

GROMACS - Bug #882

trjconv creates infinite trajectory

02/13/2012 04:53 PM - Jan Henning Peters

Status: Closed	
Priority: Normal	
Assignee: David van der Spoel	
Category: analysis tools	
Target version: 4.6	
Affected version - extra info:	Difficulty: uncategorized
Affected version:	
Description	
I observed this problem under the following circumstances:	
<pre>- the input trajectory is concatenated .xtc file from different trajectories, i.e. containing more then one frame with t=0.0 - both options -b and -e have been supplied to trjconv (the problem is not observed if no -b op tion is used) - the -e option specifies a time greater than any timestamp in the trajectory</pre>	
Under these circumstances, trjconv continues writing out data into the output trajectory file, probably until there is no more space left on the drive (in one case I stopped it after reaching 1.4TB). The output seems to consist of continuous repetitions of the input trajectory.	

Associated revisions

Revision effe8e43 - 06/16/2012 02:10 AM - David van der Spoel

Fixes #882 - looping bug in trxio.c

This led to infinite output files in the case of a corrupt input file.

Change-Id: I25d61752d901012e9ce5e6adae1679c2ef99467a

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Revision 81e3359c - 06/20/2012 01:12 AM - Mark Abraham

Merge "Fixes #882 - looping bug in trxio.c" into release-4-5-patches

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History

#1 - 02/13/2012 07:22 PM - David van der Spoel

Can you provide an example (not 1.4Tb) and exact command lines to reproduce this? Which gmx version? I guess this bug will exist in most versions.

#2 - 02/15/2012 11:04 AM - Jan Henning Peters

- File *bugtest.gro* added

- File *bugtest_s10.xtc* added

Using the attached file and the command line

```
trjconv -s bugtest.gro -f bugtest_s10.xtc -b 10000 -e 150000 -o error.xtc
```

,I can reproduce the bug using the following two versions of gromacs:

4.0.7

4.5.5-dev-20110921-e25c350

(I agree that this will probably happen in most versions)

Also, when I tried to further reduce the size of the files (bugtest_s10.xtc is a "-skip 10" version of the full trajectory), the behaviour changed - using the same command on a "-skip 100" trajectory (alternatively on a "-skip 10" version of the attached trajectory), trjconv freezes without creating the output file.

#3 - 04/11/2012 12:39 PM - Rossen Apostolov

- Priority changed from Normal to High

- Target version set to 4.5.6

#4 - 04/16/2012 11:40 AM - Rossen Apostolov

- Priority changed from High to Normal

#5 - 04/26/2012 09:34 PM - David van der Spoel

- Target version changed from 4.5.6 to 4.6

This is a very nasty bug that sits very deep in the trajectory reading routine, in trxio.c:

```
if (bTimeSet(TBEGIN) && (fr->time < rTimeValue(TBEGIN))) {
    if (xtc_seek_time(status->fio, rTimeValue(TBEGIN), fr->natoms)) {
        gmxfatal(FARGS, "Specified frame doesn't exist or file not seekable");
    }
}
```

what this does is seek the begin time (-b 10000) if the present time is less than the begin time. However, when the time in the trajectory suddenly jumps backward, trjconv realizes it is before the -b time, and starts seeking again: from the beginning. Hence the loop.

Unfortunately this code is rather difficult and I would rather not touch it at this point in time. What needs to be done is that xtc_seek_time gets an additional flag telling it to seek forward only, that is not to start from a file offset of zero again. Upping the target version to 4.6, but 5.0 seems more likely.

#6 - 04/26/2012 11:55 PM - Szilárd Páll

Can't we aim for 4.5.6? The consensus anyway seems to be that 4.5.6 and 4.6 should come out at the same time and the 4.5.x should enter into a "critical bugfixes only" state.

#7 - 08/05/2012 12:49 AM - Roland Schulz

- Status changed from New to Closed

Files

bugtest.gro	3.49 KB	02/15/2012	Jan Henning Peters
bugtest_s10.xtc	823 KB	02/15/2012	Jan Henning Peters