Gromacs - Bug #1405

some trjconv -b and -t0 combinations lead to a never-ending stream of output to the new xtc

12/12/2013 05:57 PM - Chris Neale

| Status: | Closed |
| Priority: | Normal |
| Assignee: | Roland Schulz |
| Category: | |
| Target version: | 4.6.5 |
| Affected version: | 3.3.3, 4.0.7, 4.5.5, 4.6.1, 4.6.3, 4.6.5 show this behaviour |

**Description**

I have provided a test system with a .xtc for a box of water that goes from 0 to 10 ps with a save frequency of 0.2 ps.

1. These go on forever, constantly writing frames
   - trjconv -f MD.xtc -o out.xtc -b 6 -t0 2
   - trjconv -f MD.xtc -o out.xtc -b 6 -t0 0

1. But these work fine:
   - trjconv -f MD.xtc -o out.xtc -b 6
   - trjconv -f MD.xtc -o out.xtc -t0 0

1. These also work fine (smaller number for -b, in this case <3)
   - trjconv -f MD.xtc -o out.xtc -b 1 -t0 0
   - trjconv -f MD.xtc -o out.xtc -b 2 -t0 0

**Related issues:**

Related to Gromacs - Bug #1406: trjconv -t0 -b leads to frame skipping

**Associated revisions**

Revision 81d10b25 - 06/20/2014 12:36 PM - Roland Schulz

Fix that seeking was wrong if frame time was modified

The trjconv -t0 option causes fr->time to be modified and this then causes the skipping to be incorrect. Alternative we could document that fr->time shouldn't be modified and change that trjconv makes a copy of fr before changing time. This change has the advantage it is less likely to reintroduce the problem.

Fixes #1405, #1406

Change-Id: lbd692dfeccdf175450fc43f7f35b774bf4446b316

Revision fa0aef8b - 11/26/2014 06:33 PM - Mark Abraham

Fix trjconv modifying fr.time unnecessarily

The was a bug where trjconv modified the input frame time, which caused issues with xtc seeking. This has recently been fixed by commit 81d10b25, but it's better not to mess with the input frame and only modify the output frame.

11/19/2015
Refs #1405, #1406

Change-Id: lb7c8655e916c12f8cc51523a6756cc7988e6e6

History

#1 - 12/13/2013 03:43 AM - Rossen Apostolov
- Related to Bug #1406: trjconv -t0 -b leads to frame skipping added

#2 - 06/14/2014 03:12 AM - Gerrit Code Review Bot
Gerrit received a related patchset ‘1’ for Issue #1405.
Uploader: Roland Schulz (rolandd@rschulz.eu)
Change-Id: lbd692dfecdf17545fc43f7b35b774bf4446b316
Gerrit URL: https://gerrit.gromacs.org/3592

#3 - 06/14/2014 05:57 AM - Roland Schulz
- Status changed from New to Fix uploaded
- Assignee set to Roland Schulz

#4 - 06/18/2014 04:20 PM - Gerrit Code Review Bot
Gerrit received a related patchset ‘1’ for Issue #1405.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: lb7c8655e916c12f8cc51523a6756cc7988e6e6
Gerrit URL: https://gerrit.gromacs.org/3616

#5 - 06/20/2014 02:15 PM - Roland Schulz
- Status changed from Fix uploaded to Resolved
- % Done changed from 0 to 100

Applied in changeset 81d10b25f5a4cf2c84b7975e492e2284e392b17.

#6 - 06/20/2014 04:30 PM - Erik Lindahl
- Status changed from Resolved to Closed

#7 - 06/23/2014 05:52 PM - Gerrit Code Review Bot
Gerrit received a related patchset ‘1’ for Issue #1405.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: lb7c8655e916c12f8cc51523a6756cc7988e6e6
Gerrit URL: https://gerrit.gromacs.org/3666

Files
ongoing.tgz 776 KB 12/12/2013 Chris Neale