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:
Affected version - extra info: 3.3.3,4.0.7,4.5.5,4.6.1, 4.6.3, 4.6.5 show this behaviour
Affected version: 4.6.5

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 -b 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: lbd692dfecdf175450fc43f7f35b774bf4446b316

Revision fa0aef68b - 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.

Refs #1405, #1406
Change-Id: lbf7a8555e916c12f8cc51523a67556cc7988e6e6

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 (roland@rschulz.eu)
Change-Id: Ibd692dfecdf175450f43f7b35b774bf4446b316
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: Ibf7c8655e916c12f8cc51523a67556cc7988e6e6
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 81d10b25f5a4d2c84b7975e492e2284e392b17.

#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: Ibf7c8655e916c12f8cc51523a67556cc7988e6e6
Gerrit URL: https://gerrit.gromacs.org/3666

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