Gromacs - Bug #1851

Incorrect LINCS dH/dl contribution

11/09/2015 03:54 PM - Berk Hess

<table>
<thead>
<tr>
<th>Status:</th>
<th>Resolved</th>
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<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>5.0.8</td>
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Description

Due to a (stupid) typing bug the constraint contribution of LINCS to dH/dlambdab was taken not divided by dt^2. This nearly always leads to an orders of magnitude smaller contribution. This then becomes negligible compared to other terms.

Associated revisions

Revision edb944fe - 11/09/2015 04:37 PM - Berk Hess

Correct LINCS dH/dl contribution

The LINCS constraint contribution to dH/dlambdab was missing a factor 1/delta_t^2 and thus orders of magnitude too small.

Fixes #1851

Change-Id: l864726d9a86a34207d2a02ad0803874fbfb33966

History

#1 - 11/09/2015 03:58 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #1851.
Uploader: Berk Hess (hess@kth.se)
Change-Id: l864726d9a86a34207d2a02ad0803874fbfb33966
Gerrit URL: https://gerrit.gromacs.org/5307

#2 - 11/09/2015 04:05 PM - Berk Hess

- Status changed from New to Fix uploaded

#3 - 11/11/2015 04:45 PM - Berk Hess

- Status changed from Fix uploaded to Resolved

Applied in changeset edb944fe82a066f14987076df0d6d14fa796198.