GROMACS - Bug #1747

gmx solvate clobbers temp.top (not given as a command line input)

05/25/2015 03:58 AM - Chris Neale

Status:	Closed		
Priority:	Low		
Assignee:	Mark Abraham		
Category:	preprocessing (pdb2gmx,grompp)		
Target version:	5.0.6		
Affected version - extra info:	all since 3.3 or earlier	**Difficulty:**	uncategorized
Affected version:	5.0.5		

Description

gromacs 5.0.5 gmx solvate seems to create its own file called temp.top, which causes any existing temp.top to be moved to #temp.top.1# . The original file is not lost, but this is unexpected and (so far as I know) undocumented behaviour. I suggest that if gmx solvate needs to create a temporary .top file then this should ideally be a guaranteed unused filename, or at the very least something much more unlikely to be in use than temp.top. Details from a test demonstration follow.

```
$ ls
empty.gro  temp.top  waterbox.top

####################

$ cat empty.gro
title
0
5 5 5

####################

$ cat waterbox.top
; Include forcefield parameters
#include "charmm27.ff/forcefield.itp"

; Include water topology
#include "charmm27.ff/tips3p.itp"

#ifdef POSRES_WATER
; Position restraint for each water oxygen
[ position_restraints ]
;  i funct       fcx        fcy        fcz
   1    1       1000       1000       1000
#endif

; Include topology for ions
#include "charmm27.ff/ions.itp"

[ system ]
; Name
Gnomes, ROck Monsters And Chili Sauce

[ molecules ]
; Compound        #mols

####################

$ gmx solvate -cp empty.gro -cs spc216.gro -p waterbox.top -o waterbox.gro
GROMACS:    gmx solvate, VERSION 5.0.5

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GROMACS:      gmx solvate, VERSION 5.0.5
Executable:   /project2/p/pomes/cneale/GPC/exe/intel/gromacs-5.0.5/exec_serial/bin/gmx
Library dir:  /project2/p/pomes/cneale/GPC/exe/intel/gromacs-5.0.5/exec_serial/share/gromacs/top
Command line:
  gmx solvate -cp empty.gro -cs spc216.gro -p waterbox.top -o waterbox.gro

Reading solute configuration
Warning: Number of atoms in empty.gro is 0
title
Containing 0 atoms in 0 residues
Initialising inter-atomic distances...
Note: no atoms in empty.gro
Reading solvent configuration
"216H2O,WATJP01,SPC216,SPC-MODEL,300K,BOX(M)=1.86206NM,WFVG,MAR. 1984"
solvent configuration contains 648 atoms in 216 residues

Initialising inter-atomic distances...

WARNING: Masses and atomic (Van der Waals) radii will be guessed
         based on residue and atom names, since they could not be
         definitively assigned from the information in your input
         files. These guessed numbers might deviate from the mass
         and radius of the atom type. Please check the output
         files if necessary.

NOTE: From version 5.0 gmx uses the Van der Waals radii
from the source below. This means the results may be different
compared to previous GROMACS versions.

++++ PLEASE READ AND CITE THE FOLLOWING REFERENCE ++++
A. Bondi
van der Waals Volumes and Radii
J. Phys. Chem. 68 (1964) pp. 441-451
-------- -------- --- Thank You --- -------- --------

Will generate new solvent configuration of 3x3x3 boxes
Generating configuration
Sorting configuration
Found 1 molecule type:
    SOL (   3 atoms):  5832 residues
Calculating Overlap...
box_margin = 0.25992
Removed 3393 atoms that were outside the box
Neighborsearching with a cut-off of 0.25992

NOTE: This file uses the deprecated 'group' cutoff_scheme. This will be
removed in a future release when 'verlet' supports all interaction forms.
```

```
NOTE: This file uses the deprecated 'group' cutoff_scheme. This will be
removed in a future release when 'verlet' supports all interaction forms.

Table routines are used for coulomb: FALSE
Table routines are used for vdw:     FALSE
Cut-off's:   NS: 0.25992   Coulomb: 0.25992   LJ: 0.25992
System total charge: 0.000
Potential shift: LJ r^-12: 0.000e+00 r^-6: 0.000e+00, Coulomb 0e+00

Grid: 19 x 19 x 19 cells
Successfully made neighbourlist
nri = 19811, nrj = 130088
Checking Protein-Solvent overlap: tested 0 pairs, removed 0 atoms.
Checking Solvent-Solvent overlap: tested 14524 pairs, removed 1881 atoms.
Added 4074 molecules
Generated solvent containing 12222 atoms in 4074 residues
Writing generated configuration to waterbox.gro

Output configuration contains 12222 atoms in 4074 residues
Volume                 :         125 (nm^3)
Density                :     974.999 (g/l)
Number of SOL molecules:   4074

Processing topology

Back Off! I just backed up temp.top to ./#temp.top.1#
Adding line for 4074 solvent molecules to topology file (waterbox.top)

Back Off! I just backed up waterbox.top to ./#waterbox.top.1#

gcq#6: "It's So Lonely When You Don't Even Know Yourself" (Red Hot Chili Peppers)

###################

Note that temp.top has been backed up by the above command. However, whatever gmx solvate created
in temp.top is now gone:

$ ls temp.top
ls: cannot access temp.top: No such file or directory
```

Thank you,
Chris.

Associated revisions

Revision 4b1e5a18 - 05/26/2015 02:11 PM - Mark Abraham

Fix use of hard-coded temporary filename

Using temp.top can run into a user file of the same name, which is unfriendly. Instead, use the function we have for doing the job of making a temporary filename.

Fixes #1747

Change-Id: Ia6266e5605dd14032743e11f5dc68a520c47ce06

History

#1 - 05/25/2015 09:15 PM - Mark Abraham

- Description updated

#2 - 05/26/2015 02:56 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #1747.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: Ia6266e5605dd14032743e11f5dc68a520c47ce06
Gerrit URL: https://gerrit.gromacs.org/4657

#3 - 05/26/2015 02:59 AM - Mark Abraham

- Status changed from New to Fix uploaded

- Assignee set to Mark Abraham

- Target version set to 5.0.6

Thanks for the report.

This and some other tools have used the name "temp.top" (since pre-3.3 GROMACS) as the intermediate file for the new waterbox.top. This is not good, so changed it to do something nicer.

#4 - 05/26/2015 03:00 AM - Mark Abraham

- Tracker changed from Feature to Bug

- Affected version - extra info set to all since 3.3 or earlier

- Affected version set to 5.0.5

#5 - 05/26/2015 05:19 PM - Mark Abraham

- Status changed from Fix uploaded to Closed