

## GROMACS - Bug #2119

### gmx solvate -shell does not add anything

02/09/2017 07:14 AM - David van der Spoel

<b>Status:</b> Closed	
<b>Priority:</b> Normal	
<b>Assignee:</b> David van der Spoel	
<b>Category:</b>	
<b>Target version:</b>	
<b>Affected version - extra info:</b>	<b>Difficulty:</b> uncategorized
<b>Affected version:</b> 5.0	
<b>Description</b>	
Running the gmx solvate program with an existing box works, but the -shell option, supposed to make a spherical droplet around a solute yields zero solvent molecules.	
Example:	
Version 4.6 gives: % genbox -cp after_em.gro -cs spc216 -o b4em_sol.gro -shell 1.2 <snip> Number of SOL molecules: 1123	
Version 5.0 gives: % gmx solvate -cp after_em.gro -cs spc216 -o b4em_sol.gro -shell 1.2 <snip> Number of SOL molecules: 7039	
Version 5.1 gives: % gmx solvate -cp after_em.gro -cs spc216 -o b4em_sol.gro -shell 1.2 <snip> Number of SOL molecules: 0	

#### Associated revisions

##### Revision 54d906f1 - 02/27/2017 08:24 PM - David van der Spoel

Fixes bug in gmx solvate with -shell that yielded 0 SOL.

In the transition from genbox to the new solvate.cpp some incorrect logic was introduced.

Added test for -shell.

Implemented test for conf files that check the title and number of atoms. In principle this could be extended to other structure files.

Fixes #2119

Change-Id: I88feef55f33c7076b9c27a9831ee04d890333b76

#### History

##### #1 - 02/09/2017 08:21 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2119](#).

Uploader: David van der Spoel ([davidvanderspoel@gmail.com](mailto:davidvanderspoel@gmail.com))

Change-Id: gromacs~release-5-1~I61b04457ddcf34b789d590d610c2c365f84a17db

Gerrit URL: <https://gerrit.gromacs.org/6461>

##### #2 - 02/10/2017 07:45 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2119](#).

Uploader: David van der Spoel ([davidvanderspoel@gmail.com](mailto:davidvanderspoel@gmail.com))

Change-Id: gromacs~release-2016~l88feef55f33c7076b9c27a9831ee04d890333b76  
Gerrit URL: <https://gerrit.gromacs.org/6468>

**#3 - 02/27/2017 10:01 PM - David van der Spoel**

- Status changed from New to Resolved

Applied in changeset [54d906f155299a4b1ceeafaa6ceca1a022beb913](#).

**#4 - 12/11/2017 12:17 PM - Erik Lindahl**

- Status changed from Resolved to Closed

**Files**

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after_em.gro	4.97 KB	02/09/2017	David van der Spoel
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