Gromacs - Bug #1408
Incorrect dvdlambda : posres() in gmxlib/bondfree.c (4.6.* & 4.5.2+)

12/16/2013 09:48 AM - teruhisa komatsu

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
</tr>
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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>4.6.6</td>
</tr>
<tr>
<td>Affected version -</td>
<td>4.5.2+</td>
</tr>
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<td>extra info:</td>
<td>4.6.x</td>
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**Description**

I think I found a simple (three year old) BUG in the line 2290 of gmxlib/bondfree.c (ver 4.6.5),

- fm*dpl[m];

which should be

+fm*dpl[m];

if I understand correctly the notation etc.

Comparing this code, which calculates dvdlambda, with the code at the line 431 of the same file,

\[
dvdlambda = \text{half} \times (kB-kA) \times dx^2 + (xA-xB) \times kk \times dx;
\]

which is inside the real function hamonic(), one may notice the inconsistency.
(c.f. fm=-kk*dx[m], dpl[m] = posB - posA)

**Associated revisions**

Revision 239fe4f4 - 06/18/2014 08:47 AM - Berk Hess

Fixed sign error in posres dvdl

For position restraints the sign of the contribution of the change in reference location was incorrect. Note that the contribution of the change in force constant was and is correct.

Fixes #1408.

Change-Id: i75210c3855d13fdd58e0a698d6c5d7c7116f456b

**History**

#1 - 06/14/2014 08:22 PM - Berk Hess

- Category set to mdrun
- Status changed from New to Closed
- Assignee set to Berk Hess
This code is correct. The code on line 431 uses $x_A - x_B$, whereas $dpdl = pos_B - pos_A$. So we need a minus sign because of this difference.

#2 - 06/16/2014 09:22 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1408.
Uploader: Berk Hess (hess@kth.se)
Change-id: i75210c3855d13dd58e0a698d6c5d7c7116f456b
Gerrit URL: https://gerrit.gromacs.org/3595

#3 - 06/16/2014 09:23 AM - Berk Hess
- Status changed from Closed to Fix uploaded
- Priority changed from Normal to High
- Target version changed from 4.6.x to 4.6.6

Sorry, I missed that the force fm also had a minus sign in it. So indeed the sign is incorrect!

#4 - 06/18/2014 09:00 AM - Berk Hess
- Status changed from Fix uploaded to Resolved
- % Done changed from 0 to 100

Applied in changeset 239fe4f4e359533215dd7c2c1815e53f85751686.

#5 - 06/18/2014 10:13 AM - Erik Lindahl
- Status changed from Resolved to Closed