### Gromacs - Bug #1169

#### PME load balancing cut-off issues

02/28/2013 06:08 PM - Berk Hess

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Priority:</td>
<td>High</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Berk Hess</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version:</td>
<td>4.6.1</td>
</tr>
<tr>
<td>Affected version - extra info:</td>
<td>4.6</td>
</tr>
</tbody>
</table>

#### Affected version:

**Description**

At the initial stage of the PME load balancing the domain decomposition dynamic load balancing can make cells smaller than the cut-off. This could potentially lead to missing interaction during a very limited number of steps. But this bug mainly reduces the effectiveness of the PME load balancing.

#### Associated revisions

**Revision e348e56a - 03/05/2013 08:19 PM - Berk Hess**

fixed bug with DD cut-off check and PME DLB

During the initial stage of PME DLB, the cut-off limit check for the DD DLB was not checked correctly. This reduced the effectiveness of both DD and PME DLB and could lead to missing interactions during a very limited number of steps.

Fixes #1169

Change-Id: l0b0cac22d4abbe8a9b0c16488aeb662d7d4d9bdc

**Revision 31725cfc - 06/13/2013 09:45 AM - Berk Hess**

fixed bug with DD cut-off check and PME DLB

During the initial stage of PME DLB, the cut-off limit check for the DD DLB was not checked correctly. This reduced the effectiveness of both DD and PME DLB and could lead to missing interactions during a very limited number of steps.

Fixes #1169

Change-Id: l0b0cac22d4abbe8a9b0c16488aeb662d7d4d9bdc

#### History

**#1 - 03/06/2013 02:40 PM - Berk Hess**

- Status changed from New to Closed