Molecular Dynamics with Explicit Solvent

https://github.com/daveminh/Chem456/tree/master/static_files/tutorials/ubq_wat-md

Suggested steps for MD simulation with explicit water

- 0-propka:
  - Submit your complete PDB file to the PDB2PQR server to assign protonation states. Use the AMBER force field and AMBER output naming scheme.
- 1-model_water:
  - Modify this script and use the Modeller package in OpenMM to add water at the desired salt concentration.
- 2-simulation:
  - Copy your input files onto XSEDE Bridges using the sync_data.sh script.
  - Log into Bridges and submit the simulation using the submit_simulation.py script. Check the options.
  - Check the queue to see if your job has submitted.
  - When your job is complete, copy your output files from XSEDE Bridges using the sync_data.sh script.