

GROMACS - Bug #135

The continue option to trjcat -settime does not always work

03/13/2007 03:59 AM - Chris Neale

Status: Closed	
Priority: High	
Assignee: David van der Spoel	
Category: analysis tools	
Target version: 3.3.1	
Affected version - extra info:	Difficulty: uncategorized
Affected version:	

Description

trjcat -settime {c option} does not work as expected when appending to a file. However it works correctly when writing a new file and when using -settime {specify #ps} after calculating the number of ps by hand.

I am using gromacs-3.3.1, single precision, installed manually (not with apt-get) on ubuntu linux. Also reproduced on gromacs-3.3 and while using .trr in place of .xtc files

To be more specific:

a.xtc (200ps) and b.xtc (800ps) were both produced using grompp with tinit=0. a.xtc was produced with position restraints and b.xtc was unrestrained.

```
trjcat -f a.xtc b.xtc -o a.xtc -settime
(enter 0,c)
produces a file of 800ps (should have been 1000ps)
```

Summary of files and start times used:

File	Start time	Time step
------	------------	-----------

a.xtc 0.000 ps 1.000 ps

b.xtc Continue from last file

Will append to a.xtc rather than creating a new file

Last frame 200 time 200.000

Reading frame 0 time 0.000

lasttime 200

Reading frame 200 time 200.000

Continue writing frames from b.xtc t=201 ps, frame=0

Last frame 800 time 800.000 -> frame 500 time 701.000 ps

Last frame written was 599, time 800.000000 ps

However, it works correctly when I write to a different file

```
trjcat -f a.xtc b.xtc -o c.xtc -settime
```

(enter 0,c)

correctly produces a file of 1000ps

Summary of files and start times used:

File	Start time	Time step
------	------------	-----------

a.xtc 0.000 ps 1.000 ps

b.xtc Continue from last file

Reading frame 0 time 0.000

lasttime -12345

Continue writing frames from a.xtc t=0 ps, frame=0

Last frame 200 time 200.000 -> frame 200 time 200.000 ps

Reading frame 0 time 0.000

lasttime 200

Reading frame 1 time 1.000

Continue writing frames from b.xtc t=201 ps, frame=201

Last frame 800 time 800.000 -> frame 1000 time 1000.000 ps

Last frame written was 1000, time 1000.000000 ps

The problem can be corrected by using entering 0,200 instead of 0,c to the -settime option of trjcat.

Summary of files and start times used:

File	Start time	Time step
------	------------	-----------

a.xtc 0.000 ps 1.000 ps

b.xtc 200.000 ps 1.000 ps

Will append to a.xtc rather than creating a new file

Last frame 200 time 200.000

Reading frame 0 time 0.000

lasttime 200

Reading frame 1 time 1.000

Continue writing frames from b.xtc t=201 ps, frame=0

Last frame 800 time 800.000 -> frame 700 time 901.000 ps

Last frame written was 799, time 1000.000000 ps

gmxcheck -f a.xtc confirms that the timestamp is good "Last frame 200 time 200.000"

Related issues:

Has duplicate GROMACS - Bug #134: The continue option to trjcat -settime does...

Closed

03/13/2007

History

#1 - 03/13/2007 04:02 AM - Chris Neale

Created an attachment (id=108)

Two xtc files that reproduce the problem that I described in the post

These two xtc files were generated from the xtc files that I actually used by trjconv -e 5 in order to send you smaller files. Prior to sending the files I ensured that they still reproduce the problem.

#2 - 03/13/2007 11:39 AM - David van der Spoel

- Bug 134 has been marked as a duplicate of this bug. ***

#3 - 09/11/2007 08:48 AM - David van der Spoel

You have uploaded two files with traj with 6 frames, from 0-5 ps each. Now when you append them with the -settime option and continue, one would expect to get 12 frames from 0-11 ps right?

#4 - 09/11/2007 09:11 AM - David van der Spoel

Fixed in CVS. GROMACS expects trajectories to overlap in one frame, therefore if you wish to get all frames you would in your example have to enter 0,6 rather than 0,c.

#5 - 05/31/2014 09:54 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#135](#).

Uploader: Roland Schulz (roland@rschulz.eu)

Change-Id: I7c5569693a4b84f481f0f7afd85f0f01c33295cf

Gerrit URL: <https://gerrit.gromacs.org/3532>

Files

trjcatContinue.tar.gz

239 KB

03/13/2007

Chris Neale