

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 onto the GPU-small (sbatch run_small_simulation.job) or GPU-shared queue (sbatch run_simulation.job)
 - 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.