GROMACS - Bug #2523

Bug in solvate

05/25/2018 05:03 PM - marc Barbry

Status:	Closed		
Priority:	Normal		
Assignee:			
Category:			
Target version:			
Affected version - extra info:		**Difficulty:**	simple
Affected version:	2018.1		

Description

Hi,

I found a bug regarding bad formatted input pdb file in the solvate package.
Using a pdb file (H2o-nocell.pdb) without any cell indication just lets the program running since it get stuck in a while loop. (solvate.cpp, line ~250).
This is because the variable box[i][i] = 0.0, therefore xcg does not increment.

To reproduce the error, you can run (see attached files)

```
gmx solvate -cs H2O-nocell.pdb  -cp centered.gro  -p topol.top -o solvated.gro
```

The input file should be correctly check in order to avoid such issues.

Best regards,
Marc Barbry

Associated revisions

Revision a59917f9 - 05/30/2018 09:25 AM - Paul Bauer

Disallow use of empty box information in solvent files

An empty box information in a solvent file presented to gmx solvate
could case an infinte loop because the current coordinate would always
be incremented by zero. Disallowed by introducing new function that
checks for proper box information.

Fixes #2523

Change-Id: I461509f8aafa2048253faf85ccbe388bbbaf80a7

History

#1 - 05/29/2018 05:07 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #2523.
Uploader: Paul Bauer (paul.bauer.q@gmail.com)
Change-Id: gromacs~release-2018~I461509f8aafa2048253faf85ccbe388bbbaf80a7
Gerrit URL: https://gerrit.gromacs.org/7960

#2 - 05/31/2018 06:15 PM - Paul Bauer

- Status changed from New to Resolved

Applied in changeset a59917f9adbdb0c0fea37917bad983c22eed02ff.

#3 - 06/04/2018 12:42 PM - Paul Bauer

- Status changed from Resolved to Closed

Files

gmx-tutorial-material-bug.tar.gz	5.68 MB	05/25/2018	marc Barbry