Petaflops Computing and Computational Science to Open New Research Frontiers

The fastest computers created today are capable of speeds of about a teraflop — a trillion operations per second. Impressive as that may sound, for the most challenging problems of interest to the U.S. Department of Energy (DOE), petaflops systems—which are a thousand times faster—are needed.

Motivation

Petaflops-scale computing systems are expected to become technically feasible by the middle of this decade. The availability of such advanced systems promises to open new research frontiers to enable breakthrough science in areas previously considered intractable. Realizing that potential, however, will require significant research and development. The central technology challenge: the vast majority of high-end computers cannot scale to systems capable of 10^{15} operations per second.

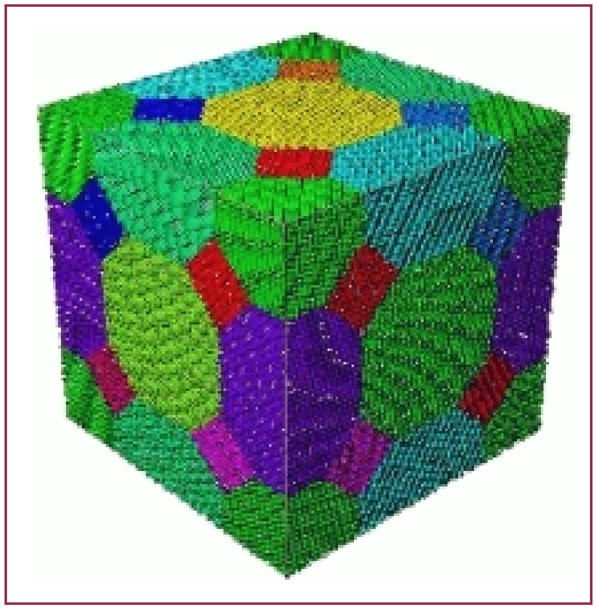

Figure 1. Structure of a 16-grain polycrystal used in deformation studies.

Vision

Argonne's Petascale Computing and Computational Science Initiative is designed to make petaflops-scale computing systems a reality and to ensure that such systems are well suited to important scientific applications. The Laboratory envisions taking an integrated approach that applies advanced computing to leading-edge scientific investigations, both theoretical and experimental (Figures 1 and 2).

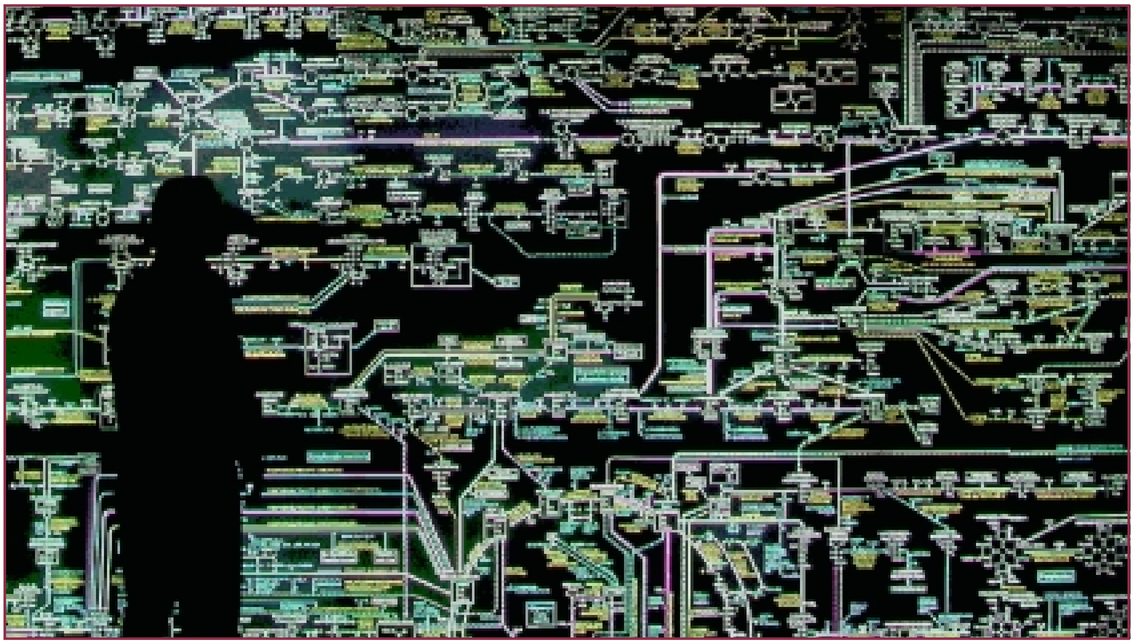

Figure 2. Researchers analyze metabolic pathways on the Active Mural.

The initiative has three major components aimed at advancing the Laboratory's leadership in large-scale scientific computing:

- A labwide computational science program, providing expertise and mid-range computing resources to the Laboratory.
- A targeted R&D program, leading to deployment of a petascale system and development of next-generation modeling capabilities.
- A new advanced computation building, incorporating digital collaborative technology and capable of housing a petaflops computing system.

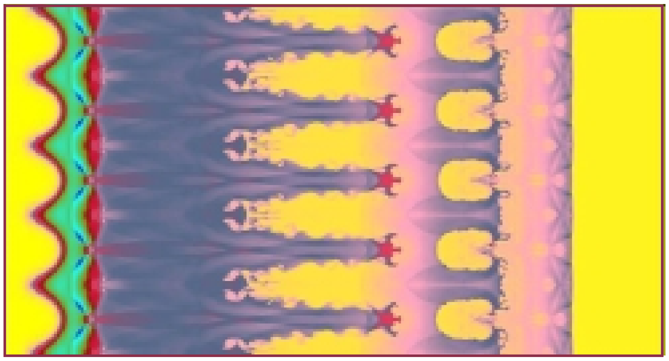

Figure 3. Simulation of instabilities generated by a laser-driven shock through a three-layer target.

Approach

Critical to the efforts of the Petascale Computing and Computational Science Initiative are partnerships: teams of computer scientists, computational scientists, and hardware developers that span laboratories, universities, and the commercial sector. Toward this end, the Laboratory, collaborating with researchers at the Center for Astrophysical Thermonuclear Flashes (Figures 3 and 4), has initiated joint programs with the Argonne/University of Chicago Computation Institute, and is working with industry on design options for specific application classes.

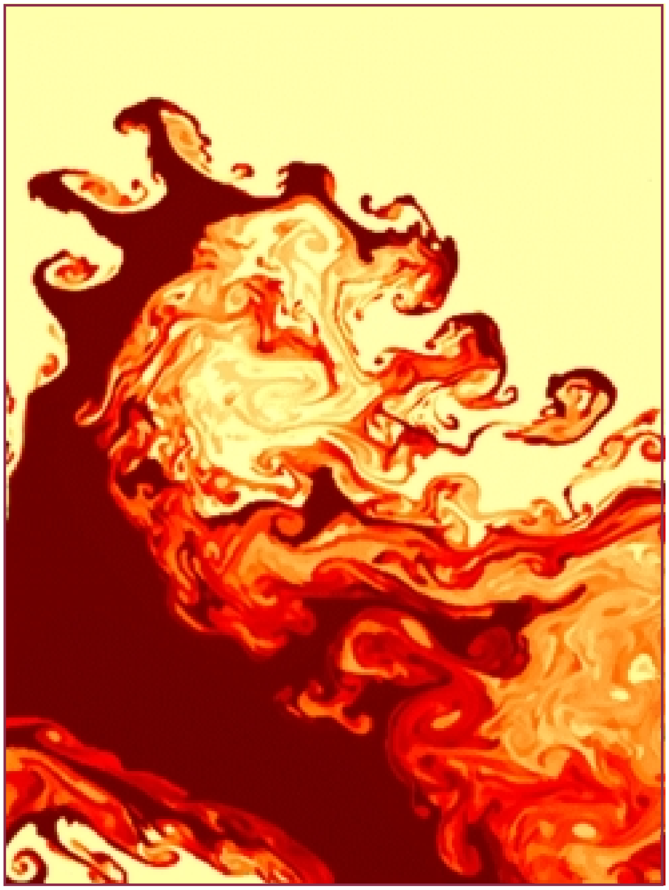

Figure 4. Argonne computer scientists collaborate with University of Chicago researchers to develop the tools needed for simulating astrophysical phenomena.

Applications

Current applications involve design of a whole-cell modeling system (in collaboration with The University of Chicago) and development of a nanoscience simulation environment that combines models at multiple temporal and spatial scales. Increased computational science efforts are anticipated in all areas of Laboratory research, including computational chemistry, reactor engineering, nuclear physics, climate modeling, and transportation.

Sponsor

U.S. Department of Energy

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