

Some complications

- Most simulations are not going to be this easy to set up
 - Crystal structures may have missing atoms, which often can be added by homology modeling
 - The added hydrogens should depend on the pH you're trying to model
 - You need to do extra work for non-standard residues, cofactors, and ligands
 - Most of the time it is better to simulate with water
 - For certain systems, you will need to build a membrane
- You usually need much longer simulations to get publishable results
 - GPU computing provides significant acceleration
 - Calculations will usually be done remotely
 - XSEDE supercomputer
 - Google/Amazon cloud
- We will help each group with all of these

Additional Resources

- In “Introduction to OpenMM” on <http://openmm.org/documentation.html>, Peter Eastman describes an OpenMM script from 5:00 to 15:03