



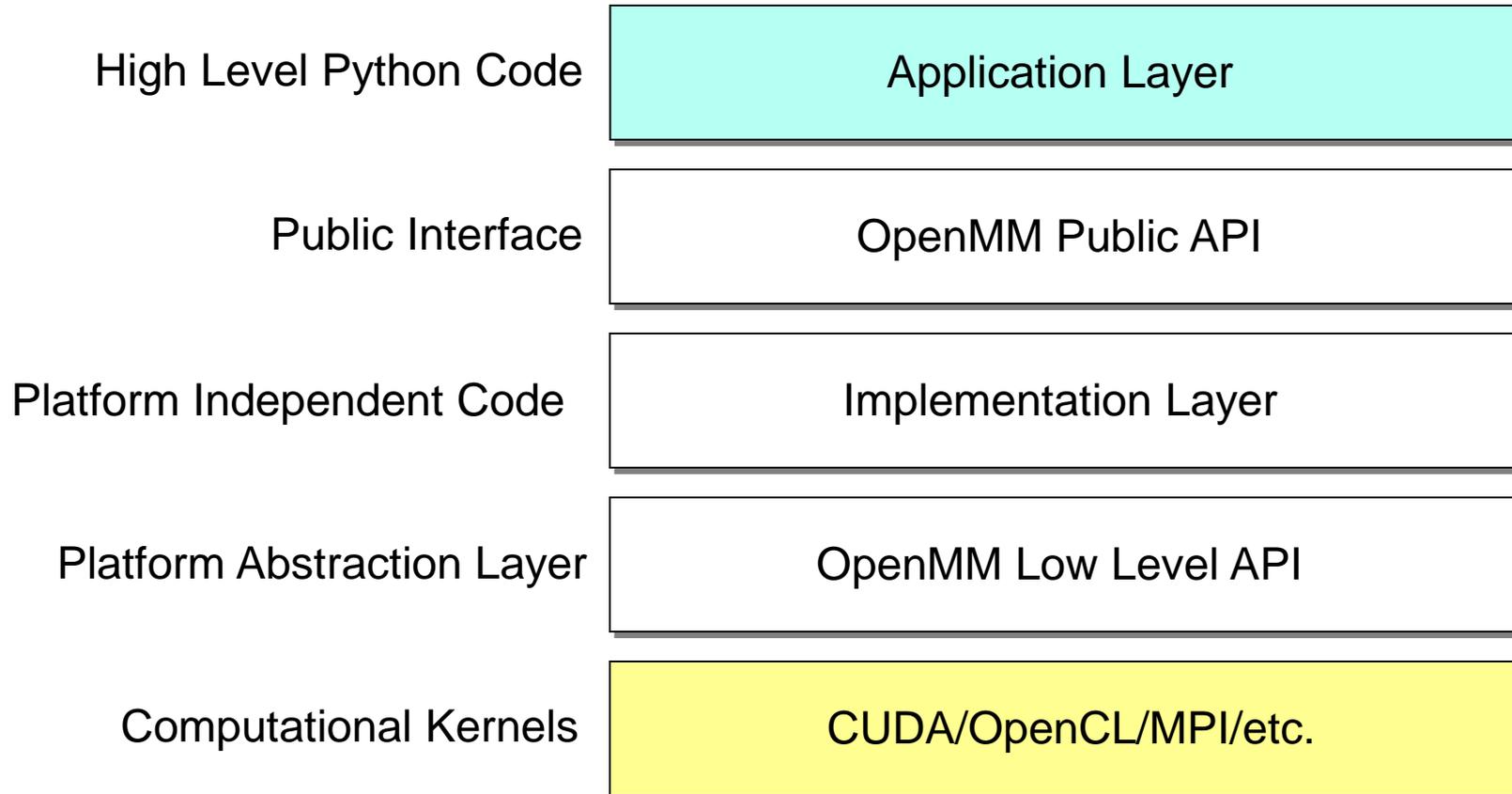
# Advanced OpenMM Features

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# The OpenMM Architecture



# Public API Classes (1 of 3)

- System
  - A collection of interacting particles
  - Defines the mass of each particle
  - Specifies distance constraints
  - Contains a list of Force objects that define the interactions
- Context
  - Contains all state information
    - Positions, velocities, other parameters

# Public API Classes (2 of 3)

- Force
  - Anything which affects the system's behavior
  - Forces, thermostats, barostats, etc.
  - A Force may:
    - Apply forces to particles
    - Contribute to the potential energy
    - Define adjustable parameters
    - Modify positions, velocities, and parameters at the start of each time step

# Public API Classes (3 of 3)

- Integrator
  - Advances the system through time
  - Both fixed and variable step size integrators are supported
- State
  - A snapshot of the state of the system
  - Immutable (used only for reporting)
  - Creating a State is the only way to access positions and velocities
  - Can optionally include forces and energies

# Example

- Create a System

```
system = System()
```

```
for particle in particles:
```

```
    system.addParticle(particle.mass[i])
```

```
for constraint in constraints:
```

```
    system.addConstraint(constraint.atom1, constraint.atom2,  
                        constraint.distance)
```

- Add Forces to it

```
bondForce = HarmonicBondForce()
```

```
for bond in bonds:
```

```
    bondForce.addBond(bond.atom1, bond.atom2, bond.length, bond.k)
```

```
system.addForce(bondForce)
```

```
# ... add Forces for other force field terms.
```

# Example (continued)

- Simulate it

```
integrator = LangevinIntegrator(297.0, 1.0, 0.002) # Temperature, friction,  
                                                # step size  
context = Context(system, integrator)  
context.setPositions(positions)  
context.setVelocities(velocities)  
integrator.step(500) # Take 500 steps
```

- Retrieve state information

```
state = context.getState(getPositions=True, getVelocities=True)  
for position in state.getPositions():  
    print(position)
```

# Platforms

- The API defines the *interface*
- A Platform provides the *implementation*
- Available Platforms:
  - Reference
  - CPU
  - OpenCL
  - CUDA

# The Platform API

- Select a Platform to use

```
platform = Platform.getPlatformByName("OpenCL")  
context = Context(system, integrator, platform)
```

- Check what Platform is being used

```
print(context.getPlatform().getName())
```

- List available Platforms

```
for i in range(Platform.getNumPlatforms()):  
    print(Platform.getPlatform(i).getName())
```

# 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

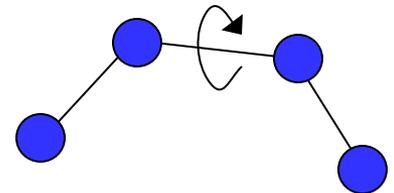
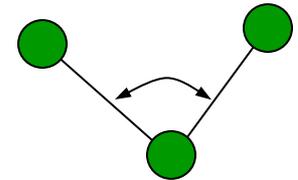
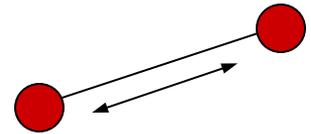
# Custom Forces

- 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

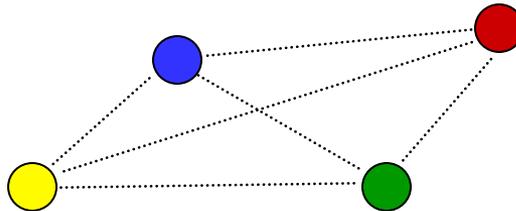


# Custom Forces Classes (continued)

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

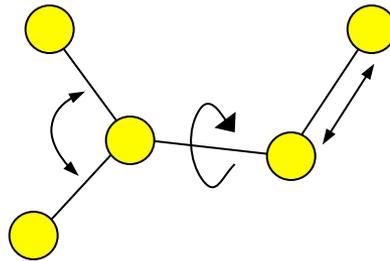


- CustomNonbondedForce
  - Nonbonded force between pairs of particles
  - Energy is a function of the distance



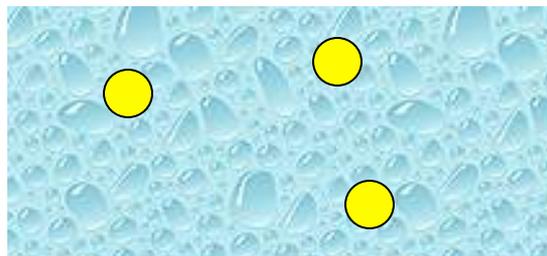
# Custom Forces Classes (continued)

- 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



# 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
- CPU and Reference platforms use 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)
```

# Example: A Spherical Potential

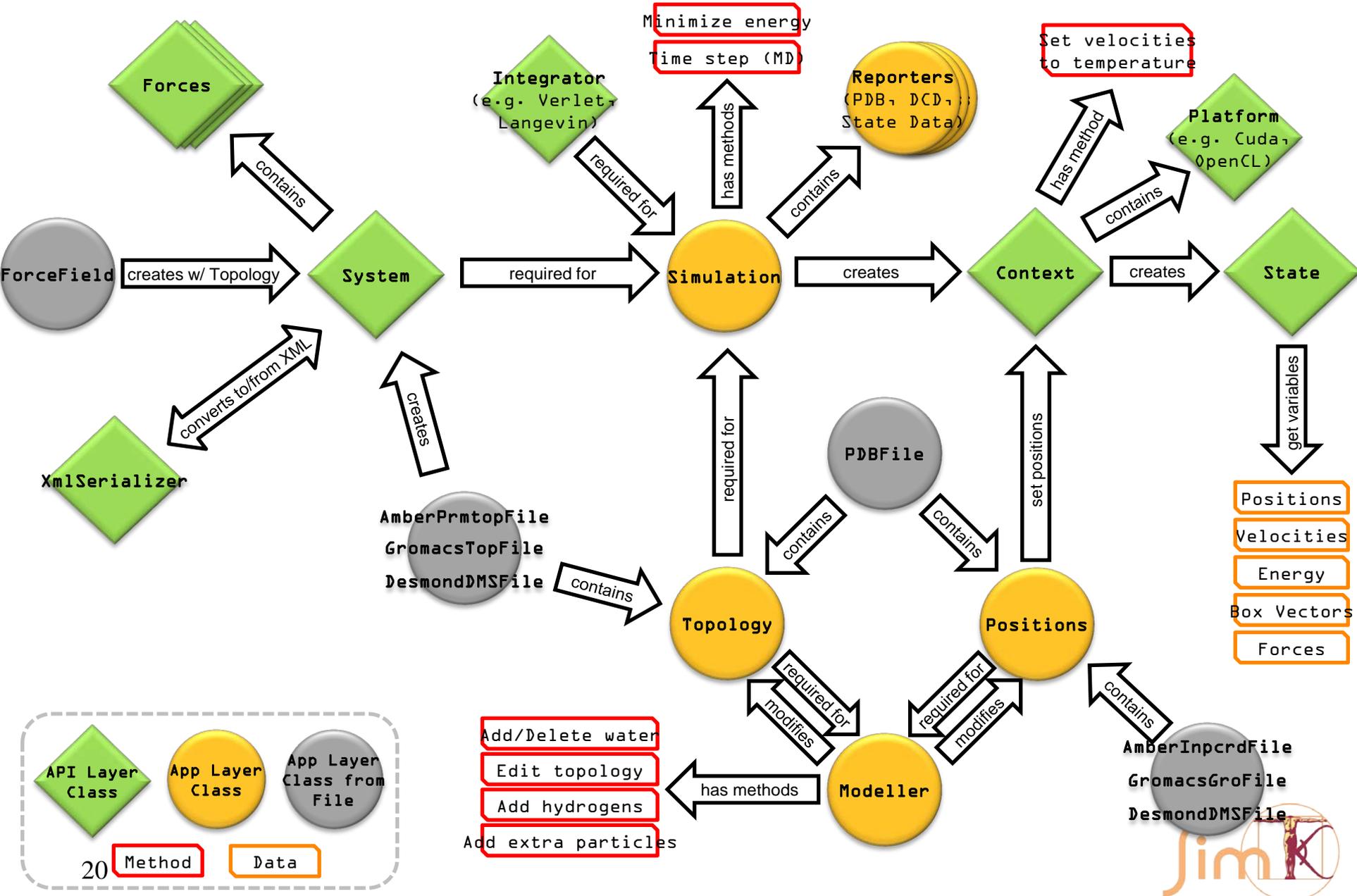
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```

# Exercises

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

# Diagram of classes in OpenMM 6.0



OpenMM: CustomExternalForce Class Reference

OpenMM: CustomExternalForce ...

https://simtk.org/api\_docs/openmm/api6\_0/python/classsimtk\_1\_1op

# OpenMM

Main Page Related Pages **Classes** Search

Class List Class Hierarchy Class Members

- ▶ AmoebaGeneralizedKirkwood
- ▶ AmoebaInPlaneAngleForce
- ▶ AmoebaMultipoleForce
- ▶ AmoebaOutOfPlaneBendForce
- ▶ AmoebaPITorsionForce
- ▶ AmoebaStretchBendForce
- ▶ AmoebaTorsionTorsionForce
- ▶ AmoebaVdwForce
- ▶ AmoebaWcaDispersionForce
- ▶ AndersenThermostat
- ▶ Integrator
- ▶ BrownianIntegrator
- ▶ CMAPTorsionForce
- ▶ CMMotionRemover
- ▶ Context
- ▶ CustomAngleForce
- ▶ CustomBondForce
- ▶ CustomCompoundBondForce
- ▶ **CustomExternalForce**
- ▶ CustomGBForce
- ▶ CustomHbondForce
- ▶ CustomIntegrator
- ▶ CustomNonbondedForce
- ▶ CustomTorsionForce
- ▶ DrudeForce
- ▶ DrudeLangevinIntegrator
- ▶ DrudeSCFIntegrator
- ▶ GBSAOBCForce

## Detailed Description

This class implements an "external" force on particles.

The force may be applied to any subset of the particles in the **System**. The force on each particle is specified by an arbitrary algebraic expression, which may depend on the current position of the particle as well as on arbitrary global and per-particle parameters.

To use this class, create a **CustomExternalForce** object, passing an algebraic expression to the constructor that defines the potential energy of each affected particle. The expression may depend on the particle's x, y, and z coordinates, as well as on any parameters you choose. Then call **addPerParticleParameter()** to define per-particle parameters, and **addGlobalParameter()** to define global parameters. The values of per-particle parameters are specified as part of the system definition, while values of global parameters may be modified during a simulation by calling **Context::setParameter()**. Finally, call **addParticle()** once for each particle that should be affected by the force. After a particle has been added, you can modify its parameters by calling **setParticleParameters()**. This will have no effect on Contexts that already exist unless you call **updateParametersInContext()**.

As an example, the following code creates a **CustomExternalForce** that attracts each particle to a target position (x0, y0, z0) via a harmonic potential:

```
CustomExternalForce* force = new CustomExternalForce("k*((x-x0)^2+(y-y0)^2+(z-z0)^2)");
```

This force depends on four parameters: the spring constant k and equilibrium coordinates x0, y0, and z0. The following code defines these parameters:

```
force->addGlobalParameter("k");
force->addPerParticleParameter("x0");
```

simtk openmm openmm CustomExternalForce

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