# GROMACS - Bug #1984

## gmx solvate (monoatomic solvents?)

06/02/2016 02:41 PM - Pim Frederix

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|---|---|---|---|
| **Status:** | Closed | | |
| **Priority:** | Normal | | |
| **Assignee:** | Teemu Murtola | | |
| **Category:** | analysis tools | | |
| **Target version:** | 5.1 | | |
| **Affected version - extra info:** | Also found in 4.0.x, 4.5.5 and 4.6.x and possibly others | **Difficulty:** | uncategorized |
| **Affected version:** | 5.0.5 | | |

**Description**

After making a box using gmx insert-molecules, I want to use gmx solvate to add solvent molecules to my system.
In my case I'm using the Martini force field which means I want to add water molecules consisting of single beads. To get the correct density I have to use flag -radius 0.20. This results in a solvated box that has a strange density inhomogeneity: the box is more dense in a cube near the centre (see image).

Command:> gmx solvate -cp FFF300_box0.gro -cs water-125A_eq.gro -o FFF300_water0.gro -radius 0.2
(or genbox -cp FFF300_box0.gro -cs water-125A_eq.gro -o FFF300_water0.gro -vdwd 0.2 for versions 4.x)

Sometimes minimization and equilibration proceeds (with box size scaling warnings in the first steps as it expands rapidly), but this might be dangerous anyway as you have many more water molecules in your system than you should think you will.

The problem persists with different solutes and "sometimes" gets reduced by using a water box of identical size to the solute box. I noticed some hacks floating around on the www, where someone mentioned this may only be the case for monoatomic solvents (Martini water), but I also get errors using Martini polarisable water (3 atoms), and anyway it seems appropriate to get to the roots of this.
This issue already existed in Gromacs 4.x as well.

### History

#### #1 - 06/02/2016 04:31 PM - Teemu Murtola

Please test with 5.1 or later, the logic in gmx solvate has changed quite a bit leading to that version and might work better.

#### #2 - 06/02/2016 05:40 PM - Pim Frederix

Amazing, it works properly with 5.1.2.

Sorry, the problem has been bothering me in so many versions of Gromacs I didn't try it with the very latest version! Thanks, great work.

#### #3 - 06/02/2016 08:08 PM - Teemu Murtola

*- Category set to analysis tools*

*- Status changed from New to Closed*

*- Assignee set to Teemu Murtola*

Closed since the issue is fixed in 5.1.

I also remember struggling with the behavior of gmx solvate/genbox with Martini with some old version, so when I essentially rewrote the logic for 5.1, I tried to make it much less surprising. Now, if you provide a solvent box, the only solvent molecules that get removed are those that overlap with your solute, or overlap with a periodic image of the solvent box (in case the size is not an exact multiple). The code no longer removes stuff elsewhere in the box, no matter what the radii of the atoms are. And if you use -maxsol, the atoms are removed throughout the box (assuming they are randomly distributed in the initial configuration). This should give you the same bulk density as in the input box, or something very close to it.

#### #4 - 07/11/2016 07:38 PM - Mark Abraham

*- Target version changed from 5.x to 5.1*

### Files

| | | | |
|---|---|---|---|
| FFF300_box0.gro | 158 KB | 06/02/2016 | Pim Frederix |

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|---|---|---|---|
| FFF300_water0.gro | 894 KB | 06/02/2016 | Pim Frederix |
| water-125A_eq.gro | 1.02 MB | 06/02/2016 | Pim Frederix |
| waterbox.tga | 1.6 MB | 06/02/2016 | Pim Frederix |