

GROMACS - Bug #305

trjconv -f traj.xtc -b X -e X -o out.gro yields an output frame when trj.xtc starts at a time greater than X

03/16/2009 02:46 PM - Chris Neale

Status: Closed	
Priority: Normal	
Assignee: Erik Lindahl	
Category: analysis tools	
Target version: 4.0	
Affected version - extra info:	Difficulty: uncategorized
Affected version:	
Description	
Hello,	
When I am trying to obtain a single frame as a .gro from a .xtc, I often use <code>trjconv -f traj.xtc -b X -e X -o out.gro</code> , where X is the time in ps of the frame that I want. If I give a traj.xtc that runs from A to B ps, there are 3 possibilities:	
1) $A < B < X$ -- trjconv correctly errors without finding frame X (Fatal error: Specified frame doesn't exist or file not seekable)	
2) $A < X < B$ -- trjconv correctly outputs my desired frame	
3) $X < A < B$ -- trjconv correctly errors without finding frame X	
Example:	
<pre>trjconv -f md668_success/dpcNx_md668.xtc -s ../md765_success/dpcNx_md765.tpr -b 140000 -e 140000 -o 140ns.gro</pre>	
...	
Will write gro: Coordinate file in Gromos-87 format	
Reading file ../md765_success/dpcNx_md765.tpr, VERSION 4.0.4 (single precision)	
Reading file ../md765_success/dpcNx_md765.tpr, VERSION 4.0.4 (single precision)	
Select group for output	
Opening library file /home/cneale/gromacs/top/aminoacids.dat	
Group 0 (System) has 20873 elements	
Group 1 (DPC) has 805 elements	
Group 2 (SOL) has 20068 elements	
Select a group: 0	
Selected 0: 'System'	
Reading frame 0 time 159800.000	
Precision of md668_success/dpcNx_md668.xtc is 0.001 (nm)	
Using output precision of 0.001 (nm)	
Last frame 0 time 159800.000	
###	
<pre>head -n 1 140ns.gro</pre>	
Generated by trjconv : TEST t= 159800.00000	
Where it would be more intuitive to me if this condition simple generated an error and no .gro output.	
This behaviour occurs in 4.0.4 and 3.3.1.	
Thanks, Chris.	

Associated revisions

Revision bb910d05 - 04/29/2010 11:58 AM - Teemu Murtola

Fix for trjconv -e option (bug #305).

The -e option for setting the last frame to analyze incorrectly included the first frame of the trajectory even if the trajectory began after the given time.

Revision 99261cfa - 04/29/2010 12:05 PM - Teemu Murtola

Fix for trjconv -e option (bug #305).

The -e option for setting the last frame to analyze incorrectly included the first frame of the trajectory even if the trajectory began after the given time.
(ported from commit bb910d05535eaec7a29be80b20d2fc2240363c5b)

History

#1 - 03/16/2009 02:48 PM - Chris Neale

oops, too much cutting and pasting left my previous description inaccurate. Correcting #3, It should have read:

- 1) A<B<X -- trjconv correctly errors without finding frame X
(Fatal error: Specified frame doesn't exist or file not seekable)
- 2) A<X<B -- trjconv correctly outputs my desired frame

- 3) X<A<B -- trjconv incorrectly outputs frame A ***

#2 - 03/17/2009 10:54 AM - Berk Hess

For what you want trjconv -dump is the easier option, which, I think, does not have this bug.

Still this bug should be fixed.

Berk

#3 - 04/29/2010 12:08 PM - Teemu Murtola

Fixed in the release and master branches.