GROMACS - Bug #68

bilayer crashing in 3.3.1 but not 3.2.1 mdrun

04/10/2006 01:18 PM - Alan Dodd

Status:	Closed		
Priority:	Normal		
Assignee:	David van der Spoel		
Category:	mdrun		
Target version:	3.3.1		
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:			

Description

Versions of Gromacs after 3.2.1 crash due to an expanding box, due to seperation of a lipid bilayer. Changing electrostatics does not stop the effect, nor does increasing tau_p, suggesting another cause? Making the leaflets more "sticky" by increasing rvdw slows the seperation down, but even at 3nm the bilayers still seperate. The bilayer has been previously equilibrated under 3.2.1 and run for a total of hundreds of ns without anything similar occuring, suggesting something in the code has changed to cause this.

I'll attach an example 3.2.1 .tpr file that crashes, along with the .edr files to compare, though I've tried several systems with almost identical results. If there are any specific comparisons you wish me to run for you, let me know.

History

#1 - 04/10/2006 01:21 PM - Alan Dodd

Created an attachment (id=33)
3.2.1 tpr file that only crashes with 3.3 onwards

#2 - 04/10/2006 01:32 PM - Alan Dodd

Created an attachment (id=34)
tar of ener files from 3.2.1 and 3.3

This example is using 3.3 (patched) rather than 3.3.1, though the same occurs, and unfortunately my rather ancient cluster crashed on the 3.2.1 run. However, 140ps is long enough to see that the bilayers seperate.

#3 - 08/21/2006 02:52 PM - David van der Spoel

Hi,

I'm getting enormous LJ-14 energies with 3.3 when testing this:

```
Energies (kJ/mol)
          Angle    Proper Dih. Ryckaert-Bell.  Improper Dih.          LJ-14
    2.87184e+04    9.63811e+03    1.25768e+04    1.73143e+03    3.27403e+06
     Coulomb-14        LJ (SR)   Coulomb (SR)   Coul. recip.      Potential
    2.42737e+04    1.68884e+03   -5.72327e+05   -2.08088e+05    2.57224e+06
    Kinetic En.   Total Energy    Temperature Pressure (bar)
    1.06528e+05    2.67877e+06    3.00081e+02    1.60075e+03
```

Is this what you get too? On the first step of the tpr?

#4 - 08/21/2006 05:31 PM - Alan Dodd

Yes. These values are comparable to other stable runs I have. In retrospect, the forcefield I'm using (ffgmx modified for lipids) appears to be relatively fragile and prone to producing errors (hence the odd 1.5fs timestep), although I never experience a problem with 3.2.1 in normal use.

#5 - 08/22/2006 12:11 PM - David van der Spoel

Is your mdrun patched for the problem with PME order != 4 ? Otherwise, retry it with pme-order =4 and ewald_tol = 1e-6

If you still have problems then please upload a new tpr file for a single molecule that runs 20 steps, and writes the energies and forces at every step. You are welcome to run gmxcheck on the output files from this tpr file with the two programs.

#6 - 08/22/2006 12:13 PM - David van der Spoel

Just as a further comment, I have run thr tpr with mdrun 3.3 (CVS) and mdrun 3.2.1 and there are very minor differences in the forces as seen from the virial.

#7 - 08/24/2006 09:18 AM - David van der Spoel

I have reproduced the problem with "standard" 3.3 code, will now retry with the latest CVS.
Did you use surface tension coupling a lot before? THis might be the culprit although I could not find any indication that something has changed.

#8 - 08/24/2006 12:41 PM - Alan Dodd

I've always used surface-tension. pme_order was definitely patched, one of the first things I checked.
Am attaching .tpr files for 20-step run as requested, along with the outputs from the runs. Both runs were created using the 3.2.1 .tpr (topol.tpr), though I have included the 3.3 version too. Am fairly sure this is using the patched version, though I'm not sure of a simple way to check - I haven't used any 3.3.* versions for several months.

#9 - 08/24/2006 12:44 PM - Alan Dodd

Created an attachment (id=67)
tar of tpr and run outputs from 3.3 and 3.2.1

#10 - 08/24/2006 05:45 PM - David van der Spoel

There definitely is an error in your topology: you have specified a pair interaction between atoms C36 and C38, which are too close together. This leads to very large 1-4 interactions (try gmxcheck -f traj.trr) and hence instability.

This does not explain why gromacs 3.3 responds different than 3.2.1, but please retest with this pair interaction taken out.

#11 - 08/30/2006 09:58 PM - David van der Spoel

The bahavior of 1-4 potentials has changed in 3.3, but only for shift and switch potentials. This does include PME, but between the two atoms in your lipid there is no Coulomb interation. This is documented here:
http://www.gromacs.org/gromacs/updates/changes-from-3.2-to-3.3-under-construction.html
Changed on 17 Jun 2005

In your input the Cut-off method is used for Van der Waals so this does not affect you.

Could you post the top file (or itp file)?

#12 - 08/31/2006 02:03 PM - Alan Dodd

Created an attachment (id=72)
.itp for DOPC

You're quite right, there is a typo in the 'pairs' section. Am testing with this fixed.

#13 - 09/01/2006 04:25 PM - Alan Dodd

With the typo fixed, the bilayers have not seperated for at least 750ps. The extra stresses must have been causing the problem.

#14 - 10/16/2006 08:24 PM - David van der Spoel

Since the system is stable I'm closing the bug.

Files

topl3.2.1.tpr	6.53 MB	04/10/2006	Alan Dodd
ener files.tar	530 KB	04/10/2006	Alan Dodd
lipidtest.tar	360 KB	08/24/2006	Alan Dodd
dopc.itp	13.6 KB	08/31/2006	Alan Dodd