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.

[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 Friedrichs, et al., "Accelerating Molecular Dynamic Simulation on Graphics Processing Units," J. Comp. Chem., in press.