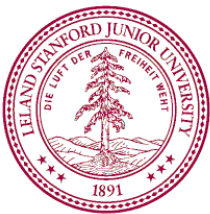# Validating OpenMM

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What is Validation?

- Make sure OpenMM works correctly...
  - Does not crash
  - Produces correct results
- Must validate *all* features across...
  - Operating systems (Linux/Mac/Windows, 32/64 bit, different OS versions)
  - GPUs (Nvidia/AMD, different generations and models)
  - OpenCL implementations (Nvidia/AMD/Apple/Intel)

Sim

Unit Tests

- Validate specific features
- Most are very simple
  - Example: Simulate a single harmonic bond with a verlet integrator, compare to the analytical result
- Some use more complicated systems
  - Example: Simulate a box of water at constant temperature and pressure, check the average box volume and kinetic energy

Unit Tests, cont.

- Unit tests are included with the source code

```
$ make test
Running tests...
Test project /Users/peastman/workspace/openmm/bin
      Start   1: TestReferenceAndersenThermostat
 1/160 Test   #1: TestReferenceAndersenThermostat .................   Passed    0.28 sec
      Start   2: TestReferenceBrownianIntegrator
 2/160 Test   #2: TestReferenceBrownianIntegrator .................   Passed    0.15 sec
      Start   3: TestReferenceCMAPTorsionForce
 3/160 Test   #3: TestReferenceCMAPTorsionForce ...................   Passed    0.02 sec
      Start   4: TestReferenceCMMotionRemover
 4/160 Test   #4: TestReferenceCMMotionRemover ....................   Passed    0.01 sec
      Start   5: TestReferenceCustomAngleForce
 5/160 Test   #5: TestReferenceCustomAngleForce ...................   Passed    0.02 sec

...
```

System Tests

- Test realistic systems
  - Proteins, DNA, RNA
  - Implicit and explicit solvent
  - From 75 to 173,181 atoms
- Three types of tests
  - Consistency across platforms
  - Force/Energy consistency
  - Integrator accuracy

Platform Consistency Tests

- Check that forces computed with Reference/CPU/CUDA/OpenCL agree

Force	Average Relative Difference
Harmonic Bond	$2.88 \cdot 10^{-6}$
Harmonic Angle	$2.25 \cdot 10^{-5}$
Periodic Torsion	$8.23 \cdot 10^{-7}$
RB Torsion	$4.82 \cdot 10^{-6}$
...	

Sim

Force/Energy Consistency Tests

- Verify that $F = -\nabla E$
  - Compute force and energy
  - Take a tiny step, evaluate energy again
  - Did it change by the right amount?

Force	Max Relative Difference
Harmonic Bond	$3.40 \cdot 10^{-5}$
Harmonic Angle	$4.96 \cdot 10^{-5}$
Periodic Torsion	$5.07 \cdot 10^{-5}$
RB Torsion	$6.32 \cdot 10^{-5}$
...	

Integrator Tests

- Deterministic integrators
  - Is energy conserved?

- Stochastic integrators
  - Is the average kinetic energy correct for the temperature?

Comparison to Other Programs

- Compare forces to Gromacs (conventional force fields) and Tinker (AMOEBA)

Force	Average Relative Difference
Harmonic Bond	$1.66 \cdot 10^{-4}$
Harmonic Angle	$6.35 \cdot 10^{-5}$
Periodic Torsion	$3.70 \cdot 10^{-5}$
Nonbonded, no cutoff	$6.13 \cdot 10^{-7}$
...	