Friday, June 26, 2009

9:00am – 9:10am  Welcome and introduction of instructors and workshop attendees
                   - Vijay Pande

9:10am – 10:10am Introduction to molecular dynamics
                - Vijay Pande

10:10am – 11:00am Introduction to OpenMM Zephyr
                - You, with guidance from Joy Ku

11:00am – 12:30pm LUNCH (on your own)

12:30pm – 1:15pm Exploring more OpenMM Zephyr features
                   - You, with guidance from Joy Ku

1:15pm – 2:15pm Introduction to advanced topics in molecular dynamics
                   - Vijay Pande

2:15 pm – 2:30pm BREAK

2:30pm – 3:30pm Exercise: Using OpenMM/mdrun to run simulations with additional parameter settings
                   - You, with guidance from Mark Friedrichs

3:30pm – 4:45pm Break-out Sessions: Use OpenMM Zephyr and OpenMM/mdrun to answer your research question

4:45pm – 5:00pm Wrap up and Q & A
               - All