

GROMACS - Bug #1450

Two-body Distance anomalously large

03/04/2014 07:15 PM - joshua layfield

Status:	Closed	
Priority:	Low	
Assignee:	joshua layfield	
Category:	mdrun	
Target version:	4.5.8	
Affected version - extra info:	I have checked this on 4.6.3 as well with the same issues.	Difficulty: uncategorized
Affected version:	4.5.4	

Description

I am trying to include a virtual particle into a simulation so that I can calculate the electric field at the midpoint of a bond. I include the virtual particle by taking an equilibrated structure of my enzymatic system and adding the virtual site using the `virtual_sites2` directive. I have confirmed that the inclusion of the virtual particle does not affect the results of an MD trajectory by analyzing structures with and without the virtual particle.

When I try run my simulation the two-body bonded distance is spuriously long.

Initial maximum inter charge-group distances:

two-body bonded interactions: 1.585 nm, LJ-14, atoms 5 13

multi-body bonded interactions: 0.434 nm, Proper Dih., atoms 5 13

Minimum cell size due to bonded interactions: 1.743 nm

The two-body bonded interaction is always ~4x longer than the multi-body bonded distance even though they are both for the same two atoms (which are always CB-CE distances in a MET residue). The multi-body bonded distance is correct based on the given structure file. I am attaching the folder that contains all of the input files.

```
grompp -f mdi.mdp -c confout.gro -p topol.top
mpirun -np 16 mdrun
```

are the commands to pre-process and run my original structure file.

```
./gro-incorporate-virtual.pl confout.gro topol.top e-stat.gro unperturbed.top perturbed.top
grompp -f mdi.mdp -c e-stat.gro -p unperturbed.top
mpirun -np 16 mdrun
```

are the series of commands to create the updated structure and topology files, pre-process the structures, and start the trajectory. When I run this I get the error that there is no domain decomposition for a minimum cell size of 2.17894 nm. I have asked on the `gmx-users` list but I have not been able to get any help there.

Thank you.

History

#1 - 03/05/2014 07:04 AM - Mark Abraham

I asked you on `gmx-users` why you are treating a beta and gamma carbon as bonded. Is that the reason for observing an anomalous distance?

#2 - 03/05/2014 04:08 PM - joshua layfield

Mark Abraham wrote:

I asked you on `gmx-users` why you are treating a beta and gamma carbon as bonded. Is that the reason for observing an anomalous distance?

In MET CB and CE interact through a 1-4 interaction.

Initial maximum inter charge-group distances:

two-body bonded interactions: 1.585 nm, LJ-14, atoms 5 13

multi-body bonded interactions: 0.434 nm, Proper Dih., atoms 5 13

Minimum cell size due to bonded interactions: 1.743 nm

As far as I understand the situation, the anomalously long distance increases the minimum cell size and limits the number of processors that can be

used.

#3 - 03/05/2014 06:46 PM - Mark Abraham

A quick look showed me that you have a [virtual_site2] constructed at 2507 from 2506 and 2505, but there was no [bond] between those two. Perhaps there was a [constraint], I didn't think to look. A virtual particle at the midpoint of a bond between two bonded atoms needs a bond if it is to make sense. Is there one?

Do the two atoms relate to the MET CB and CE and if so in what way?

#4 - 03/05/2014 08:39 PM - joshua layfield

Mark Abraham wrote:

A quick look showed me that you have a [virtual_site2] constructed at 2507 from 2506 and 2505, but there was no [bond] between those two. Perhaps there was a [constraint], I didn't think to look. A virtual particle at the midpoint of a bond between two bonded atoms needs a bond if it is to make sense. Is there one?

Do the two atoms relate to the MET CB and CE and if so in what way?

The two atoms are the donor and acceptor for a hydride transfer reaction that are located on two different substrates. There should not be a bond between them and I cannot find anything that suggests that is necessary for defining a virtual site along the non-bonded axis between these two atoms.

The two atoms are not related to the MET CB and CE either through bonding or spatial interactions. As I have investigated this further, I think that methionine just tends to have the longest 1-4 distances since the C-S bond lengths are longer than C-C and the C-S-C bond angle is larger than the C-C-C angle.

#5 - 03/06/2014 02:00 PM - Mark Abraham

joshua layfield wrote:

Mark Abraham wrote:

A quick look showed me that you have a [virtual_site2] constructed at 2507 from 2506 and 2505, but there was no [bond] between those two. Perhaps there was a [constraint], I didn't think to look. A virtual particle at the midpoint of a bond between two bonded atoms needs a bond if it is to make sense. Is there one?

Do the two atoms relate to the MET CB and CE and if so in what way?

The two atoms are the donor and acceptor for a hydride transfer reaction that are located on two different substrates.

Now I'm really confused. Your descriptions have all referred to wanting to measure the field strength at a point along a "bond," yet, the atoms in different substrates surely do not share a [bond] interaction.

There should not be a bond between them and I cannot find anything that suggests that is necessary for defining a virtual site along the non-bonded axis between these two atoms.

Indeed, it is not necessary, but your use of "bond" in your description is perhaps misleading me.

The two atoms are not related to the MET CB and CE either through bonding or spatial interactions. As I have investigated this further, I think that methionine just tends to have the longest 1-4 distances since the C-S bond lengths are longer than C-C and the C-S-C bond angle is larger than the C-C-C angle.

OK, that suggests that someone is screwing up some indexing.

From unperturbed.top

```
2505      CA    161    FOD    C4N    2505    0.138800    12.010
2506      CY    161    FOD    C6     2506    0.225975    12.010
2507      MW    161    FOD    DU     2507    0.000000     0.000
```

...

```
[ virtual_sites2 ]
; site from      func      a
2507 2506 2505    1      0.50000
```

The [bonds] setup looks like it could be two carbons in different substrates, but when I tried to see what was going on in conf.gro in VMD, all the atom indices around those numbers were in the folate.

Are you able to reproduce the weird effect with and without the vsite with just NAD+FOL in vacuum? The symptom will now be different (no MET), but finding the problem in a debugger (assuming it exists) will be about a hundred times easier.

#6 - 05/20/2014 12:02 PM - Erik Lindahl

- Status changed from New to Feedback wanted

- Priority changed from Normal to Low

No feedback for two months; Joshua, did you try the things Mark suggested?

#7 - 06/12/2014 01:19 AM - Erik Lindahl

- Status changed from Feedback wanted to Closed

Bug closed for lack of feedback. Feel free to reopen when information is added.

Files

domain-decomp.tar.gz	5.48 MB	03/04/2014	joshua layfield
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