GROMACS - Bug #1606

mdrun PME tuning can results in too short cut-offs

09/26/2014 08:36 PM - Berk Hess

<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>Berk Hess</td>
</tr>
<tr>
<td>Category</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version</td>
<td>5.0.2</td>
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<td>Affected version - extra info:</td>
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<td>Affected version:</td>
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**Difficulty:** uncategorized

**Description**

With uncommon tpr inputs where the PME grid is much finer than the requested fourier-spacing (see issue 1605), the PME tuning in mdrun can produce Coulomb cut-off shorter than the original Coulomb cut-off and shorter than the VdW cut-off. Since rcoulomb < rvdw is not supported in the Verlet cut-off scheme, this might lead to incorrect results.

**Associated revisions**

Revision d3e2d78f - 09/29/2014 05:03 PM - Berk Hess

Avoid PME tuning decreasing rcoulomb

With mdrun input with the grid much finer than fourier-spacing, PME tuning could reduce rcoulomb below the starting value.

Fixes #1606.

Change-Id: I3ae7fe38a4240251aad0b9636199b306fc7dce40

**History**

#1 - 09/26/2014 08:49 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #1606.

Uploader: Berk Hess (hess@kth.se)

Change-Id: I3ae7fe38a4240251aad0b9636199b306fc7dce40

Gerrit URL: https://gerrit.gromacs.org/4104

#2 - 09/29/2014 12:07 PM - Berk Hess

- Status changed from In Progress to Fix uploaded

#3 - 10/01/2014 04:23 PM - Mark Abraham

- Status changed from Fix uploaded to Resolved

#4 - 10/01/2014 04:30 PM - Mark Abraham

- Status changed from Resolved to Closed