**GROMACS - Bug #1155**

**Enforced rotation potential is not evaluated with Verlet cut-off scheme**

02/22/2013 06:20 PM - Carsten Kutzner

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<tr>
<td>Priority:</td>
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</tr>
<tr>
<td>Assignee:</td>
<td>Carsten Kutzner</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version:</td>
<td>4.6.2</td>
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<td>Affected version - extra info:</td>
<td>4.6</td>
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<td>Difficulty:</td>
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**Description**

If one uses the Verlet cut-off scheme in combination with a rotation potential, the calculation of the latter is silently ignored. The enforced rotation module is initialized but a call to `do_rotation` is missing in the Verlet force routine.

**Associated revisions**

- **Revision d13fc483 - 04/29/2013 08:59 PM - Carsten Kutzner**
  Evaluate enforced rotation potential with Verlet, fixes #1155
  Change-Id: l6231a9a6cd9cd4004d53b721922e5d9298af76a2

- **Revision 5cbf3915 - 06/13/2013 09:45 AM - Carsten Kutzner**
  Evaluate enforced rotation potential with Verlet, fixes #1155
  Change-Id: l6231a9a6cd9cd4004d53b721922e5d9298af76a2

**History**

- **#1 - 03/14/2013 11:43 AM - Carsten Kutzner**
  - Category set to mdrun
  - Target version changed from 4.6.1 to 4.6.2
  - % Done changed from 0 to 80

- **#2 - 04/29/2013 10:10 PM - Carsten Kutzner**
  - Status changed from New to Resolved
  - % Done changed from 80 to 100

  Applied in changeset `d13fc4831999a27c4cc6b8b969663e5d4f0cb0`.

- **#3 - 04/29/2013 10:11 PM - Carsten Kutzner**

  Applied in changeset `d13fc4831999a27c4cc6b8b969663e5d4f0cb0`.

- **#4 - 04/29/2013 10:11 PM - Carsten Kutzner**

  Applied in changeset `d13fc4831999a27c4cc6b8b969663e5d4f0cb0`.

- **#5 - 05/31/2013 10:41 AM - Mark Abraham**
  - Status changed from Resolved to Closed
  - Affected version set to 4.6.1