



# 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	$2.88 \cdot 10^{-6}$
Harmonic Angle	$2.25 \cdot 10^{-5}$
Periodic Torsion	$8.23 \cdot 10^{-7}$
RB Torsion	$4.82 \cdot 10^{-6}$
...	

# 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	$6.13 \cdot 10^{-7}$
...	