Software speeds up molecular simulations

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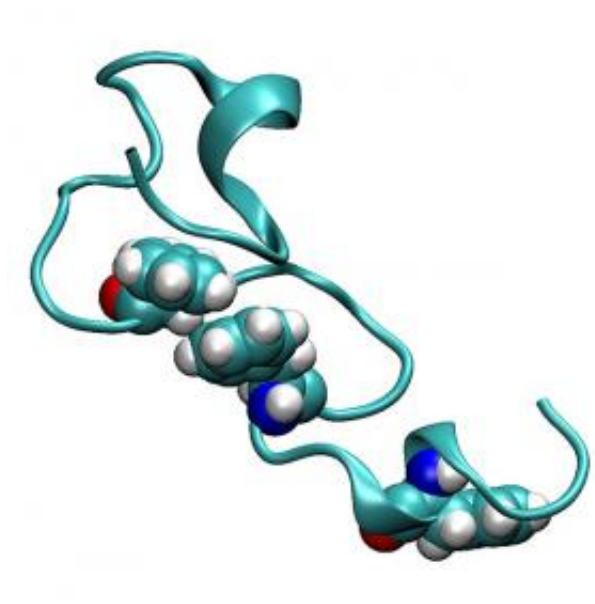

A snapshot from a molecular dynamic simulation of the folding of a mutant protein found in chicken intestines. New open-source software permits faster simulations of molecular motion on desktop computers. Courtesy of Daniel Ensign

(PhysOrg.com) -- Whether vibrating in place or taking part in protein folding to ensure cells function properly, molecules are never still. Simulating molecular motions provides researchers with information critical to designing vaccines and helps them decipher the bases of certain diseases, such as Alzheimer's and Parkinson's, that result from molecular motion gone awry.

In the past, researchers needed either supercomputers or large computer clusters to run simulations. Or they had to be content to run only a tiny fraction of the process on their desktop computers. But a new open-source software package developed at Stanford is making it possible to do complex simulations of molecular motion on desktop computers at much faster speeds than has been previously possible.

"Simulations that used to take three years can now be completed in a few days," said Vijay Pande, an associate professor of chemistry at Stanford and principal investigator of the Open Molecular Mechanics (OpenMM) project. "With this first release of OpenMM, we focused on small molecular systems simulated and saw speedups of 100 times faster than before."

OpenMM is a collaborative project between Pande's lab and Simbios, the National Center for Physics-based Simulation of Biological Structures at Stanford, which is supported by the National Institutes of Health. The project is described in a paper that was scheduled to be posted online Feb. 3 in the "Early View" section of the *Journal of Computational Chemistry*.

The key to the accelerated simulations OpenMM makes possible is the advantage it takes of current graphics processors (GPUs), which cost just a few hundred dollars. At its core, OpenMM makes use of GPU acceleration, a set of advanced hardware and software technologies that enable GPUs, working in concert with the system's central processor (CPU), to accelerate applications beyond just creating or manipulating graphics.

The icing on the molecular-simulation cake is that the software has no allegiance to any particular brand of GPU, meaning it is, as computer geeks like to say, "brand agnostic." OpenMM will enable molecular dynamics (MD) simulations to work on most of the high-end GPUs used

today in laptop and desktop computers.

This is a boon to MD developers. Converting their code to run on just one GPU product is a challenging project by itself. And until now, if developers wanted to accelerate their MD software on different brands of GPUs, they would have to write multiple versions of their code. OpenMM provides a common interface.

"OpenMM will allow researchers to focus on the science at hand instead of the hardware," Pande said. "Researchers will see a jump in productivity and resourcefulness from computers they already own." With OpenMM, researchers can use GPUs to perform massively parallel calculations.

OpenMM fits squarely with Simbios' mission of providing computational tools to stimulate research in biology and medicine, according to Russ Altman, principal investigator of Simbios and chair of the Department of Bioengineering at Stanford. "OpenMM will be a tool that unifies the MD community," he said. "Instead of difficult, disparate efforts to recode existing MD packages to enjoy the speedups provided by GPUs, OpenMM will bring GPUs to existing packages and allow researchers to focus on discovery."

OpenMM incorporates specially developed algorithms that allow MD software to take full advantage of the GPU architecture. In fact, the OpenMM code is at the heart of the GPU implementations of the Folding@home project, which uses the horsepower of GPUs and CPUs in computers around the world to simulate protein folding. The current release uses an implicit solvent model, in which all the surrounding fluid, such as water, is represented as one continuous medium, rather than having each water molecule represented individually (an explicit solvent model). Future releases will allow the modeling of explicit solvent.

A free workshop on OpenMM and OpenMM Zephyr (simtk.org/home/zephyr), an easy-to-use application for running and visualizing accelerated MD simulations, will be offered sometime in the next three months. Anyone interested in learning about using OpenMM and OpenMM Zephyr will be welcome. A workshop on Feb. 12 is already filled. For more information on the workshop, or a symposium on molecular dynamics held the day after each workshop, email simbiosfeedback(at)stanford.edu.

Source: Stanford University