GROMACS - Bug #635

position restraints output with gmxdump -sys is wrong

01/07/2011 02:30 PM - Floris Buelens

Status: Rejected
Priority: Low
Assignee: Berk Hess
Category: analysis tools
Target version: 
Affected version: 

Description
gmxdump output for position restraints is incorrect when the option -sys is used. Tested with 4.0.5 and 4.5.3. Steps to reproduce:
wget 'http://www.pdb.org/pdb/download/downloadFile.do?fileFormat=pdb&compression=NO&structureId=1AKI' -O 1AKI.pdb
wget http://www.bevanlab.biochem.vt.edu/Pages/Personal/justin/gmx-tutorials/lysozyme/Files/minim.mdp
pdb2gmx -f 1AKI.pdb -o 1AKI_processed.gro -water spce
editconf -f 1AKI_processed.gro -o 1AKI_newbox.gro -c -d 1.0 -bt cubic
genbox -cp 1AKI_newbox.gro -cs spc216.gro -o 1AKI_solver.gro -p topol.top
[add -DPOSRES]
grompp -f minim.mdp -c 1AKI_solver.gro -p topol_top -o em.tpr
gmxdump -s em.tpr > gmxdump.mdp
gmxdump -sys -s em.tpr > gmxdump_sys.mdp

now gmxdump.mdp has a healthy Position Rest. section starting like this:

Position Rest.:
  nr: 2002
  iatoms:
  0 type=409 (POSRES) 0
  1 type=410 (POSRES) 4
  2 type=411 (POSRES) 6
  3 type=412 (POSRES) 9
  4 type=413 (POSRES) 12
  5 type=414 (POSRES) 15

and gmxdump_sys.mdp looks like:

Position Rest.:
  nr: 2002
  iatoms:
  0 type=0 (LJ_SR) 0 1
  1 type=4 (LJ_SR) 2 6
  2 type=3 (LJ_SR) 9 4
  3 type=12 (LJ_SR) 5 15
  4 type=6 (LJ_SR) 18 7
  5 type=22 (LJ_SR) 8 23

The first functype=POSRES entry starts with index 409. With -sys the entries start from type 0 and the whole section is messed up.

Associated revisions

Revision ced146e9 - 01/13/2013 10:37 PM - Mark Abraham

Noting that and why gmxdump -s -sys is broken

Not worth fixing. You could pass a boolean from gmxdump into the set_posres_params to avoid executing the problematic line, but that would hit a lot of other code paths that also call gmx_mtop_to_t_topology.

Refs #635
commenting out this line:

```c
/* Set the parameter index for idef->iparams_posre */
il->iatoms[i*2] = i;
```

in mtop_util.c seems to fix gmxdump -sys functionality but I would guess this has some knock-on effects...?

---

#2 - 06/08/2011 04:47 PM - Rossen Apostolov
- Assignee set to Berk Hess
- Target version changed from 4.5.1 to 4.5.5

#3 - 09/21/2011 08:41 PM - Szilárd Páll
- Target version changed from 4.5.5 to 4.5.6

#4 - 01/13/2013 10:33 PM - Mark Abraham
- Category set to analysis tools
- Status changed from New to Feedback wanted
- Target version changed from 4.5.6 to future

I made [https://gerrit.gromacs.org/2035](https://gerrit.gromacs.org/2035) to note that this bug exists and comment where the code is that triggers it. But with the likelihood of massive code changes, and the low impact of the bug, it is not worth fixing.

#5 - 01/09/2014 01:54 PM - Rossen Apostolov
- Status changed from Feedback wanted to Rejected
- Affected version set to 4.5.3

As Mark pointed out, it's not worth fixing, thus closing the report.

#6 - 07/11/2016 08:46 PM - Mark Abraham
- Target version deleted (future)