the wellspring of the next generation for science directions of computation."



COMPUTER IMAGE – Volume rendering of the energy dissipation through the current in the development of magneto-rotational instability, believed to be important in accretion of matter onto a central compact object such as a black hole.

Six projects were allocated over 10 million processor hours through the Argonne and IBM collaboration:

- University of Washington: High Resolution Protein Structure Prediction
- University of California-Davis: Computational Spectroscopy of Aqueous Solutions
- Oak Ridge National Laboratory: Large-Scale Simulations of Fracture in Disordered Media: Statistical Physics of Fracture
- Pratt and Whitney: High-Fidelity LES Simulations of an Aircraft Engine Combustor to Improve Emissions and Operability
- University of Alaska-Fairbanks: Modeling the Response of Terrestrial Ecosystems to Climate Change and Disturbance
- University of California-San Diego: Simulation and Modeling of Synuclein-based Protofibril Structures as a Means of Understanding the Molecular Basis of Parkinson's Disease

Through this collaboration Argonne will provide 10 percent of its Blue Gene/L hours to INCITE, and IBM will provide 5 percent of BGW's hours to INCITE. The BGW system is the second fastest computer in the world, with a capacity of 91 teraflops — 91 trillion calculations per second.

"It's often hard for researchers to get big enough allocations on supercomputers for the most challenging projects," Bair said. "With the extended joint time on the two Blue Gene systems, DOE researchers can attack cutting-edge problems in science and engineering that were previously unfeasible on traditional systems." A computation needing 500,000 hours could run on 1,000 processors for 500 hours, or about 21 days. Running the same project on a single-processor desktop computer would take about 20 years.

INCITE seeks computationally intensive research projects of large scale that can make high-impact scientific advances through the use of a large allocation of computer time and data storage. In its first two years, INCITE has enabled scientists to create unprecedented simulations and gain greater insight into problems in chemistry, combustion, astrophysics, genetics and turbulence. This year, for the first time, proposals from the private sector were also encouraged.

"The overwhelming response to the INCITE program reflects the computational leadership of the Department of Energy," said Raymond L. Orbach, DOE Under Secretary for Science. "The combination of leadership capability machines and software code development allows unprecedented opportunities for researchers across all fields of science and engineering. The Office of Science welcomes proposals from all who are prepared to enter this exciting new realm for scientific discovery."

Blue Gene

"Argonne's Mathematics and Computer Science Division is focusing on petascale computation — creating the tools and applications for addressing the challenges of very large science and engineering problems with computers soon capable of 10^{15} operations per second," said Bair. "Blue Gene has design features that make it especially attractive for computational science. We're evaluating it to see how broadly applicable it is to science and engineering problems."

In the past year scientists from across the nation have identified more applications for Blue Gene than originally expected. Such broad applicability indicates that the supercomputer could well become a mainstay for leadership computing.

The Blue Gene/L is the most powerful computer Argonne has ever had. "It's an example of a machine that's opening many doors in science," Bair said. "Number one is at Lawrence Livermore National Lab. Number two is BGW at IBM. Of the 100 most powerful computers, 19 are Blue Genes, and of those, one is Argonne's."

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