Running Simulations with OpenMM

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OpenMM is...

A. An application for running molecular simulations
B. A library of simulation routines for use by applications
C. A domain specific language for molecular simulation
D. All of the above

What is OpenMM?

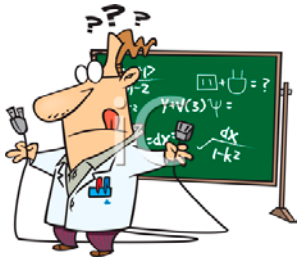
- A toolkit for high performance molecular simulations
  - A low level computational library (C++)
  - A high level application layer (Python)

- Supports GPUs (NVIDIA and AMD) and CPUs
  - Computations implemented in OpenCL and CUDA

User Types

Biologists/Chemists: Use the application layer to run simulations

Application Developers: Use the computational library to add simulation features to their programs



Algorithm Developers: Use Python, C++, custom forces to implement new algorithms within the application layer

Running Simulations

- The “application layer” is really a set of Python libraries
- You write a Python script to run a simulation

No programming experience required!

Example Script

```
from simtk.openmm.app import *
from simtk.openmm import *
from simtk.unit import *

pdb = PDBFile('input.pdb')
forcefield = ForceField('amber99sb.xml', 'tip3p.xml')
system = forcefield.createSystem(pdb.topology, nonbondedMethod=PME,
   nonbondedCutoff=1*nanometer, constraints=HBonds)
integrator = LangevinIntegrator(300*kelvin, 1/picosecond,
   0.002*picoseconds)
simulation = Simulation(pdb.topology, system, integrator)
simulation.context.setPositions(pdb.positions)
simulation.minimizeEnergy()
simulation.reporters.append(PDBReporter('output.pdb', 1000))
simulation.step(10000)
```

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Tell Python about the OpenMM libraries we'll be using

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Load the PDB file

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```

Select the force field to use

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```

Construct the system to simulate

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simulation.minimizeEnergy()
simulation.reporters.append(PDBReporter('output.pdb', 1000))
simulation.step(10000)
```

Select the integration method and parameters

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```

Let's do a simulation!

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simulation.minimizeEnergy()
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simulation.step(10000)
```

Set the initial atom positions

Example Script

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simulation.minimizeEnergy()
simulation.reporters.append(PDBReporter('output.pdb', 1000))
simulation.step(10000)
```

Better run an energy minimization first

Example Script

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simulation.minimizeEnergy()
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simulation.step(10000)
```

Save a frame to a PDB file every 1000 steps

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simulation.step(10000)
```

Simulate!

Starting from AMBER Files

```
from simtk.openmm.app import *
from simtk.openmm import *
from simtk.unit import *

prmtop = AmberPrmtopFile('input.prmtop')
inpcrd = AmberInpcrdFile('input.inpcrd')
system = prmtop.createSystem(nonbondedMethod=PME,
   nonbondedCutoff=1*nanometer, constraints=HBonds)
integrator = LangevinIntegrator(300*kelvin, 1/picosecond,
   0.002*picoseconds)
simulation = Simulation(prmtop.topology, system, integrator)
simulation.context.setPositions(inpcrd.positions)
simulation.minimizeEnergy()
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```

Starting from AMBER Files

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integrator = LangevinIntegrator(300*kelvin, 1/picosecond,
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simulation = Simulation(prmtop.topology, system, integrator)
simulation.context.setPositions(inpcrd.positions)
simulation.minimizeEnergy()
simulation.reporters.append(PDBReporter('output.pdb', 1000))
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