Preparing a script to run MD

Why write a script?

- Molecular dynamics simulations require a lot of information about
  - Input data
    - coordinates
    - topology
      - which atoms are included in energy terms
      - parameters for functions in energy terms
  - System description
    - periodicity
    - constraints
  - Integrators
    - algorithms to propagate forward in time
    - adjust box size
    - adjust kinetic energy (temperature)
  - Simulation
    - how long to run
    - how much output data to store
- OpenMM can be run from widely-used computer programming languages, python and C++, facilitating extension and combination with other code