

GROMACS - Bug #1667

gmx convert-tpr writes wrong number of mol in output tpr

12/29/2014 04:45 PM - Alexey Shvetsov

Status: New	
Priority: Normal	
Assignee: David van der Spoel	
Category:	
Target version:	
Affected version - extra info:	Difficulty: uncategorized
Affected version: 5.0.4	
Description	
<p>I notice when i tried to remove solvent from tpr file and write new one with gmx convert-tpr that output file always contain all molecules merged, so effective number of mols are 1. However in this case output should contain 10 mols (9 proteins and 1 rna)</p>	
<pre>gmx convert-tpr -s hk_162_39_ring9_rna.md_npt.tpr -nsteps -1 -o tmp.tpr -n index.ndx GROMACS: gmx convert-tpr, VERSION 5.0.4 Executable: /usr/bin/gmx Library dir: /usr/share/gromacs/top Command line: gmx convert-tpr -s hk_162_39_ring9_rna.md_npt.tpr -nsteps -1 -o tmp.tpr -n index.ndx</pre>	
<pre>Reading topology and stuff from hk_162_39_ring9_rna.md_npt.tpr Reading file hk_162_39_ring9_rna.md_npt.tpr, VERSION 5.1-dev-20140712-06ff230-dirty-unknown (single precision) Setting nsteps to -1 Group 0 (System) has 644440 elements Group 1 (Protein) has 70200 elements Group 2 (Protein-H) has 35289 elements Group 3 (C-alpha) has 4482 elements Group 4 (Backbone) has 13446 elements Group 5 (MainChain) has 17937 elements Group 6 (MainChain+Cb) has 22050 elements Group 7 (MainChain+H) has 22275 elements Group 8 (SideChain) has 47925 elements Group 9 (SideChain-H) has 17352 elements Group 10 (Prot-Masses) has 70200 elements Group 11 (non-Protein) has 574240 elements Group 12 (RNA) has 5579 elements Group 13 (NA) has 272 elements Group 14 (CL) has 195 elements Group 15 (Water) has 568194 elements Group 16 (SOL) has 568194 elements Group 17 (non-Water) has 76246 elements Group 18 (Ion) has 467 elements Group 19 (NA) has 272 elements Group 20 (CL) has 195 elements Group 21 (Water_and_ions) has 568661 elements Group 22 (Protein_RNA) has 75779 elements Select a group: 22 Selected 22: 'Protein_RNA' Will write subset Protein_RNA of original tpx containing 75779 atoms Reduced block cgs from 644440 to 75779 index-, 644440 to 75779 a-entries Reduced block mols from 189875 to 10 index-, 644440 to 75779 a-entries Reduced block excl from 644440 to 75779 index-, 2605914 to 900865 a-entries Reduced ilist ANGLES from 138078 to 138078 entries Reduced ilist PDIHS from 208589 to 208589 entries Reduced ilist PIDIHS from 15444 to 15444 entries Reduced ilist LJ14 from 197721 to 197721 entries Reduced ilist CONSTR from 76744 to 76744 entries</pre>	

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Reduced ilst SETTLE from 189398 to      0 entries
Writing statusfile with starting step    0 and length      -1 steps...
                                time      0.000 and length    -0.002 ps

alexxy@mdstore ~/Models/np/hk_162_39_ring9_rna/312K $ gmxcheck -s1 tmp.tpr -m /tmp/
GROMACS:      gmx check, VERSION 5.0.4
Executable:   /usr/bin/gmx
Library dir:  /usr/share/gromacs/top
Command line:
  gmxcheck -s1 tmp.tpr -m /tmp/

Reading file tmp.tpr, VERSION 5.0.4 (single precision)

Back Off! I just backed up /tmp/.tex to /tmp/#.tex.2#

gcq#147: "I'm An Oakman" (Pulp Fiction)

alexxy@mdstore ~/Models/np/hk_162_39_ring9_rna/312K $ cat /tmp/.tex
\section{Methods}
\subsection{Simulation system}
A system of 1 molecules (75779 atoms) was simulated.

\subsection{Simulation settings}
A total of -2e-06 ns were simulated with a time step of 2 fs.
Neighbor searching was performed every 500 steps.
The PME algorithm was used for electrostatic interactions.
with a cut-off of 1.2 nm.
A reciprocal grid of 216 x 216 x 96 cells was used with 4th order B-spline interpolation.
A single cut-off of 2.485 was used for Van der Waals interactions.
Temperature coupling was done with the Nose-Hoover algorithm.
Pressure coupling was done with the Parrinello-Rahman algorithm.

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Related issues:

Related to GROMACS - Feature #1861: Add support for trajectories of part of t...	Closed
Related to GROMACS - Feature #1864: write tng files with energies	New

History

#1 - 12/29/2014 05:07 PM - Justin Lemkul

- Priority changed from Normal to Low

Does this affect anything other than the methods output? Since you're manipulating the .tpr anyway, whatever -m produces is probably useless, anyway.

#2 - 12/29/2014 07:17 PM - Alexey Shvetsov

Its just an example. Actualy selections like mol_cog, mol_com and so on dont works with reduced topology

#3 - 12/29/2014 07:20 PM - Justin Lemkul

- Priority changed from Low to Normal

OK, so there is a substantive problem in interfacing the subset .tpr file with other tools like gmx select - that is a much more informative report, because it distinguishes it from being some trivial output bug to something that impacts further analysis.

#4 - 12/29/2014 07:39 PM - Alexey Shvetsov

i'm preparing patch for convert-tpr to correctly copy molblock info

#5 - 01/02/2015 04:53 PM - Mark Abraham

- Description updated

#6 - 06/20/2015 02:27 AM - Peter Kasson

Quick ping: Alexey, do you have a patch here? It sounds like you've thought about how to fix this...if you don't have a patch but do have a quick pointer to the code and/or files reproduce, I can try to push something out.

#7 - 06/20/2015 09:40 AM - Alexey Shvetsov

I dont have correctly working solution for this issue. Seems like to solve it its better to recreate tpr

Easy steps to reproduce it

1. Get tpr of multimeric system (e.g two proteins in a box with water)
2. Create index group (also default Protein will work)
3. Use convert-tpr to reduce tpr file with Protein index group
4. Try to use any new tool with dynamic selections (if you'll try to use mol_com for example you will see only one mol)

Resulting tpr will have only one molblock (however in case of two protein it should have at least 2), I didnt find correct and easy way to reduce tpr system with selected index group (so it will have right number of molblocks and right contents for them) =\

#8 - 06/20/2015 09:42 AM - Alexey Shvetsov

- File con-tpr-partial-fix.patch added

Partially working patch.. however it doesnt fully fix issue
I may also upload it to gerrit

#9 - 06/24/2015 10:21 PM - Berk Hess

Do you have a strong need for this functionality?
This is ancient functionality that we would rather remove.

#10 - 06/24/2015 11:14 PM - Alexey Shvetsov

Its good question. Its only needed for new tools (with dynamic selections) and reduced trajectory (e.g. with dropped solvent). For example if full trajectory quite large (e.g. 500+Gb) its very usefull. Otherwise its not needed.

#11 - 06/29/2015 07:55 PM - Peter Kasson

Does convert-tpr work properly if System is selected and only fail if an index specifying less than the full system is used?

#12 - 11/24/2015 06:21 PM - David van der Spoel

- Assignee set to David van der Spoel

I will try to fix it. It can be convenient for analysis.

#13 - 11/24/2015 09:49 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#1667](#).
Uploader: David van der Spoel (davidvanderspoel@gmail.com)
Change-Id: I15450b734fe96710eee0744f34b5bdae919c632c
Gerrit URL: <https://gerrit.gromacs.org/5377>

#14 - 11/24/2015 09:56 PM - Berk Hess

I didn't realize people were working on fixing this.
I think it would be a far better solution to remove this tool that produces buggy topologies and allow the new analysis framework to use a full tpr with a partial xtc file. It could even check that the xtc file atom count matches that of the xtc group in the tpr.
Teemu, how much work would that be?

#15 - 11/24/2015 10:31 PM - David van der Spoel

Since we do not have atom information in xtc files it would be creating new problems too.

I've recently used this tool for mdrun -rerun, setting specific charges to zero.

Now I would like to take all-atom simulations, remove the hydrogens from the tpr and trr file and analyze them (and the patch in gerrit makes this possible).

#16 - 11/25/2015 06:39 AM - Teemu Murtola

I think it should be straightforward, even if quite a bit of work, to add support for specifying the index group for the atoms that are contained in the trajectory for the new framework. Most of the work is in the selection code, in particular in various consistency checks. And I don't think this would create any problems that aren't already there: the user now needs, and would still need, keep track of what atoms there are in the trajectory.

#17 - 11/25/2015 08:14 AM - Teemu Murtola

The option to clear charges from a tpr should be trivial to put in grompp, and is not really in any way related to this issue.

Getting rid of t_topology is a massive amount of work, with probably 50+ tools, all selection code, and probably a lot of analysis utility code

depending on it...

I think Berk's suggestion of supporting a trajectory with an arbitrary subset of atoms in the tools, without touching the topology, would probably be simplest for most problems.

#18 - 11/25/2015 08:58 AM - David van der Spoel

The latter could be fixed in tng if we store original atom numbers. That does not guarantee that the tpr matches the tng files but it would be an improvement.

#19 - 11/25/2015 09:05 AM - Teemu Murtola

David van der Spoel wrote:

The latter could be fixed in tng if we store original atom numbers. That does not guarantee that the tpr matches the tng files but it would be an improvement.

Sure, that would help, and would simplify the use of tools that would support such a subset. But not much has happened with the tng support after it was hastily introduced just before 5.0.

#20 - 11/25/2015 09:15 AM - David van der Spoel

I guess that should be the topic of another redmine, but apparently one can not store velocities to tng during mdrun, and energies would be nice too.

#21 - 11/25/2015 09:48 AM - Berk Hess

Related to [#1861](#)

#22 - 11/25/2015 09:49 AM - Berk Hess

- Related to Feature #1861: Add support for trajectories of part of the system to new analysis framework added

#23 - 06/27/2016 08:29 PM - Mark Abraham

- Related to Feature #1864: write tng files with energies added

#24 - 06/27/2016 08:29 PM - Mark Abraham

- Target version deleted (5.x)

Files

con-tpr-partial-fix.patch	4.57 KB	06/20/2015	Alexey Shvetsov
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