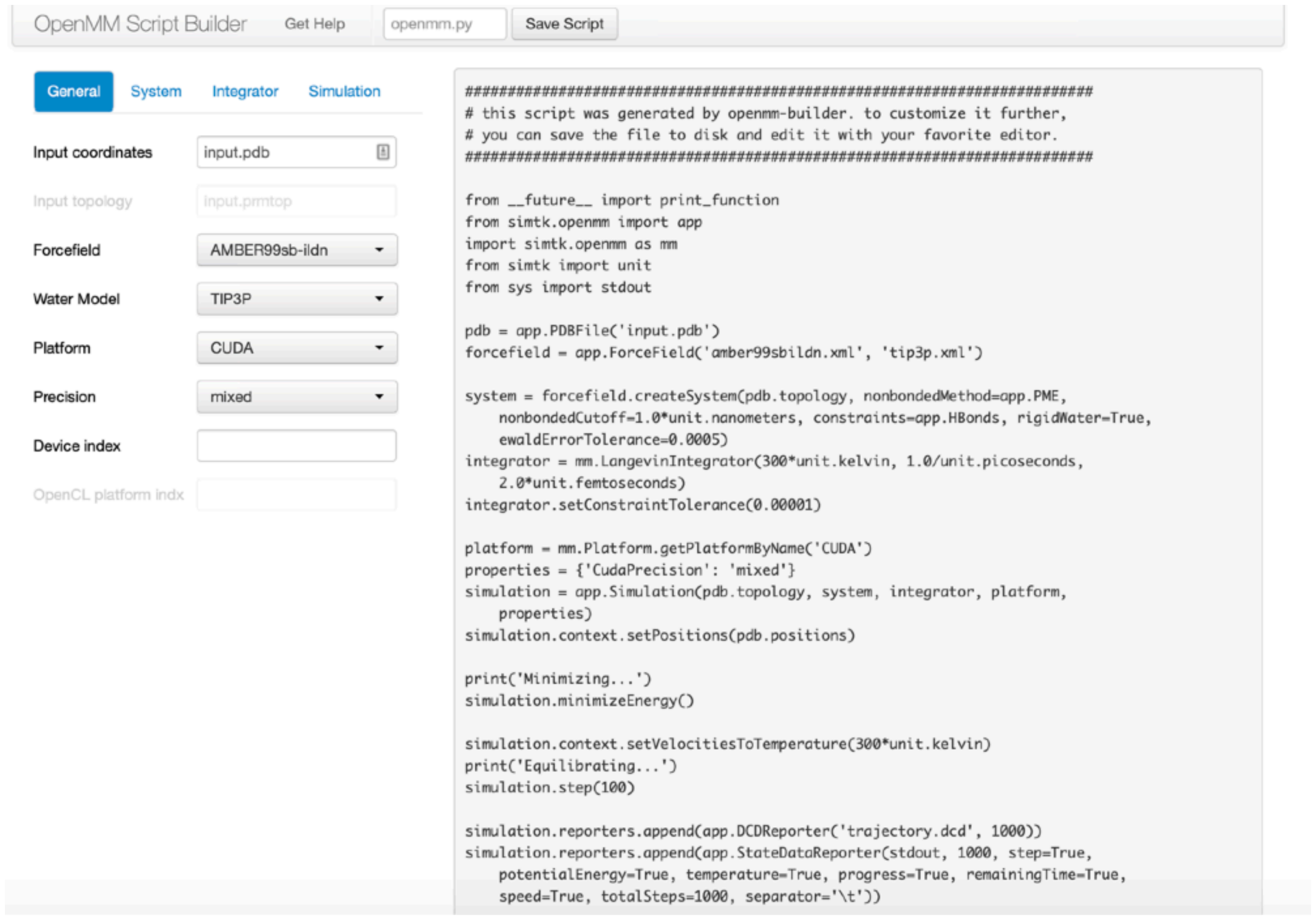
Why write a script?

- 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

- This is the default script in the OpenMM script builder: http://builder.openmm.org
- Let’s go through what the parameters mean and I’ll give you values for a simple simulation of ubiquitin, a protein that we looked at during the VMD tutorial
- If you hover your mouse over the parameter names, it’ll also give a brief description
- A more detailed description of simulation parameters is available at http://docs.openmm.org/latest/userguide/application.html#simulation-parameters



Input coordinates: input.pdb
Input topology: input.prmtop
Forcefield: AMBER99sb-ildn
Water Model: TIP3P
Platform: CUDA
Precision: mixed
Device index:
OpenCL platform indx:

```
##########################################################################
# this script was generated by openmm-builder. to customize it further,
# you can save the file to disk and edit it with your favorite editor.
##########################################################################

from __future__ import print_function
from simtk.openmm import app
import simtk.openmm as mm
from simtk import unit
from sys import stdout

pdb = app.PDBFile('input.pdb')
forcefield = app.ForceField('amber99sbildn.xml', 'tip3p.xml')

system = forcefield.createSystem(pdb.topology, nonbondedMethod=app.PME,
    nonbondedCutoff=1.0*unit.nanometers, constraints=app.HBonds, rigidWater=True,
    ewaldErrorTolerance=0.0005)
integrator = mm.LangevinIntegrator(300*unit.kelvin, 1.0/unit.picoseconds,
    2.0*unit.femtoseconds)
integrator.setConstraintTolerance(0.00001)

platform = mm.Platform.getPlatformByName('CUDA')
properties = {'CudaPrecision': 'mixed'}
simulation = app.Simulation(pdb.topology, system, integrator, platform,
    properties)
simulation.context.setPositions(pdb.positions)

print('Minimizing...')
simulation.minimizeEnergy()

simulation.context.setVelocitiesToTemperature(300*unit.kelvin)
print('Equilibrating...')
simulation.step(100)

simulation.reporters.append(app.DCDReporter('trajectory.dcd', 1000))
simulation.reporters.append(app.StateDataReporter(stdout, 1000, step=True,
    potentialEnergy=True, temperature=True, progress=True, remainingTime=True,
    speed=True, totalSteps=1000, separator='\t'))
```