Why OpenMM?

- Many choices of software for molecular dynamics
  - https://en.wikipedia.org/wiki/Comparison_of_software_for_molecular_mechanics_modeling
  - https://www.rcsb.org/pages/thirdparty/modeling_and_simulation
- OpenMM is
  - free
  - GPU-accelerated
  - can be used in python scripts/C++ programs

Interactive MD exercise