The OpenMM API

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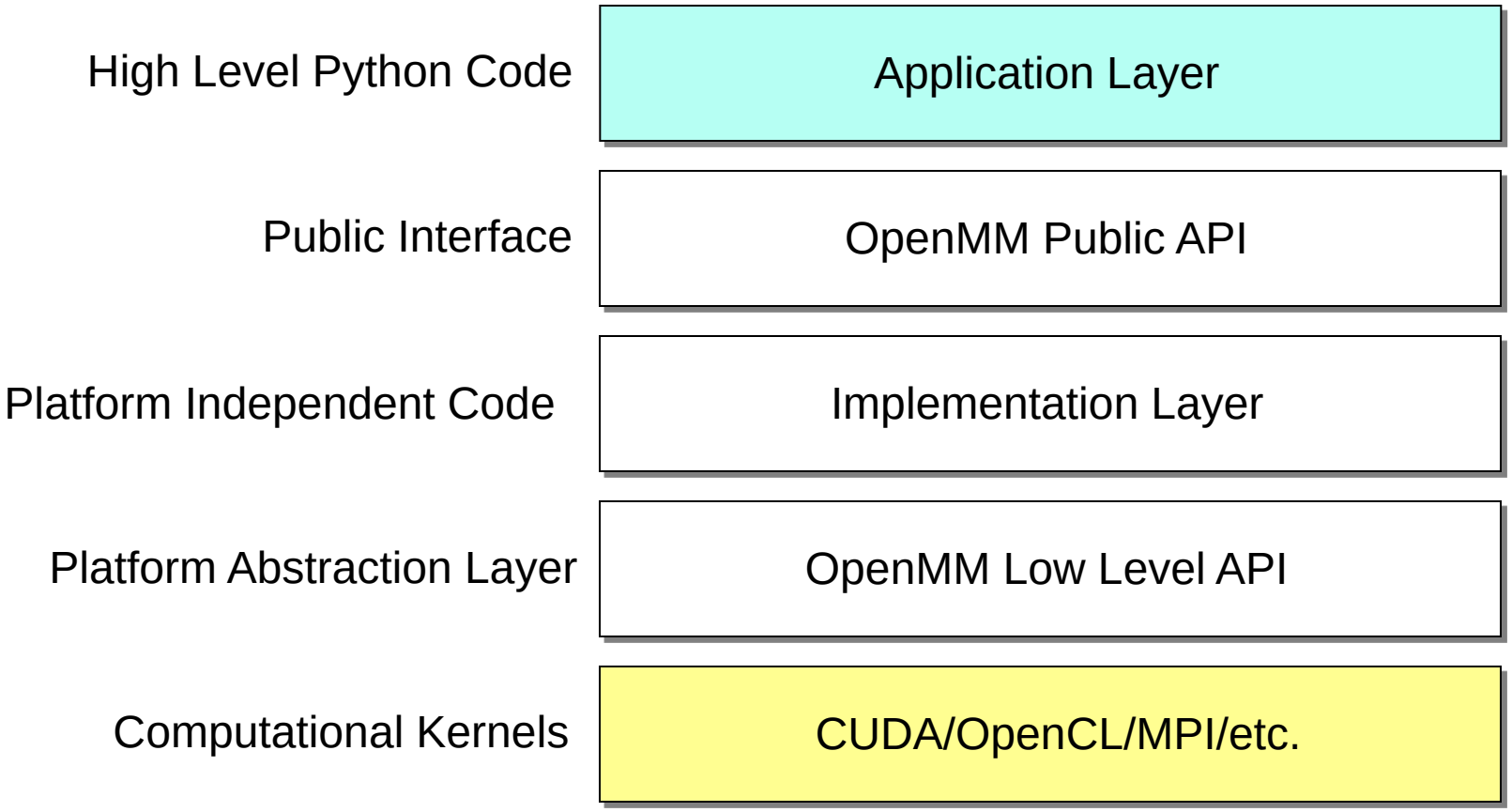
OpenMM Workshop, March 26, 2013

The OpenMM Architecture



Why Use the API?

- Application Developers
  - This is how you use OpenMM within your programs
- Chemists/Biologists
  - It's available to your control scripts... if you want it
  - There's a lot you can do with it!

Goals of the API

- Simple
  - Easy to learn
  - Easy to use
- Extensible
  - Add new force fields, integration methods, etc.
  - Support new hardware platforms
- Can be implemented efficiently on a variety of hardware platforms
- Easy to incorporate into existing codebases

Choice of Language

- The OpenMM API is written in C++
- API wrappers are provided for Python, C, and Fortran
  - Provide access to most features
  - Plugins can only be written in C++

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
  - OpenCL
  - CUDA

The Platform API

- Select a Platform to use

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

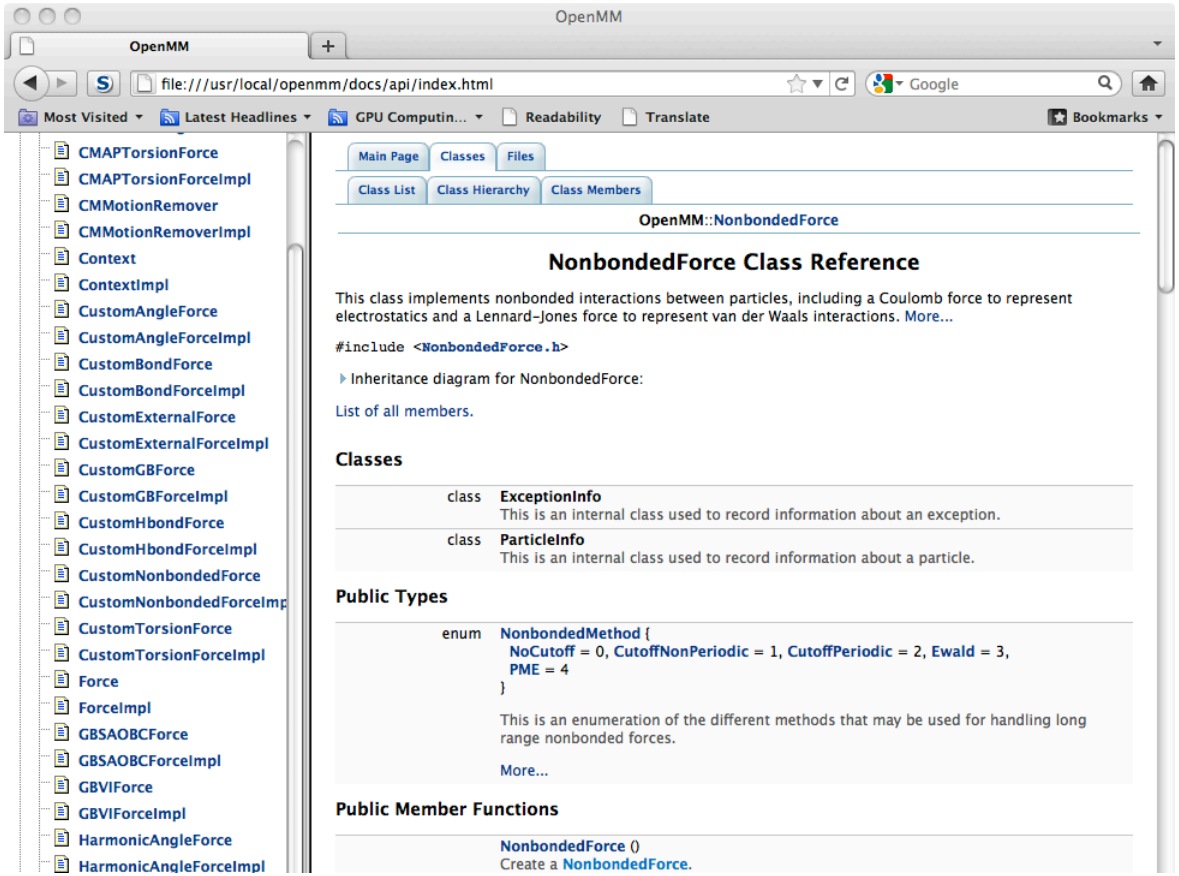
- Check what Platform is being used

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

- List available Platforms

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

Documentation



See .../openmm/docs/C++ API Reference.html and .../openmm/docs/Python API Reference.html

Also online (see OpenMM download page)

Python Help

- Can use help() to get docs for a class, function, object, etc.

```
help(Context)
help(Context.getState)
help(simulation.context)
```

- Use dir() to list every field and method of an object

```
dir(simulation)
```

C++/Python Differences

- Context.getState() uses boolean arguments instead of flags

  C++:

```
context.getState(State::Positions | State::Velocities);
```

  Python:

```
context.getState(getPositions=True, getVelocities=True)
```

C++/Python Differences, cont.

- Multiple return values are returned directly, not as arguments

C++:

```
int particle1, particle2;
double length, k;
f.getBondParameters(i, particle1, particle2, length, k);
```

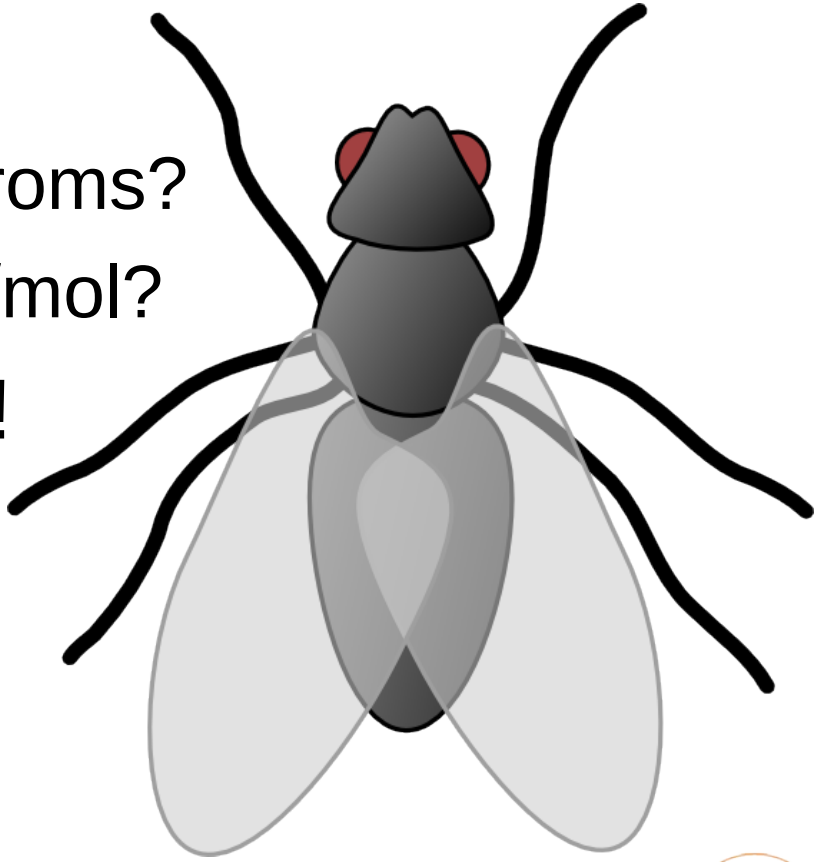
Python:

```
(particle1, particle2, length, k) = f.getBondParameters(i)
```

- Quantities have explicit units

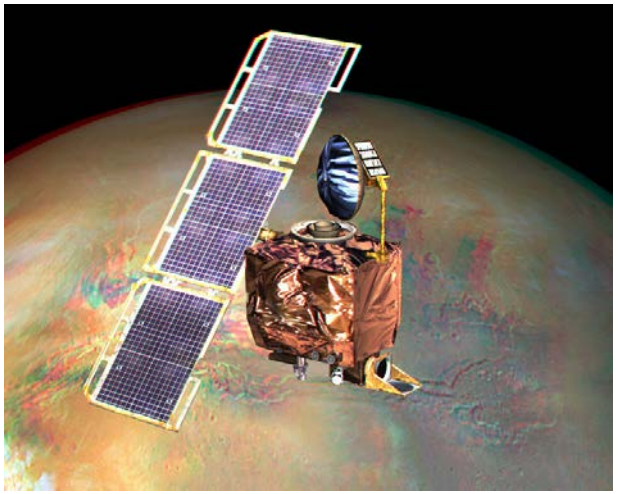
Why Units?

- Many different units are common in MD
  - Time in ps or fs?
  - Distance in nm or Angstroms?
  - Energy in kcal/mol or kJ/mol?
- You *will* make mistakes!
- This *will* produce bugs!



...and you're not alone!

- Mars Climate Orbiter
  - Crashed into Mars in 1999
  - Cost $125 million



- Air Canada Flight 143
  - Ran out of fuel in midair in 1983

Both caused by errors in unit conversions

Units in OpenMM

- Just multiply each value by its units

```
>>> size = 5*nanometers
>>> print size
5 nm
>>> accel = 9.8*meters/second**2
>>> print accel
9.8 m/(s**2)
```

- Can convert to any compatible unit

```
>>> print size.in_units_of(angstroms)
50.0 A
>>> print size.value_in_unit(angstroms)
50.0
```

Units in OpenMM, continued

- Conversions happen automatically when doing math

```
>>> print 5*nanometers+25*angstroms
7.5 nm
>>> print 5*nanometers+25*picoseconds
Traceback (most recent call last):
...
TypeError: Cannot add two quantities with incompatible units
   "nanometer" and "picosecond".
```

- Can apply units to lists, tuples, and arrays

```
>>> x = (1.0, 1.5, 0.0)*nanometers
>>> positions = state.getPositions().in_units_of(angstrom)
```

Units in OpenMM, continued

- Units are optional (but recommended!) on input values
- Output values always have units
- Default OpenMM units:
  - nm, ps, K, amu (g/mole), kJ/mole, e
  - These form a consistent unit system!

Which Language to Use?

- Python
  - Faster development
  - Interactive mode for experimenting
  - Explicit units
- C++
  - Faster execution
  - Easier to call from other languages
  - Can write plugins

Diagram of classes in OpenMM 5.0