

BY JOY KU, PHD

OpenMM: Bringing GPU Acceleration Capabilities to Molecular Dynamics

Over the last three years, the lab of **Vijay Pande, PhD**, at Stanford University has optimized their molecular dynamics (MD) algorithms to take advantage of the fast computing that's possible with GPUs, or graphics processing units (see this issue's Under the Hood column for more information about GPUs). Now, through their collaboration with Simbios that capability will be made freely available to the whole community via a library called Open Molecular Mechanics, or OpenMM.

"OpenMM will be a tool that unifies the MD community," says **Russ Altman, MD, PhD**, principal investigator of Simbios and a professor of bioengineering, genetics, medicine, and computer science at Stanford University. "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."

There are tens of MD packages available today: GROMACS, NAMD, and Amber to name just a few. Currently, if an applications developer wanted to accelerate their MD software using GPUs, they would have to write multiple versions of their code since each GPU manufacturer uses a different set of commands. OpenMM would provide a common interface, hiding the details of programming the different GPUs.

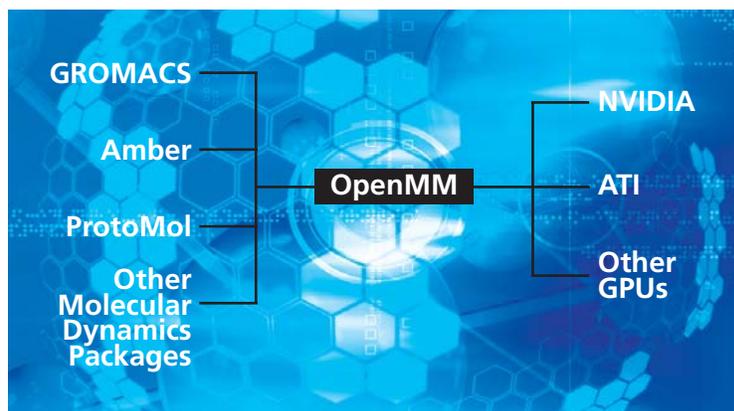
"The user wouldn't even have to think about any of the GPU craziness," says Pande, associate professor of chemistry and of structural biology at Stanford University and lead of the OpenMM project. "All they would know is that they want to do a force calculation or an energy calculation and they'll just know it's going to be done fast on a variety of hardware."

How fast? "On GPUs, we routinely get speedups by a factor of 100 and in some cases, close to a factor of 1000," says Pande. "Those types of speedups can really change how your work gets done. Things that used to take three years can now get done in a day."

DETAILS

OpenMM is part of Simbios' new protein folding driving biological problem (DBP). Hundreds of the protein folding trajectories generated by the Pande lab are also being made available as part of this DBP. See <https://simtk.org/home/foldvillin>.

To learn more about OpenMM, visit <https://simtk.org/home/openmm>. The first open code release of OpenMM is planned for Fall 2008 and will be available for download from this Web site.



OpenMM makes it easy to use GPUs to speed up different molecular dynamics packages.

Grant Krafft, PhD, Chairman and Chief Science Officer of Acumen Pharmaceuticals, Inc., has benefited directly from faster simulations. His company uses Pande's simulation software to help them design molecules to treat and prevent Alzheimer's.

"With the expanded capabilities of these simulations, we can get a more complete picture of which molecular assemblies prefer to form," Krafft says. "What's really important is that they don't incorporate approximations that many other molecular dynamics calculations have to incorporate, approximations that would lead to errors."

OpenMM makes it possible for other scientists to achieve similar results with their preferred MD code without much more programming and without an expensive supercomputer or a cluster. The only additional hardware that might be needed would be a high-end GPU board, which costs just a few hundred dollars these days and is straightforward to install.

The first release of the OpenMM library is planned for the fall of 2008. The release will include integration of the OpenMM library into the GROMACS MD package.

"Nobody's really coming close to what Vijay's doing in terms of duration of folding and dynamics studies," says Krafft. But with the release of OpenMM, those capabilities could easily become available to all. □

