OpenMM Workshop: Background and Logistical Details

An Introduction to Molecular Dynamics & OpenMM Zephyr (for scientists):

Researchers are increasingly using molecular dynamics (MD) simulations to model molecular motion and help expand our knowledge and understanding of biology. Examples of how MD simulations have been used include:

- Providing hypotheses for biological phenomena that cannot currently be observed experimentally and guiding new experiments [1, 2, 3]
- Identifying which engineered molecules would be stable or would bind with another molecule [3]
- Augmenting information provided by static structures, i.e., from x-ray crystallography [4]

The potential uses for MD simulations are exciting, but getting started can be overwhelming and time-consuming. OpenMM Zephyr was designed to get researchers running MD simulations quickly.

OpenMM Zephyr is a freely downloadable application with a graphical user interface that allows users to easily run the OpenMM version of GROMACS, a widely used MD package, and visualize the results. The OpenMM version significantly speeds up GROMACS on recent versions of NVIDIA and ATI graphics processing units (GPUs) – graphics cards—with speed ups of over **100X** in some cases.* This makes it more reasonable to simulate larger molecules and/or longer processes.

OpenMM Overview (for MD developers):

OpenMM is a freely downloadable, high performance, extensible library that allows molecular dynamics (MD) simulations to run on high performance computer architectures, such as graphics processing units (GPUs). Significant performance speed ups of over **100X** in some cases were achieved using OpenMM.*

The library performs full protein Hamiltonian calculations without any cutoffs (full $O(N^2)$ treatment). The January release includes a version of GROMACS that uses OpenMM to speed up its calculations on recent versions of NVIDIA and ATI GPUs. The current release supports implicit solvent models (Onufriev, Bashford, Case GB), with explicit solvent models to be incorporated into the next release.

OpenMM Workshop Details:

The workshop will be held on February 12-13, 2009 at Stanford University. The first day of the workshop is geared towards MD developers. A detailed presentation of OpenMM and its integration into GROMACS will be given, followed by a hands-on session to explore integration of OpenMM into other MD codes. We will also discuss techniques used to achieve significant speed increases for MD codes running on GPUs.

The second day is devoted to researchers using or interested in using MD simulations, including novices to MD simulations. Experts in the field will introduce the theory of MD, and a hands-on demo of OpenMM Zephyr will be given. More advanced topics, such as force fields and implicit versus explicit solvent models, will be discussed in the afternoon.

For more details, go to http://simbios.stanford.edu/EventsOfInterest/OpenMMWorkshop.htm.

Registration is free but required and spaces are limited. You may register for one day or both. To register, go to http://simbios.stanford.edu/EventsOfInterest/OpenMMWorkshopReg.htm.

About Simbios:

OpenMM and OpenMM Zephyr are supported by Simbios, an NIH National Center for Physics-Based Simulation of Biological Structures, as part of its protein folding research efforts. To learn more about Simbios and its research and software tools, visit http://simbios.stanford.edu.

[1] PE Marszalek, et al., “Mechanical unfolding intermediates in titin molecules,” Nature, 1999 Nov 4; 402(6757):100-103.
[2] HD Herce, AE Garcia, “Molecular dynamics simulations suggest a mechanism for translocation of the HIV-1 TAT peptide across lipid membranes,” PNAS, 2007; 104:20805-20810
[3] PM Kasson, VS Pande, “Structural basis for influence of viral glycans on ligand binding by influenza hemagglutinin,” Biophysical Journal, 2008; 95:L48-L50.
[4] DS Glazer, RJ Radmer, RB Altman, “Combining molecular dynamics and machine learning to improve protein function recognition,” Pac Symp Biocomput, 2008; 332-343.

*OpenMM accelerated code running on Nvidia GeForce GTX 280 GPU vs. conventional code with Amber9 running on Intel Xenon 2.66 GHz CPU. MS Friedrichsm, et al., "Accelerating Molecular Dynamic Simulation on Graphics Processing Units," J. Comp. Chem., in press.