



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)

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/CUDA/OpenCL agree

Force	Average Relative Difference
Harmonic Bond	1.982e-05
Harmonic Angle	1.153e-05
Periodic Torsion	1.506e-05
RB Torsion	3.878e-06
...	

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	7.512e-03
Harmonic Angle	4.170e-03
Periodic Torsion	1.434e-02
RB Torsion	3.540e-03
...	

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	1.658e-04
Harmonic Angle	6.347e-05
Periodic Torsion	3.701e-05
Nonbonded, no cutoff	6.125e-07
...	