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

<table>
<thead>
<tr>
<th>Force</th>
<th>Average Relative Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Harmonic Bond</td>
<td>1.982e-05</td>
</tr>
<tr>
<td>Harmonic Angle</td>
<td>1.153e-05</td>
</tr>
<tr>
<td>Periodic Torsion</td>
<td>1.506e-05</td>
</tr>
<tr>
<td>RB Torsion</td>
<td>3.878e-06</td>
</tr>
<tr>
<td>...</td>
<td></td>
</tr>
</tbody>
</table>
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?

<table>
<thead>
<tr>
<th>Force</th>
<th>Max Relative Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Harmonic Bond</td>
<td>7.512e-03</td>
</tr>
<tr>
<td>Harmonic Angle</td>
<td>4.170e-03</td>
</tr>
<tr>
<td>Periodic Torsion</td>
<td>1.434e-02</td>
</tr>
<tr>
<td>RB Torsion</td>
<td>3.540e-03</td>
</tr>
<tr>
<td>...</td>
<td></td>
</tr>
</tbody>
</table>
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)

<table>
<thead>
<tr>
<th>Force</th>
<th>Average Relative Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Harmonic Bond</td>
<td>1.658e-04</td>
</tr>
<tr>
<td>Harmonic Angle</td>
<td>6.347e-05</td>
</tr>
<tr>
<td>Periodic Torsion</td>
<td>3.701e-05</td>
</tr>
<tr>
<td>Nonbonded, no cutoff</td>
<td>6.125e-07</td>
</tr>
<tr>
<td>...</td>
<td></td>
</tr>
</tbody>
</table>