GROMACS - Bug #2551

COM motion removal moves frozen atoms

06/07/2018 02:27 PM - Berk Hess

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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</thead>
<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>2018.2</td>
</tr>
<tr>
<td>Affected version:</td>
<td>2018</td>
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| Difficulty: | uncategorized |

Description

Due to optimizations in the integrator in release-2018, COM removal velocity corrections could lead to accumulation of velocity of particles that should be frozen.

This is related to #2542

Associated revisions

Revision 1645a388 - 06/12/2018 09:21 AM - Berk Hess

Avoid COM removal moving frozen atoms

Fixes #2551

Refs #2542

Change-Id: lfd7523661248594cce7329dfd686e814b78c9c32c

History

#1 - 06/07/2018 02:31 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #2551.
Uploader: Berk Hess (hess@kth.se)
Change-Id: gromacs~release-2018~lfd7523661248594cce7329dfd686e814b78c9c32c
Gerrit URL: https://gerrit.gromacs.org/7982

#2 - 06/07/2018 02:32 PM - Berk Hess

- Status changed from In Progress to Fix uploaded

I uploaded a fix to gerrit: https://gerrit.gromacs.org/#/c/7974/
Please test.

#3 - 06/08/2018 08:51 AM - Berk Hess

I tested this on your input and it fixes the issue.

#4 - 06/12/2018 10:15 AM - Berk Hess

- Status changed from Fix uploaded to Resolved

Applied in changeset 1645a388673d7bb83479196372d3de21ce59816b.

#5 - 06/12/2018 03:10 PM - Mark Abraham

- Status changed from Resolved to Closed