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>
<tr>
<td>Priority</td>
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<tr>
<td>Assignee</td>
<td>David van der Spoel</td>
</tr>
<tr>
<td>Category</td>
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<td>Target version</td>
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<td>5.0</td>
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<tr>
<td>Difficulty</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
<nclip>
```

Number of SOL molecules: 1123

Version 5.0 gives:

```
% gmx solvate -cp after_em.gro -cs spc216 -o b4em_sol.gro -shell 1.2
<nclip>
```

Number of SOL molecules: 7039

Version 5.1 gives:

```
% gmx solvate -cp after_em.gro -cs spc216 -o b4em_sol.gro -shell 1.2
<nclip>
```

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.

Implemented 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 54d906f155299a4b1ceefaaa6ceca1a022be913.

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

Files

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<td>4.97 KB</td>
<td>02/09/2017</td>
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