Hi,

I have experienced some strange behaviour. I am running a test simulation to check freeze groups in gromacs-5.0.2 (using amber03w ff with TIP4P2005 water). And I am getting LINCSWarnings for atoms which should be frozen...

Same situation is with Gromacs-4.6.7, but in Gromacs-4.6.5 simulation runs O.K.

I have attached grompp files.

Thanks,

Best,

tomek

Associated revisions

Revision 405cc128 - 11/26/2014 12:37 AM - Berk Hess

Fixed twin-range + freeze + constraints

With twin-range cut-offs, atoms which are both frozen and constrained would experience very large or NaN forces, leading to constraint warnings and errors.

Fixes #1639.

Change-Id: I1871a87054fec1149c9ed75872451d79a8ac2d2

History

#1 - 1/24/2014 10:13 AM - Berk Hess

- Status changed from New to Accepted
- Assignee set to Berk Hess

The issue is with the combination of three things: freeze-groups, constraints and twin-range interactions.

Solution 1: If you want to freeze the whole protein, you should not also constrain it, use constraints = none.

Solution 2: You are using twin-range interactions, which I don't know if that's on purpose. This can easily happen accidentally. You can set rcoulomb and rlist equal to rvdw=1.2. This will make the simulation slower, but more accurate.

I don't know if it is worth fixing this bug, since twin-range interaction are only supported with the group scheme, which is already deprecated.

#2 - 1/24/2014 03:38 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #1639.

Uploader: Berk Hess (hess@kth.se)

Change-Id: I1871a87054fec1149c9ed75872451d79a8ac2d2

Gerrit URL: https://gerrit.gromacs.org/4236

#3 - 1/24/2014 03:40 PM - Berk Hess

- Category set to mdrun
- Status changed from Accepted to Fix uploaded
- Target version set to 5.0.3
The fix turned out to be trivial, so I pushed up a fix. Still solution 1 will circumvent the issue and give slightly better performance as well.

#4 - 12/09/2014 04:18 PM - Mark Abraham
- Status changed from Fix uploaded to Closed

Files

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