New Stanford software takes Folding@home's biological research to supercomputers

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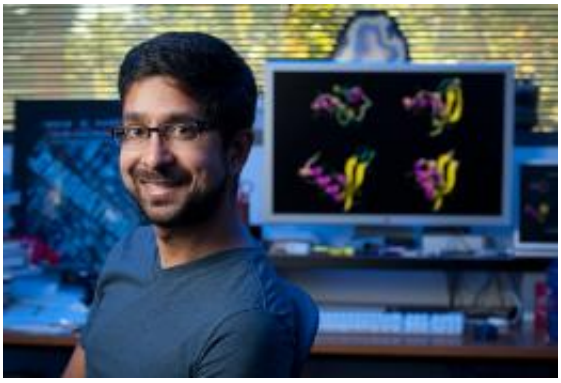

Chemistry Professor Vijay Pande's group recently used Folding@home simulations to investigate new therapeutic approaches for Alzheimer's.

Vijay Pande's chemistry and structural biology group at Stanford has become known for Folding@home, a distributed computing project that borrows computing time from home computers to simulate how proteins take shape.

Now, other researchers will be able to take advantage of the computing technology that Pande's group has developed over the last decade. The new distributed framework for supercomputers, called Copernicus, was presented this week at SC11, an international supercomputing conference, in Seattle.

Copernicus was developed in collaboration with the labs of Erik Lindahl at Sweden's KTH Royal Institute of Technology and Stockholm University and Peter Kasson at the University Virginia.

"We're bringing Folding@home to supercomputers," said Pande, a professor of chemistry.

Proteins control nearly all of life's functions, but how they self-assemble, or fold, is an unsolved problem in biology. Understanding how folding goes awry could lead to cures for diseases caused by protein misfolding, like Alzheimer's and Parkinson's.

By modeling protein folding, Pande says, "We hope to get exquisite detail and information that you might not be able to get from experiments."

Folding@home uses processor time donated by millions of home computer and video game console users. It has advanced the field of molecular dynamics by cutting protein-folding simulation times from years to days. Recently, Pande's group used Folding@home simulations to investigate new therapeutic approaches for Alzheimer's.

The vast computing resources of Folding@home have been available to Pande and his collaborators. With open-source Copernicus software, other researchers can run simulations, including molecular models, using processer time on multiple supercomputers or computing clusters, rather than home computers.

"It opens the door to huge crowds of people using these methods, which have matured with Folding@home," Pande said.

With an interest in solving protein structures and having large computing clusters on hand, pharmaceutical companies are an example of one

potential Copernicus user-group.

The advantage of Copernicus comes from how it uses the fast communication available between supercomputers, combined with statistical sampling techniques, to run parallel simulations within or between computing clusters or between supercomputers.

Copernicus allows for each additional processor in the system to aid the calculation to run faster and faster, something known as strong scaling. Previously, when using supercomputers to understand molecular dynamics, it has been very difficult to achieve strong scaling on a single machine.

"This method should be able to use any supercomputer on the planet completely," Pande said. "Strong scaling to these extremes is unusual."

Folding@home is useful for molecular simulations that take place on relatively long timescales. But Copernicus will be a tool for shorter problems where researchers want a quick solution.

Computationally, using Copernicus is like taking a Lamborghini to run out for milk. Folding@home, on the other hand, "is kind of like a rocket. It takes a big deal to launch it and once you launch, it goes really far," Pande said. "You don't use it to go to the corner store."

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