**GROMACS - Bug #2613**

**Pairlist buffer set incorrectly with BD**

08/16/2018 01:32 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>core library</td>
</tr>
<tr>
<td>Target version:</td>
<td>2018.3</td>
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<td>Affected version - extra info:</td>
<td></td>
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<td>Affected version:</td>
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<td>Difficulty:</td>
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**Description**

The Verlet list buffer estimation uses incorrect masses for constrained particles and vsites with BD and bd_fric > 0. This results in incorrect buffer sizes and usually a too small buffer for typical atomistic simulations with constraints.

**Associated revisions**

Revision de5aaa57 - 08/20/2018 12:02 PM - Berk Hess

Fix Verlet buffer estimate with BD

With BD and bd_fric>0, the masses used for estimating the pairlist buffer based on estimated motion of constrained atoms and virtual sites were, incorrectly, the actual masses instead of 1.

Fixes #2613

Change-Id: I5378c5f5566ccda28554b5a6c7d7c403228aa794

**History**

#1 - 08/16/2018 01:43 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #2613.

Uploader: Berk Hess (hess@kth.se)

Change-Id: gromacs~release-2018~I5378c5f5566ccda28554b5a6c7d7c403228aa794

Gerrit URL: https://gerrit.gromacs.org/8195

#2 - 08/17/2018 10:43 AM - Berk Hess

- Status changed from In Progress to Fix uploaded

#3 - 08/20/2018 10:30 PM - Berk Hess

- Status changed from Fix uploaded to Resolved

Applied in changeset de5aaa572243889fc61f4ca45303a1b36503bedb.

#4 - 08/21/2018 10:33 AM - Paul Bauer

- Status changed from Resolved to Closed