GROMACS - Bug #2637

gmx solvate tears apart molecules

09/06/2018 10:56 AM - Stephan Mohr

Status:	New		
Priority:	High		
Assignee:			
Category:			
Target version:			
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:	2018.3		

Description

I try to solve a molecule with a solvent (a mixture of methane, propane and decane) that I have prepared previously. However, gmx solvate seems to tear apart some of the solvent molecules.
I run the following command:
gmx solvate -cp molecule.gro -cs solvent.gro -o molecule_solvated.gro

All files are attached. If you look at the resulting file molecule_solvated.gro, you can observe that some molecules are torn apart (for instance, within residue 12, atoms C2 and C8 (overall these are atoms numbers 369 and 375)).
In the pure solvent these problems are not present.

Any help is appreciated!

Best regards,
Stephan Mohr

History

#1 - 09/06/2018 11:04 AM - Paul Bauer

Hello, having a look at it!
One question, it looks like the solvent in solvent.gro is already split over the periodic boundaries (e.g Resid 59). Did you try making the solvent molecules whole first?

#2 - 09/06/2018 12:46 PM - Stephan Mohr

Paul Bauer wrote:

> Hello, having a look at it!
> One question, it looks like the solvent in solvent.gro is already split over the periodic boundaries (e.g Resid 59). Did you try making the solvent molecules whole first?

Hi Paul, thanks a lot for looking at it!
No, I did not make the solvent molecules whole first. Might this be the reason (and so it is not a bug, but rather a bad usage from my side)?

#3 - 09/10/2018 02:23 PM - Paul Bauer

I think so, gmx solvate does not take anything into consideration, it simply makes copies of the solvent boxes until the volume has been filled, it does not care about what states the molecules are in.

Did you try making the molecules whole first in your solvent box? It might be an idea for a future feature that the tool does some checks if possible.

#4 - 09/11/2018 07:43 PM - Stephan Mohr

Indeed, eliminating the periodic wrap around of the molecules seems to solve the problem!

As you say, it might be nice to have this feature directly integrated, but for the moment this two-step procedure solves my problem.
Thanks a lot for your help!

Files

molecule.gro	3.46 KB	09/06/2018	Stephan Mohr
solvent.gro	553 KB	09/06/2018	Stephan Mohr