Custom Forces in OpenMM

Peter Eastman

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Forces in OpenMM

- “Standard” forces cover the most widely used force fields
  - HarmonicBondForce, HarmonicAngleForce, NonbondedForce, etc.
- But what if you need something that isn’t provided?
  - Could write a plugin, but that’s hard and a lot of work

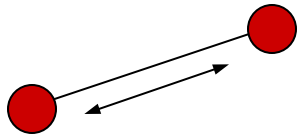
Custom Forces

- Combine *some* of the flexibility of a plugin with *most* of the simplicity of standard forces
- You specify the energy function, it does the rest

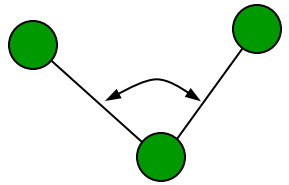
```
CustomNonbondedForce("A*exp(-B*r)-C/r^6")
```

Custom Forces Classes

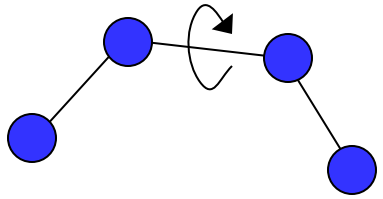
- CustomBondForce
  - Bonded force between two particles
  - Energy is a function of the distance



- CustomAngleForce
  - Bonded force between three particles
  - Energy is a function of the angle



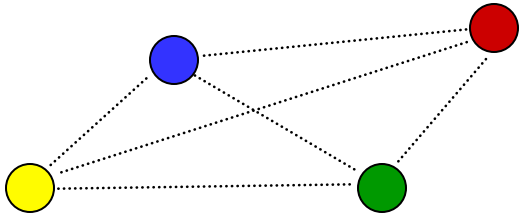
- CustomTorsionForce
  - Bonded force between four particles
  - Energy is a function of the dihedral angle



Custom Forces Classes (continued)

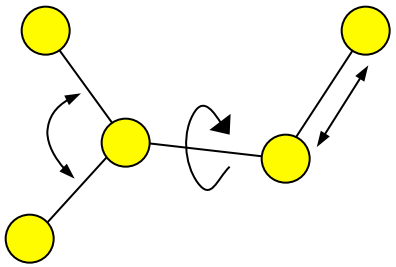
- CustomExternalForce
  - Force applied to each particle independently
  - Energy is a function of the particle position

- CustomNonbondedForce
  - Nonbonded force between pairs of particles
  - Energy is a function of the distance



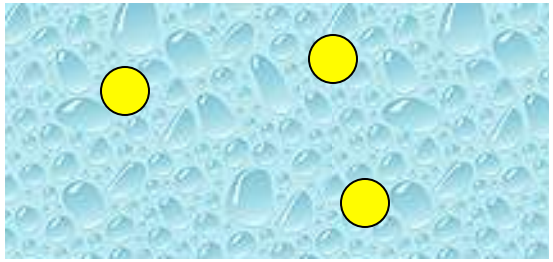
Custom Forces Classes (continued)

- CustomCompoundBondForce
  - Bonded force between an arbitrary number of particles
  - Energy can depend on positions, distances, angles, and dihedrals

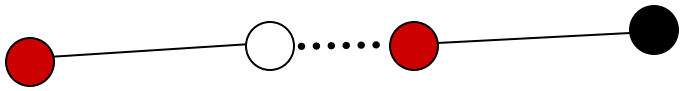


Custom Forces Classes (continued)

- CustomGBForce
  - Supports various implicit solvent models



- CustomHbondForce
  - Supports various hydrogen bonding models



Example: Harmonic Restraints

- Restrain particular atoms from moving

$$E(x,y,z) = 10 \cdot \left((x - x_0)^2 + (y - y_0)^2 + (z - z_0)^2 \right)$$

```
# Create the force
force = CustomExternalForce(“10*((x-x0)^2+(y-y0)^2+(z-z0)^2)")
force.addPerParticleParameter("x0")
force.addPerParticleParameter("y0")
force.addPerParticleParameter("z0")

# Bind particle 5 to the location (0, 1, -0.5) nm
force.addParticle(5, (0, 1, -0.5)*nanometers)
```

Lennard-Jones Combining Rules

- Lennard-Jones potential represents Van der Waals interactions

$$E(r) = 4\varepsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right)$$

- The combining rule determines ε and σ from the particle parameters
- NonbondedForce uses Lorentz-Bertelot combining rule

$$\varepsilon = \sqrt{\varepsilon_1 \varepsilon_2} \qquad \sigma = 0.5(\sigma_1 + \sigma_2)$$

Jorgensen Combining Rules

- Some force fields (e.g. OPLS) use Jorgensen combining rules

$$\varepsilon = \sqrt{\varepsilon_1 \varepsilon_2} \qquad \sigma = \sqrt{\sigma_1 \sigma_2}$$

```
force = CustomNonbondedForce(
   "4*eps*((sig/r)^12-(sig/r)^6); eps=sqrt(eps1*eps2);
   sig=sqrt(sig1*sig2)")
force.addPerParticleParameter("eps")
force.addPerParticleParameter("sig")
force.addParticle([0.1, 0.3])
```

Other Features

- Global parameters
  - Have a single value for all bonds/particles
  - Can change during a simulation
- Tabulated functions
  - Use tabulated values to define a function, then use it in expressions
  - Only supported by CustomNonbondedForce, CustomGBForce, and CustomHbondForce

Performance of Custom Forces

- OpenCL and CUDA platforms generate a new kernel at runtime to evaluate the expression
  - Little or no performance difference from standard forces
- Reference platform uses an interpreter to evaluate expressions
  - Much slower than standard forces

Example: A Spherical Potential

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

pdb = PDBFile('waterSphere.pdb')
forcefield = ForceField('amber99sb.xml', 'tip3p.xml')
system = forcefield.createSystem(pdb.topology,
   nonbondedMethod=NoCutoff)
force = CustomExternalForce('10*max(0, r-1)^2; r=sqrt(x*x+y*y+z*z)')
for i in range(system.getNumParticles()):
    force.addParticle(i, ())
system.addForce(force)
integrator = LangevinIntegrator(1000*kelvin, 1/picosecond,
   0.002*picoseconds)
simulation = Simulation(pdb.topology, system, integrator)
simulation.context.setPositions(pdb.positions)
simulation.reporters.append(PDBReporter('output.pdb', 100))
simulation.step(5000)
```

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```

Exercises

- Run the script and view the results in VMD
- Increase the sphere radius to 2 nm. What happens?
- Reduce the temperature to 300K. What happens? Why?

Custom Integrators

- Define integration algorithm as an arbitrary series of computations
- Supports many types of integrators
  - Deterministic
  - Stochastic
  - Metropolized
  - Generalized Langevin
  - Multiple time step
  - ...

Example: Velocity Verlet

```
integrator = CustomIntegrator(0.001)
integrator.addComputePerDof("v", "v+0.5*dt*f/m")
integrator.addComputePerDof("x", "x+dt*v")
integrator.addComputePerDof("v", "v+0.5*dt*f/m")
```

- CustomIntegrator automatically recalculates forces when necessary
- Supports arbitrary global and per-DOF variables