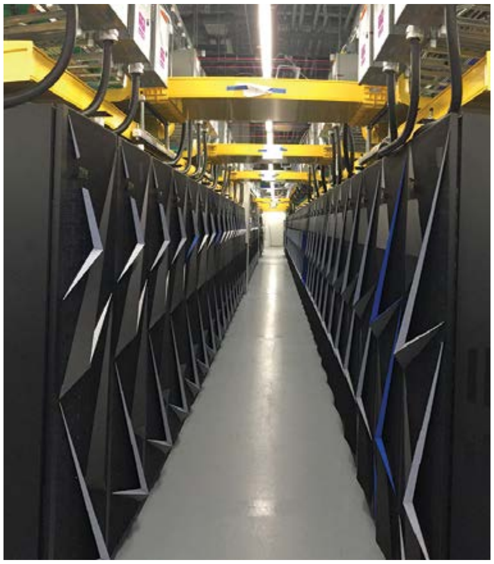
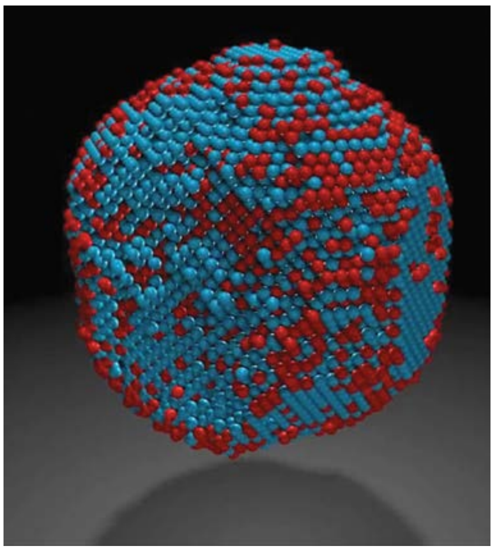
The *HIGH-STAKES RACE* in HIGH-PERFORMANCE COMPUTING





Very fast computers are increasingly critical to maintain national security and for many areas of science and industry to model chemical processes or predict material properties. U.S. leadership in high-performance computing is now challenged by China, as each country seeks to build faster computers by increasing the number of processing units that operate in parallel. It turns out, however, that raw computing speed is not the only thing that counts. Specialized software that can make effective use of these massively parallel computers—by dividing up problems among all those processing units and reassembling the results—is equally important. And here the U.S. holds a substantial lead, thanks to decades of research supported initially by the Basic Energy Sciences (BES) office of DOE (and now by many agencies).

The Breakthrough

Developing novel computer software—designed for use on massively parallel supercomputers—that transformed multiple areas of science.

- Transforming theoretical chemistry by modeling how individual molecules break and form chemical bonds, including the intermediate states of chemical reactions that are hard to measure experimentally.
- Predicting the properties of metal alloys and complex magnetic materials with atom-by-atom calculations.
- Simulating the combustion that occurs when fuel is injected into an engine, including how the air and fuel mix and how that affects the rate and completeness of burning.

The Impact

Accelerated development of new industrial materials and cleaner diesel engines, as well as a significant U.S. advantage in high-performance computing.

- Accelerated development of biofuels, solar cells, and advanced batteries, as well as more rapid development of new plastics by the petrochemical industry.
- Transformed ability to design new nanoscale materials for applications such as next-generation data storage devices.
- Improved efficiency in diesel engines and a remarkable reduction in pollutant emissions in recent decades, because on-board computers now adjust when fuel is injected to optimize combustion as engines warm up or conditions change.

The Takeaway

A pioneering fundamental research effort into the development of software for massively parallel computers—begun when it was clear that such computers were the future but well before any existed—has given the U.S. a significant edge in high-performance computing.

ABOUT THE IMAGES

The Summit supercomputer just completed at Oak Ridge National Laboratory in Tennessee has more than 36,000 separate processor units operating in parallel and is expected to process some 200 million billion operations per second.
(OAK RIDGE NATIONAL LABORATORY)

A magnetic nanoparticle composed of 23,000 iron (red) and platinum (blue) atoms is a promising material for next-generation data storage devices. A supercomputer analysis of its magnetic structure—calculated separately atom by atom—is helping to optimize its properties.
(JIANWEI MIAO / UNIVERSITY OF CALIFORNIA AT LOS ANGELES)

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