Extracting and analyzing data from OpenMM simulations

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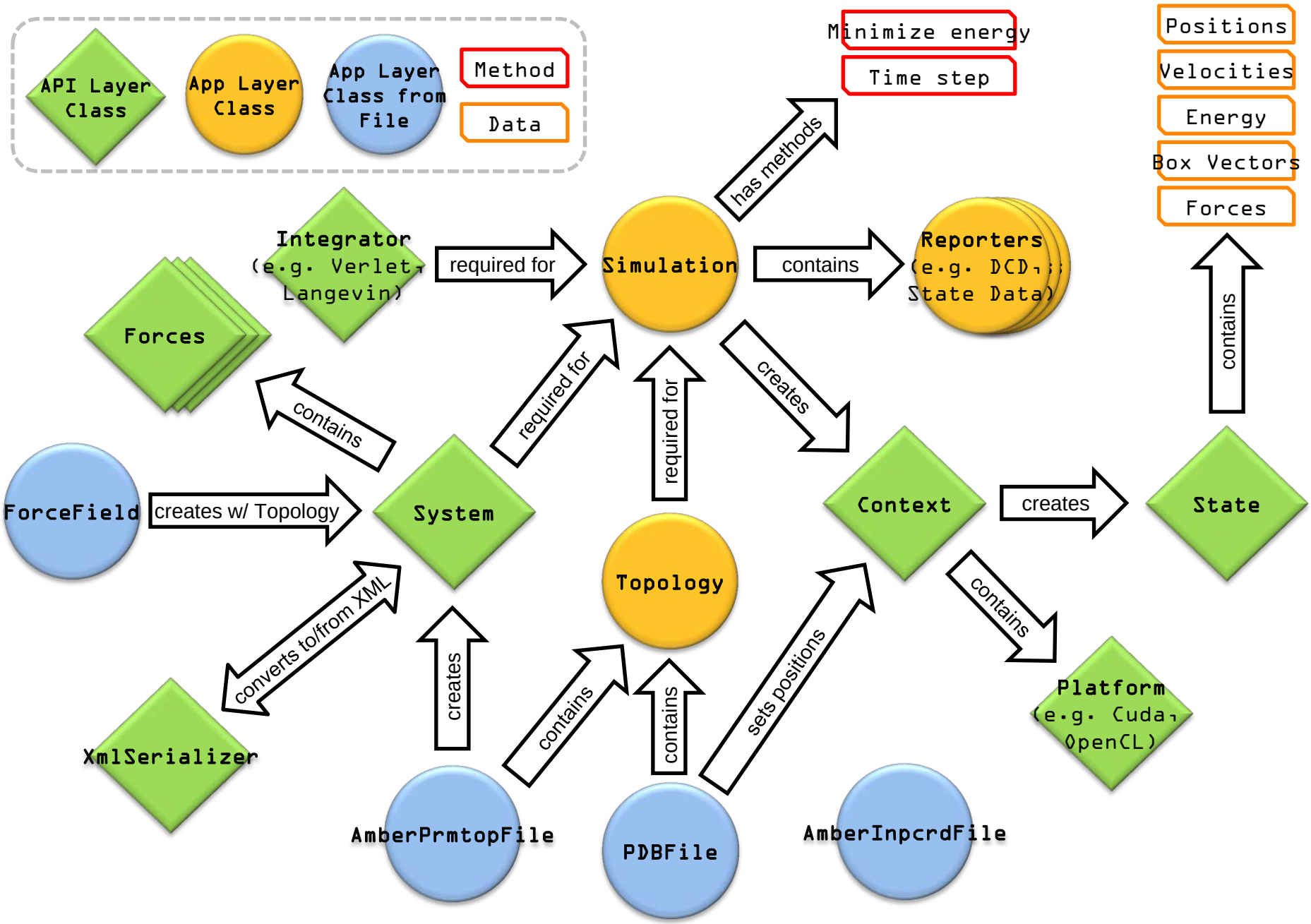
Diagram of classes in OpenMM 5.0



Interrogating physical variables

The `simulation.reporters.append()` method adds a Reporter function to a simulation.

Reporter functions are called at fixed time intervals and write useful information to the terminal or to a file.

Types of reporters:

1. PDBReporter: Write the current coordinates to a PDB file
2. DCDReporter: Write the current coordinates to a DCD file
3. StateDataReporter: Print essential information about the State (simulation time, kinetic/potential energy, temperature)

To add a reporter:

Provide the output file name (or `stdout`) and reporting

Interrogating physical variables

The `simulation.context.getState()` method provides access to all physical variables

```
# Read PDB File
pdb = PDBFile('input_exercise1.pdb')
# Read force field
forcefield = ForceField('amber99sb.xml', 'tip3p.xml')
# Create system
system = forcefield.createSystem(pdb.topology)
# Create integrator
integrator = VerletIntegrator(0.002*picoseconds)
# Create simulation
simulation = Simulation(pdb.topology, system, integrator)
# Set positions
simulation.context.setPositions(pdb.positions)
# Get state!
state = simulation.context.getState(getEnergy=True)
# Print quantity!
print state.getPotentialEnergy()
```

Let's write a new Reporter function.

Goal: You wish to observe a particular variable from your simulation as it runs.

1) Open the file `myreporter.py` containing the framework for a new reporter. In the `report` method, the `state` object has been provided for you.
2) Extract the position of the alpha carbon atom in Angstrom from the `state` object, and name it `output`.
3) Add the new reporter to the simulation specified in to `exercise1a.py`. Direct the output to your screen (`stdout`) and provide the reporting interval.
4) Run the exercise and view your output.
5) Try with more advanced variables (dihedral angle, density of the system)