GROMACS - Bug #2094

Solvation Consistency with MARTINI forcefield water across GROMACS versions with user-specified VDW size

12/27/2016 10:53 PM - Tyler Reddy

Status:	New		
Priority:	Normal		
Assignee:			
Category:			
Target version:			
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:	2016.1		

Description

Although it is known that GROMACS database VDW size parameters for solvation changed with the 5.0 series, it is not clear to me why one would get different solvation results between GROMACS 4.6.5 and GROMACS 2016.1 when explicitly specifying the VDW particle size to be used. Indeed, the defaults used in GROMACS were never appropriate for the MARTINI FF so we've always explicitly specified the VDW size that is to be used. For me, this resulted in a hydration of rhombic dodecahedral container (with many lipids already present) with a deficit of 3.3 million water particles for 2016.1 versus 4.6.5. Since I'm already specifying a VDW radius that is roughy consistent with the particle radius used in the MARTINI FF, I don't understand what particle size I'm supposed to use in 2016.1 to reproduce the proper solvation I was getting with 4.6.5. If this is working as intended, then how is it an improvement that I would have to artificially decrease the VDW radius below the value used by the forcefield in newer versions of GROMACS -- that doesn't seem right.

Perhaps this is a bug, and for that reason I have simplified the test case from my usual large viral systems to a cubic container with a single lipid, downloaded from the MARTINI website. I've attached the files needed to reproduce the behaviour I demonstrate below.

Using GROMACS 4.6.5:
Command: genbox -cp POPC-em.gro -cs water.gro -o hydrated_POPC.gro -vdwd 0.24
Result: "Generated solvent containing 139 atoms in 139 residues"

Using GROMACS 2016.1:
Command: gmx solvate -cp POPC-em.gro -cs water.gro -o hydrated_POPC.gro -radius 0.24
Result: "Generated solvent containing 134 atoms in 134 residues"

That minor difference appears to grow massively with more solute & more solvent in a real / large system, as I've described above.

There is one flag that differs between the two commands -- radius vs. vdwd. The 2016 docs describe "radius" as "Default van der Waals distance." The 4.6 docs describe 'vdwd' as "Default van der Waals distance." That sounds like the same thing to me. Perhaps the docs need some clarification on what has changed if this is a backward-incompatible change, so that end users don't have to feel compelled to juggle GROMACS versions for different tasks.

If I had to speculate, perhaps the updated database for VDW sizes is sometimes finding values for particles in the MARTINI FF & therefore not falling back to the default size that is user-specified as it was in previous versions. But if you're going to provide values that recognize based on name, then that seems risky because there are a lot of different FFs out there... If this is what is going on, is there a way to completely override the database VDW values in newer versions & is this clearly explained in the docs?

Associated revisions

Revision 6be1d47d - 02/07/2017 02:55 PM - Mark Abraham

Introduced system preparation section to user guide

This gives us somewhere we could document the use and limitations of
vdwradii.dat better.

Enchanced documentation of solvate and insert-molecules, similarly.

Refs #2094

Change-Id: I019948472dfc308c1acd74d4fce271ba4d481ead

History

#1 - 12/28/2016 11:02 AM - Teemu Murtola

There have been several changes to gmx solvate between those releases, the vdw radii changes being just one of them. It would help if you could identify which solvent molecules you expect to be kept by gmx solvate that are not kept by the 2016 version (compared to the 4.6 version). The algorithm that selects what to keep has changed, for the most part to keep as much as possible of the original pre-equilibrated water configuration, instead of adding or removing solvent molecules from the middle of the solvent.

It is certainly possible that there is a bug, but that's hard to say without such analysis. It should be possible to get rid of the default radii by creating an empty vdwradii.dat into the working directory to investigate whether they could play a role here.

#2 - 01/20/2017 02:00 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #2094.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~release-2016~I019948472dfc308c1acd74d4fce271ba4d481ead
Gerrit URL: https://gerrit.gromacs.org/6427

#3 - 01/20/2017 04:56 PM - Mark Abraham

Tyler Reddy wrote:

> If I had to speculate, perhaps the updated database for VDW sizes is sometimes finding values for particles in the MARTINI FF & therefore not falling back to the default size that is user-specified as it was in previous versions. But if you're going to provide values that recognize based on name, then that seems risky because there are a lot of different FFs out there... If this is what is going on, is there a way to completely override the database VDW values in newer versions & is this clearly explained in the docs?

Indeed, the approach of having such a name-based database of radii is risky for lots of reasons. I've tried to create some docs for the mechanics of vdwradii.dat at the above linked patch, and Jenkins will build the docs from that. Is there anywhere better anyone can think of where to try to document the behaviour of such .dat files?

Files

POPC-em.gro	586 Bytes	12/27/2016	Tyler Reddy
water.gro	27 KB	12/27/2016	Tyler Reddy