Fusion researchers use Titan supercomputer to burst helium bubbles

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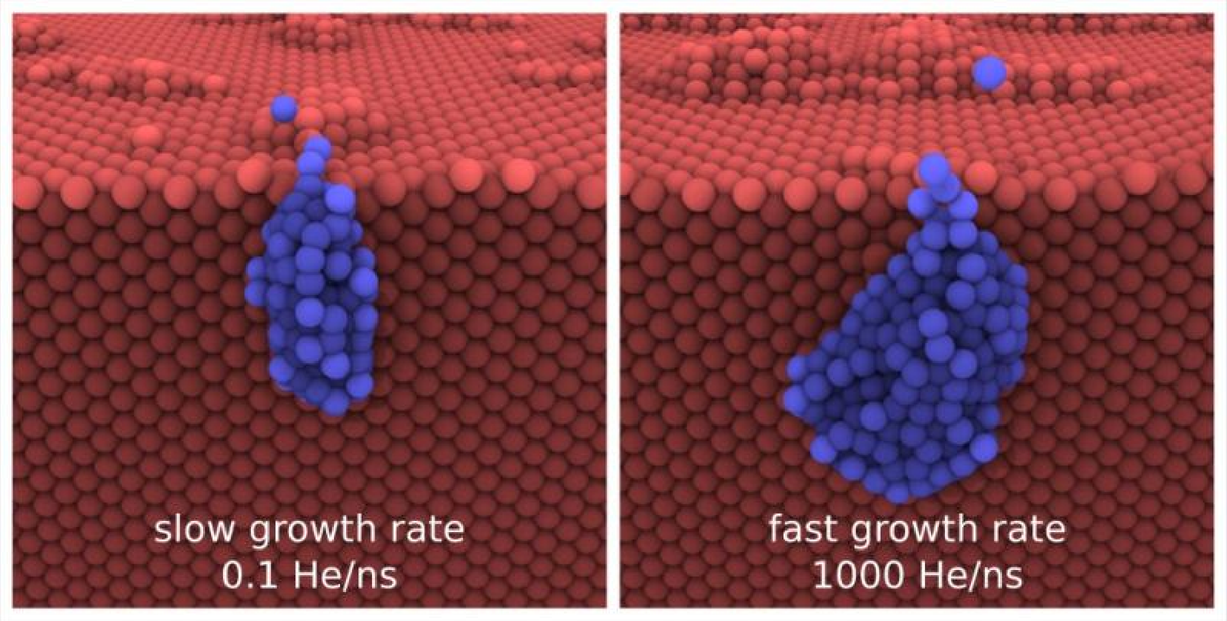

Using their ParRep method on the Titan supercomputer, Los Alamos National Laboratory researchers were able to simulate the surface morphology for helium bubbles growing inside of a fusion reactor's divertor wall for two different growth stages. The combination of Titan and the ParRep method completed simulations in 30 minutes that would have taken months using traditional molecular dynamics approaches. Credit: Luis Sandoval, Arthur Voter, Blas Uberuaga, and Danny Perez

Scientists look to the stars when it comes to developing clean, virtually limitless energy. Though humanity understands how stars power themselves—nuclei of hydrogen and its isotopes fuse together in extreme conditions, releasing bursts of energy in the process—they have been unable to replicate this massive fusion process on Earth in a way practical for power production.

As part of a Scientific Discovery through Advanced Computing (SciDAC) project, a partnership between the US Department of Energy's (DOE's) Advanced Scientific Computing Research Leadership Computing Challenge and Fusion Energy Sciences programs, researchers are using the Oak Ridge Leadership Computing Facility's (OLCF's) Titan supercomputer to try to get closer to producing sustainable fusion for electricity.

The project, led by Brian Wirth, a researcher with the University of Tennessee and DOE's Oak Ridge National Laboratory, brings researchers from various organizations together to work on different aspects of the ITER experimental fusion reactor under construction in southeastern France. An international collaboration, ITER will be by far the largest fusion reactor ever built. Participating countries hope the reactor will serve as proof of concept for future fusion power plants.

"Essentially fusion is the ultimate energy source," Wirth said. "The stars fuse hydrogen isotopes together, and that produces all of the periodic table, and we're trying to replicate that with the fusion program here on Earth."

ITER is a tokamak, or doughnut-shaped, reactor. Scientists will use two hydrogen isotopes, deuterium and tritium, and create a plasma, the fourth state of matter. They then will send the plasma around the tokamak at high speeds and at very high temperatures—anywhere between 10 million and 100 million degrees kelvin. When deuterium and tritium collide in such an extreme environment, they fuse together. This fusion process transforms two hydrogen isotopes into a helium atom, releasing energy and an excess neutron.

"Our particular project is focused on the divertor," Wirth said, referencing the part of ITER that serves as a cache for heavier, more energetic particles from fusion byproducts and reactor material that can pollute the plasma, lower its temperature, and ultimately make it difficult to sustain the fusion reaction. "ITER will hopefully answer a major question for fusion, whether we can make and sustain the plasma conditions at high-enough density and hot-enough temperature, but we still don't have the materials and technology to make a reactor to extract electricity out of."

Wirth and his collaborators are using Titan, a Cray XK7 supercomputer capable of 27 petaflops, or 27 quadrillion calculations per second, to shed light on how fusion plasma interacts with the materials used to build the reactor. The team received computing time at the OLCF, a DOE Office of Science User Facility, through the Advanced Scientific Computing Research Leadership Computing Challenge program.

Testing the toughness of tungsten

Researchers designing ITER plan to use tungsten—one of the toughest materials known—for the divertor. However, despite tungsten's relative strength, there is still concern about how the plasma could affect the divertor over time.

As helium particles bombard the tungsten wall, they begin to form clusters within the material. Once a helium atom is embedded in the wall, it attracts other helium particles. When enough helium is bunched together, it can "knock out" a tungsten atom from its normal position within the material, forming a nanoscale cavity, or hole, within the tungsten. This forms the nucleus of a helium bubble that can then grow very large, reducing the durability of the material. These bubbles also serve as traps for tritium, which reduce the amount involved in the fusion reaction and introduce a radiological hazard.

In addition to tritium retention, helium bubbles cause other problems. As they cluster together and push out tungsten atoms, the divertor's surface is left with a fuzz-like nanostructure, literally appearing like steel wool, but on the nanoscale. The concern is that these nanoscale wires can erode into the plasma, degrading its quality, cooling the reaction, and making the reaction far more difficult to maintain.

A Los Alamos National Laboratory (LANL)-based team made up of Luis Sandoval, Danny Perez, Blas Uberuaga, and Arthur Voter is working to understand more fully how tungsten behaves in such harsh conditions. The group hopes that by better understanding the interactions between helium bubbles and tungsten, they can predict the evolution of the material and maybe even mitigate concerns over tungsten in the reactor.

"If ITER researchers can't mitigate tungsten turning into a fuzz-like structure, they may have to turn to another material for a reactor that's halfway built," Voter said. "We're working on one small part here to try to understand something more about how, when the helium bubbles come to the surface, they contribute to this fuzzy roughness."

Particle interactions in parallel

Many computational scientists use molecular dynamics (MD) simulations to model particle interactions. Though MD can model complex and relatively large atomic systems, its sequential nature—in which calculations must be done one at a time—makes it computationally expensive to reach experimentally relevant time scales. Therefore, the LANL team is using an alternative to traditional MD and is getting a massive speedup in time-to-solution in the process.

The team is using the Parallel Replica (ParRep) method, developed at LANL in the 1990s with the support ofDOE's Office of Basic Energy Sciences (which also supports Voter's work on this fusion project). Applying an implementation of ParRep in the LAMMPS code, they achieve that drastic speedup—a simulation using more than half of Titan's computing power can be done in 30 minutes using the LANL method, whereas it would have taken 7 months using traditional MD simulations.

In traditional MD, researchers calculate forces on all particles in a particular model. Then, researchers choose a very small time increment—typically about a femtosecond (one quadrillionth of a second)—and run this force calculation repeatedly to observe particles in motion, by integrating Newton's equations of motion. Even with leadership-class computing resources like Titan, running a simulation of a few thousand tungsten and helium atoms in a fusion reactor for a microsecond would require many weeks of computation with MD.

ParRep works in similar fashion to traditional MD but streamlines the process on molecular systems that only occasionally change their average position—like atoms in the divertor wall. As opposed to other parallelization strategies for MD, which parallelize the spatial dimensions, ParRep parallelizes the time domain. To grasp the essence of the algorithm, think of 100 people holding egg cartons that only have one egg each. Each person shakes his or her carton until one egg in any one of the 100 cartons hops from one hole to another. When this event happens, everyone else stops shaking. You would then multiply the time it took by 100 (because 100 people were shaking cartons), and that would give you the average time it would take to see that event if only one person were shaking one egg carton.

Though ParRep was developed in the 1990s, Sandoval says powerful computers are required to take full advantage of the method. "The method was first developed almost 20 years ago, but it's only because of access to machines like Titan that we can do these simulations," he said.

By using ParRep, Sandoval was able to simulate many microseconds of time rather than pico- or nanoseconds (10^{-12} and 10^{-9}, respectively). This speedup allows researchers to more fully understand how helium particles interact with the divertor wall. In particular, the LANL team found that the evolution of bubbles, when simulated over these realistic time scales, is qualitatively different from what is observed when traditional MD is used. The team's findings were published in the March 11 issue of *Physical Review Letters*.

Ultimately, the LANL work will serve as the foundation for the larger SciDAC project. The SciDAC group is developing a suite of computer codes that will together create a more comprehensive fusion materials simulation. "Part of our SciDAC is learning the most important processes that occur over nanosecond or microsecond timescales, and learning how to integrate them into a continuum code," Wirth said. "Our ultimate objective is to develop a continuum-level code that we've got confidence simulates the most important aspects of fusion materials physics when we don't have experimental facilities that can tell us that."

Though ITER is still far from completion, the Wirth collaboration plans to continue to refine its code suite and try to solve as many problems as possible before ITER goes online.

Provided by Oak Ridge National Laboratory

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