

- 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>

The screenshot shows the OpenMM Script Builder web interface. The top bar includes the title "OpenMM Script Builder", a "Get Help" link, and buttons for "openmm.py" and "Save Script". The interface is divided into four tabs: "General" (selected), "System", "Integrator", and "Simulation".

Under the "General" tab, the following parameters are visible:

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

On the right side, the generated Python script is displayed. It starts with a header comment and then defines the simulation setup:

```
#####
# 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'))
```

- For “Input coordinates”, enter 1ubq.pdb
- “Forcefield” is the set of parameters and functions that describes the energy of a system. Let’s keep “AMBER99sb-ildn”
- “Water Model” includes
  - descriptions that vary in the number of point charges
  - a description that doesn’t actually model water at all, but its effect on the electrostatic energy and a penalty for forming surfaces. For computational speed, let’s pick this “Implicit Solvent” version
- “Platform” describes the version of the code and the hardware it will run on
  - “Reference” is meant to be the most readable code
  - “CUDA” and “OpenCL” are meant for GPUs, which make MD simulations much faster. “CUDA” only works with Nvidia GPUs and “OpenCL” on others
  - “CPU” is a faster version of Reference.
  - Since the laboratory machines don’t have GPUs, let’s use “CPU”
- The other options are GPU-specific

General System Integrator Simulation

Input coordinates

Input topology

Forcefield

Water Model

Platform

Precision

Device index

OpenCL platform indx

General System Integrator Simulation

Input coordinates

Input topology

Forcefield

Water Model

Platform

Precision

Device index

OpenCL platform indx

General System Integrator Simulation

Input coordinates

Input topology

Forcefield

Water Model

Platform   
TIP3P  
TIP4P-Ew  
TIP5P  
Implicit Solvent (OBC)

Precision

Device index

OpenCL platform indx

General System Integrator Simulation

Input coordinates

Input topology

Forcefield

Water Model

Platform   
Reference  
OpenCL  
CPU  
CUDA

Precision

Device index

OpenCL platform indx