Anton Supercomputer Proves Its Mettle

By Elizabeth K. Wilson

Shaw Research's supercomputer Anton is designed to simulate the dynamics of biological macromolecules.

Credit: Courtesy of Matthew Monteith

The supercomputer Anton is online and ready to fold proteins. D. E. Shaw Research, which designed and built the massively parallel Anton, has at last verified the machine's much-publicized capabilities, reporting Anton's first major long-time-scale protein dynamics simulations.

The computer performed two types of simulations of well-studied systems: In the first, Anton's 100-microsecond simulations of the protein domain FiP35 show that the domain folds and unfolds in the same progression of steps each time—a surprise to some researchers. The second simulation involved a longer, one-millisecond study of the dynamics of the already folded protein bovine pancreatic trypsin inhibitor (BPTI), which explored the intricate motions of protein in water. Results were published in *Science* (**2010,** *330,* 341).

"This work demonstrates that their machine really can do the tasks they proposed," says Vijay Pande, an associate chemistry professor at Stanford University and creator of the folding@home project, which harnesses volunteers' home computers to carry out computationally intensive protein calculations.

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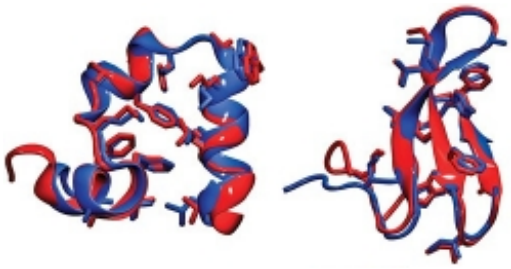

Folding Two Ways

A comparison of protein folding results from X-ray crystallography (blue) and Anton's molecular dynamics simulations (red) of the protein domain villin (left) and FiP35.

Credit: © Science/AAAS

Anton was built solely for the purpose of molecular dynamics (MD) simulations of the behavior of large biological molecules. The machine, which was completed more than a year ago, stakes its claim to fame on its ability to perform lengthy simulations that aren't possible on current supercomputers. The new results mark the first significant test of Anton's prowess.

MD simulations, which track the motions of every atom in a large molecule, are limited in their time scales by computer power and architecture. It can take months for a supercomputing system to simulate only tens of microseconds of a protein's dynamics. But many proteins fold on the millisecond time scale.

Anton, its creators report, is capable of performing millisecond-long simulations of systems containing tens of thousands of atoms in 100 days—100 times faster than with current supercomputers.

David E. Shaw, chief scientist at Shaw Research, tells C&EN that Anton is now simulating proteins with more

complicated folding behavior. "We now have some encouraging preliminary results on the folding of certain proteins that are known to fold more slowly than those investigated in the *Science* paper," he says.

Klaus J. Schulten, director of the Theoretical & Computational Biophysics Group at the University of Illinois, Urbana-Champaign, cautions that an intimate understanding of biomolecule behavior is still a ways off. Although Anton's capabilities are a "major advancement," the problems that Anton, and indeed MD simulations in general, can solve well are very specific: the behavior of proteins in water, he tells C&EN.

Once a simulation starts, it can't be adjusted. "You cannot change conditions on the fly; it has to be hands off," Schulten says. Only about 10% of protein-folding problems can be done this way, he adds.

Recently, Shaw Research donated another Anton machine to the Pittsburgh Supercomputing Center for research use by universities and other nonprofit institutions through the National Resource for Biomedical Supercomputing.

Schulten's group is one of 45 that were allotted time on the machine by the National Science Foundation. His group began simulations last week, and "it's working very well," he says.

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