# GROMACS - Bug #2119

## gmx solvate -shell does not add anything

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

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<tbody>
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<td>Priority:</td>
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<tr>
<td>Assignee:</td>
<td>David van der Spoel</td>
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<tr>
<td>Category:</td>
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<td>Target version:</td>
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<td>Affected version</td>
<td>5.0</td>
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## Description
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)
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)
#3 - 02/27/2017 10:01 PM - David van der Spoel
- Status changed from New to Resolved

Applied in changeset 54d906f155299a4b1ceefaa6ccea1a022beeb913.

#4 - 12/11/2017 12:17 PM - Erik Lindahl
- Status changed from Resolved to Closed

Files

+ after_em.gro 4.97 KB 02/09/2017 02/22/2020 2/2