Breakthrough 3D simulations win prestigious 2005 Gordon Bell Prize

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A team of scientists led by physicist Fred Streitz has been awarded the 2005 Gordon Bell Prize for pioneering materials science simulations conducted on the world's fastest supercomputer at Lawrence Livermore National Laboratory.

The winner was announced at the conclusion of the Supercomputing 2005 conference held earlier this month in Seattle, Wash. Other team members included James Glosli, Mehul Patel, Bor Chan, Robert Yates and Bronis de Supinski of Lawrence Livermore, and James Sexton and John Gunnels of IBM. The title of their entry was "100+ Tflop/s Solidification Simulations on BlueGene/L."

Named for one of the founding fathers of supercomputing, the prestigious Gordon Bell Prize is awarded to innovators who advance high-performance computing.

Running a newly developed, three-dimensional molecular dynamics code (ddcMD) on BlueGene/L – the IBM machine that ranks No. 1 on the list of the world's Top500 supercomputers – the team investigated solidification in tantalum and uranium at extreme temperatures and pressure with simulations ranging in size from 64,000 atoms to 524 million atoms.

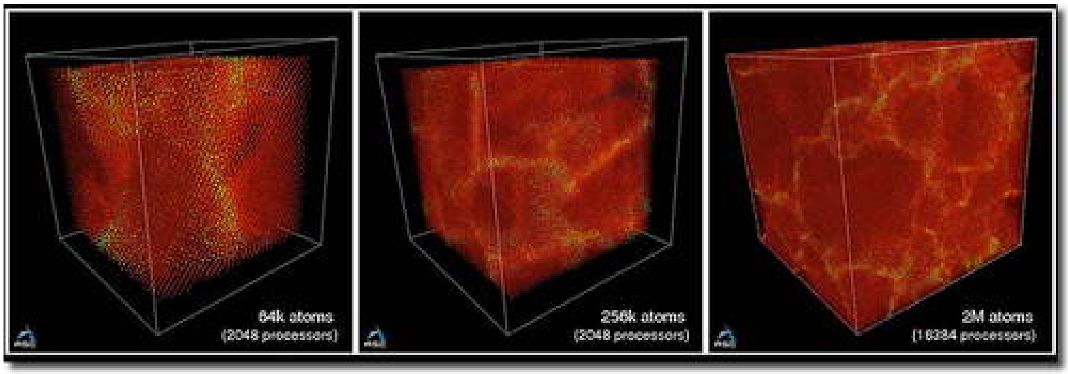

Image: Simulations recently completed on BlueGene/L with LLNL's new parallel ddcMD code: Molten tantalum at 5000°K is isothermally compressed, resulting in solidification to a polycrystalline phase. The 0.75-nanosecond, 2-million-atom simulation on the right, obtained in a 30-hour run, yields the first realistic grain-size distribution emerging entirely from the melt, making it possible to model natural nucleation and growth processes as well as to create grain structures that reflect the directional quantum-mechanical bonding of the atoms – a result that was unobtainable without BlueGene/L.

"These simulations allow us for the first time to examine the process of solid formation at high temperature and pressure from the atomistic level. We can actually watch, atom by atom, as macroscopic grains grow out of the liquid and form structures," said Streitz. "This allows us to better understand the properties of these metals and has important implications for the development of stronger metals, such as those that might be used for aircraft or automobile components as well as other applications."

In the largest simulation of its kind, the team achieved a performance rate of up to 107 teraflop/s (trillion operations per second) with a sustained rate of 101.7 teraflop/s over a seven-hour run on the IBM machine's 131,072 processors. This performance, using what will be a workhorse application for BlueGene/L to do work vital to the National Nuclear Security Administration's (NNSA) mission, exceeds the best performance by any other computer on the industry standard LINPACK benchmark.

"BlueGene/L is ideally suited for precisely the kinds of molecular dynamics studies that the program needs to do at this time to better understand the behavior of materials at high temperature and pressure," said Bruce Goodwin, Associate Director for Defense and Nuclear Technologies at LLNL. "By working with IBM to develop this machine, we created simultaneously a solution that provides both the best sustained performance and the lowest cost per floating point operation. This is an ideal combination. Usually, one gets one or the other. In this case, we got both, and while we planned it this way, we are delighted that it worked out so well."

Simulations of the solidification of metals such as tantalum and uranium under high temperatures and pressures provide valuable insights into the properties of these materials important to the National Nuclear Security Administration's (NNSA) stockpile stewardship program to ensure the safety, security and reliability of the nation's nuclear deterrent without underground testing.

The simulations were conducted by NNSA's Advanced Simulation and Computing (ASC) program, a tri-lab effort uniting the computing know-how of Sandia, Los Alamos and Lawrence Livermore national laboratories.

NNSA scientists need the detailed information about the properties of the materials in nuclear weapons that 3D simulations provide to understand the effects of aging on those weapons systems as they age well beyond their intended design life.

Source: Lawrence Livermore National Laboratory

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