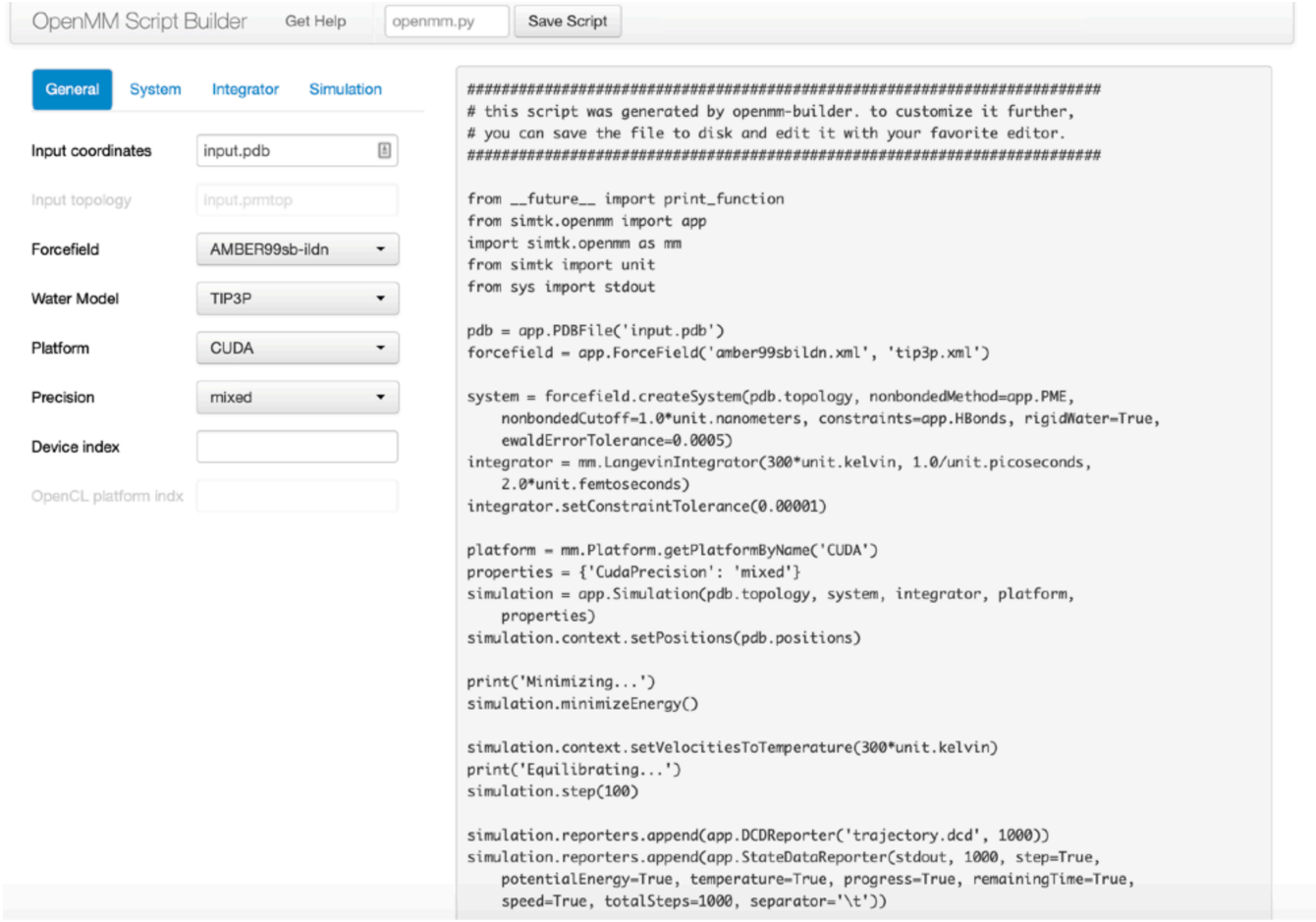
- This is the default script in the OpenMM script builder: http://builder.openmm.org
- Let's go through what the parameters mean and I'll give you values for a simple simulation of ubiquitin, a protein that we looked at during the VMD tutorial
- If you hover your mouse over the parameter names, it'll 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



- 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