GROMACS - Bug #1878
Pull weighting broken
12/11/2015 04:39 PM - Berk Hess

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<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>
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<td>Target version:</td>
<td>5.1.2</td>
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<td>Affected version - extra info:</td>
<td>5.1.1</td>
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<tr>
<td>Difficulty:</td>
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Description
Using the option pull-group?-weights leads to using the first atom in the system for all atoms in the pull group. This gives (obviously) incorrect results.

Associated revisions
Revision 72bec06b - 12/11/2015 04:36 PM - Berk Hess
Fix bug with pull group weights
Using pull-group?-weights would set all pull indices to 0.
Fixes #1878
Change-Id: lff4c4ef9814313f948fbec3279d5815ce96216ef

History
#1 - 12/11/2015 04:40 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1878.
Uploader: Berk Hess (hess@kth.se)
Change-Id: lff4c4ef9814313f948fbec3279d5815ce96216ef
Gerrit URL: https://gerrit.gromacs.org/5446

#2 - 12/12/2015 02:30 AM - Berk Hess
- Status changed from In Progress to Resolved

Applied in changeset 72bec06b61ad6dda7228a1584bd35a13c880554.

#3 - 01/12/2016 04:22 PM - Mark Abraham
- Status changed from Resolved to Closed