Setting C6 parameter zero within combination rules 2 and 3

12/03/2013 09:10 AM - Suman Chakrabarty

Status: Closed
Priority: Normal
Assignee:
Category:
Target version:
Affected version - extra info: Affected version: 4.6.3

Description

According to the page 117 of the manual, "when sigma and epsilon need to be supplied (rule 2 and 3), it would seem it is impossible to have a non-zero C12 combined with zero C6 parameter. However, providing a negative sigma will do exactly that, such that C6 is set to zero and C12 is calculated normally. This situation represents a special case in reading the value of sigma".

However, this special option of setting negative sigma is not working as intended. Gromacs is reading sigma value with sign, so effectively $\sigma_{ij} = (\sigma_i + \sigma_j)/2$ (for comb rule 2) is being translated as $\sigma_{ij} = (\sigma_i - \sigma_j)/2$, if $\sigma_j$ was provided with a negative sign.

In case of combination rule 3, the same procedure leads to "segmentation fault" and mdrun crashes at the 0th step with all energy terms being "nan". This might originate from the fact that we are attempting square root of a negative number, if the sigma is being read with a negative sign.

So basically the special case of reading a negative sigma value needs to be checked for a possible bug.

Associated revisions

Revision 000c6b9e - 06/10/2014 03:31 PM - Erik Lindahl
Process negative sigma correctly with combrule 2 or 3

The initial combination rule code (for sigma/epsilon) did not take negative sigma rules into account, which caused segfaults instead of the values reaching the code in convparm.c that handles $\sigma<0$ during conversion to $c6/c12$ (where it is used to signal $c6=0$).

Fixes #1391.

Change-Id: I437f06d67c5ecfb58d236590288ad122bcd5f2df0

History

#1 - 06/09/2014 08:00 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1391.
Uploader: Erik Lindahl (erik@kth.se)
Change-Id: I437f06d67c5ecfb58d236590288ad122bcd5f2df0
Gerrit URL: https://gerrit.gromacs.org/3561

#2 - 06/09/2014 08:06 PM - Erik Lindahl
- Status changed from New to Fix uploaded
- Priority changed from High to Normal

#3 - 06/10/2014 03:45 PM - Erik Lindahl
- Status changed from Fix uploaded to Resolved
- % Done changed from 0 to 100

Applied in changeset 000c6b9e5d94d9e2c5efb592cb038d9775a0c21.

#4 - 06/11/2014 11:36 PM - Erik Lindahl
- Status changed from Resolved to Closed

Files

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