Gromacs - Bug #1660

pbc=xy with 2 walls segvs with the Verlet scheme

12/15/2014 08:31 PM - Berk Hess

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<tbody>
<tr>
<td>Priority:</td>
<td>Normal</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>5.0.5</td>
</tr>
<tr>
<td>Affected version:</td>
<td>4.6</td>
</tr>
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<td>extra info:</td>
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**Description**

Since this case is bounded, it is allowed to run, and should be able to run, with the Verlet cut-off scheme, even though general pbc=xy is not yet supported.

**Associated revisions**

Revision 30782acb - 12/22/2014 02:33 AM - Berk Hess

Fixed pbc=xy + 2 walls + Verlet scheme

Fixes #1660.

Change-Id: ld28f5d164c24d9bc6cb80f8fa8f4cba5e95262995

**History**

#1 - 12/15/2014 08:32 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #1660.
Upload: Berk Hess (hess@kth.se)
Change-Id: ld28f5d164c24d9bc6cb80f8fa8f4cba5e95262995
Gerrit URL: https://gerrit.gromacs.org/4316

#2 - 12/15/2014 09:24 PM - Berk Hess

- Status changed from In Progress to Fix uploaded
- Target version changed from 5.0.4 to 5.0.5

#3 - 01/08/2015 05:43 PM - Mark Abraham

- Status changed from Fix uploaded to Closed