GROMACS - Bug #1339

Center of mass drift with Nose-Hoover, MTTK and md-vv

09/19/2013 10:20 PM - ABolfazl Noorjahan

Status:	New		
Priority:	Normal		
Assignee:	Michael Shirts		
Category:	mdrun		
Target version:	future		
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:	4.6		

Description

Simulation of single long polymer chain shows huge center of mass drift during microsecond simulation.
The very same system has been simulated with md integrator and nose-hoover and parrinello-rahman with identical settings and no significant drift has been detected.
Here I have attached the simulation files and the architecture used for running simulation. The plot of the center of mass velocity is larger than 10 mb, so I could not attach it.
I have seen your discussion in bug#165, so thought yo might be interested in this one too.

Related issues:

Related to GROMACS - Feature #1137: Proposal for integrator framework (do_md)...	**New**

History

#1 - 09/19/2013 10:22 PM - ABolfazl Noorjahan

- File topol.top added

I am attaching the topol.top file in case if you need it.

#2 - 09/20/2013 05:04 PM - David van der Spoel

Is it center of mass of the whole system? That is, is the box changing shape?

#3 - 09/20/2013 08:07 PM - Szilárd Páll

Have you tried 4.6.3?

#4 - 09/20/2013 09:38 PM - ABolfazl Noorjahan

Yes, the center of mass of the whole system (which is a polymer chain with 400 monomer) is drifting. The box shape stays cubic and with a bit oscillation due to pressure control (The density is constant with correct value for polymer chain at all specified temperatures.).

I did simulations with 4.6 on a cluster and the only version available was 4.6 and below. If you think that may cause problem I can request an upgrade and repeat the calculations.

#5 - 09/21/2013 01:32 AM - Michael Shirts

What's the shortest time scale over which it is statistically significant?

ABolfazl Noorjahan wrote:

> Yes, the center of mass of the whole system (which is a polymer chain with 400 monomer) is drifting. The box shape stays cubic and with a bit oscillation due to pressure control (The density is constant with correct value for polymer chain at all specified temperatures.).
>
> I did simulations with 4.6 on a cluster and the only version available was 4.6 and below. If you think that may cause problem I can request an upgrade and repeat the calculations.

#6 - 09/21/2013 02:09 AM - ABolfazl Noorjahan

- File 1.ps added

- File 2.ps added

- File 3.ps added

Here I am attaching the Velocity of center of mass during time. I tried to zoom in to see the time scale on which the diversion starts.

#7 - 09/21/2013 08:50 AM - David van der Spoel

Is your molecule cyclic?

#8 - 10/06/2013 05:02 AM - Michael Shirts

David van der Spoel wrote:

> Is your molecule cyclic?

It's a single polyethylene chain. I'm not sure what to make of that, other than perhaps something odd might happen with temperature groups. Note that it's using h-bonds, not all bonds.

Currently, it looks like an abrupt 1 nm vdw cutoff, which could give artifacts.

I'd like to see it run with (and I am trying a short version of this now).

nstcalctcoupl = 1
nstcalpcoupl = 1
nstcalcenergy = 1
nstcomm = 1

To remove any weird issues with properties being calculated only every N steps.

#9 - 10/06/2013 06:15 AM - Michael Shirts

I started running this but realized that it may take a rather long time to check this -- it's running on my laptop at 2 ns/day, and it's not clear the issues would really be distinguishable for 1-2 days. Error cases that can be distinguished are usually better. . .

So far (20-30 ps in), it appears that the COM velocities are about 10x times larger for md-vv, using nstcomm = 100. For md/pr, it's down at 5^10-6, while for md-vv, it's more like 5^10-5, occasionally 1^10-4. This seems somewhat suspicious. I'll keep investigating.

#10 - 10/06/2013 06:52 AM - Michael Shirts

Interestingly, it seems to be happening when nstcomm = 1 as well, and also when MTTK is off. If it's just that it's outputting the velocities at a different place in the loop, then that's not a big deal. I'll let it go overnight and see if the drift continues, and investigate the code further.

#11 - 05/22/2014 07:06 PM - Erik Lindahl

- Assignee changed from David van der Spoel to Michael Shirts

- Target version changed from 4.6.x to 5.x

#12 - 06/18/2015 08:53 PM - Erik Lindahl

- Target version changed from 5.x to future

Any update on the investigation? ;-)

#13 - 03/06/2018 11:09 PM - Mark Abraham

- Related to Feature #1137: Proposal for integrator framework (do_md) in future GROMACS added

Files

md.mdp	764 Bytes	09/19/2013	ABolfazl Noorjahan
run.pbs	738 Bytes	09/19/2013	ABolfazl Noorjahan
md.gro	162 KB	09/19/2013	ABolfazl Noorjahan
topol.top	719 KB	09/19/2013	ABolfazl Noorjahan
1.ps	335 KB	09/21/2013	ABolfazl Noorjahan
2.ps	569 KB	09/21/2013	ABolfazl Noorjahan
3.ps	348 KB	09/21/2013	ABolfazl Noorjahan