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.
