GROMACS - Bug #1832
'gmx trjconv -dump t' gives no output if t < frame timestep
09/28/2015 06:03 PM - Viveca Lindahl

Status: Closed
Priority: Low
Assignee: 
Category: analysis tools
Target version: 
Affected version - extra info:
Affected version: 5.1

Description
With time between xtc frames = 1000 ps

gmx trjconv -s topol.tpr -f traj_comp.xtc -dump 500

gives the t=1000 frame

but

gmx trjconv -s topol.tpr -f traj_comp.xtc -dump 499

gives no output.

Related issues:
Related to GROMACS - Task #2115: trjconv does too many things, and combinatio...
New

Associated revisions
Revision d27e9055 - 01/03/2018 08:37 PM - Erik Lindahl
Fix trjconv for tdump<frame timestep

Set frame timestep before starting the loop by reading first two frames and rewinding, and make sure we always write something to the dump output based on best-guess (if there is at least one input frame present).

Fixes #1832.

Change-Id: Ic1db912c966448e68b307cfc1fd492f4677e7ab4

History
#1 - 09/28/2015 06:19 PM - Viveca Lindahl
Correction: there is actually 'trajout.xtc' output, but it's empty and doing e.g. gmx check on it generates an error:

Assertion failed:
Condition: bOK
Inconsistent results - OK status from read_first_xtc, but 0 atom coords read

#2 - 02/06/2017 04:20 PM - Mark Abraham
- Related to Task #2115: trjconv does too many things, and combinations of them work poorly added

#3 - 01/03/2018 12:12 PM - Gerrit Code Review Bot
Gerrit received a related patchset ‘1’ for Issue #1832.
Uploader: Erik Lindahl (erik.lindahl@gmail.com)
Change-Id: gc86d4448e68b307cfc1fd492f4677e7ab4
Gerrit URL: https://gerrit.gromacs.org/7422

#4 - 01/03/2018 12:13 PM - Erik Lindahl
- Status changed from New to Fix uploaded

#5 - 01/04/2018 11:13 AM - Erik Lindahl
- Status changed from Fix uploaded to Resolved

Applied in changeset d27e905528c781d5fb08528d34a748840d055cd8.

#6 - 01/04/2018 05:30 PM - Erik Lindahl
- Status changed from Resolved to Closed