GROMACS - Bug #2482

Atoms/molecules in freezegrps move and system crashes

04/18/2018 06:17 PM - Tai Bui

Status:	Feedback wanted		
Priority:	Normal		
Assignee:			
Category:			
Target version:			
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:	2018.1		

Description

I am using gromacs version 2018 and 2018.1. However I figured that when I froze a group of atoms/molecules (water) using freezegrps (NVT ensemble), the frozen atoms could still move and the simulation terminated due to too many LINCS warnings. This problem never happened before for previous versions of gromacs that I used (version 5.*).

History

#1 - 04/18/2018 06:22 PM - Tai Bui

- File 200ns-NVT-Eq-Gromacs5.1.4.tpr added

#2 - 04/18/2018 06:37 PM - Mark Abraham

gmx check -s1 200ns-NVT-Eq-Gromacs5.1.4.tpr -s2 200ns-NVT-Eq-from-200ns.tpr suggests there are meaningful differences in the .tpr files. Were they actually generated consistently with each other, e.g. from a common source? What does 2018.1 do with the 5.1 .tpr file?

#3 - 04/18/2018 06:44 PM - Tai Bui

The simulation in 2018.1 version used the final configuration (out.gro) from the simulation using version 5.1 as the initial configuration. In the .mdp file for version 2018.1 I just removed energygrps so I can run simulations on GPU.

#4 - 04/25/2018 09:46 AM - Berk Hess

- Status changed from New to Feedback wanted

- Priority changed from High to Normal

I don't see any significant motion in the water.

The instability could easily be caused by a different configuration. When you freeze a large part of the system, free molecules could get "stuck" in between frozen atoms and become unstable.
Please try running with the same coordinates as the 5.1 file and report if that also crashes or not.

#5 - 04/25/2018 11:57 AM - Tai Bui

- File 2018.1.tpr added

- File 2016.5.tpr added

- File 2015.1.5.tpr added

Hi Berk,

I have run on few different systems, and test on different version of gromacs. Here I attached tpr files (version 5.1.5, 2016.5, 2018.1) using the same coordinates. The sample system contains only frozen water which is part of my original system -> to run faster.

I checked the output and see that:

- Version 5.1.5: it seems like no atom is moving at all as expected.
- Version 2016.5: I found just few atoms rotated a little bit (not much) after few ns.
- Version 2018.1: A lot of atoms/molecules moved/rotated => distroyed my configuration (gas hydrates)

If you can, please run these tpr files and check the results. Thanks

#6 - 04/25/2018 02:36 PM - Berk Hess

Note that you can run your 2015.1.5.tpr in versions 2016 and 2018 as well.

I don't understand why there would be a different between versions in frozen atom handling.
What likely causes the waters to move is that the constraints are still acting.
Could you try without the constraints by copying your water model itp file, removing the [SETTLE] section in the copied version and including the copied version in your top file?

#7 - 05/18/2018 07:13 PM - Tai Bui

Berk Hess wrote:

> Note that you can run your 2015.1.5.tpr in versions 2016 and 2018 as well.
>
> I don't understand why there would be a different between versions in frozen atom handling.
> What likely causes the waters to move is that the constraints are still acting.
> Could you try without the constraints by copying your water model itp file, removing the [SETTLE] section in the copied version and including the copied version in your top file?

Hi Berk,

You are right. I am using tip4p-ice model. When I removed [constraints] from the ti4pice itp file and run again, it worked without any problem. But it's not a good solution, because it is not convenient when we want to freeze a group of molecules, while the rest is free to move.

Best regards,

Files

200ns-NVT-Eq-from-200ns.log	151 KB	04/18/2018	Tai Bui
200ns-NVT-Eq-from-200ns.tpr	950 KB	04/18/2018	Tai Bui
200ns-NVT-Eq-Gromacs5.1.4.tpr	1.04 MB	04/18/2018	Tai Bui
2018.1.tpr	163 KB	04/25/2018	Tai Bui
2016.5.tpr	163 KB	04/25/2018	Tai Bui
2015.1.5.tpr	163 KB	04/25/2018	Tai Bui