GROMACS - Bug #1406

trjconv -t0 -b leads to frame skipping

12/12/2013 06:10 PM - Chris Neale

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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</thead>
<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Roland Schulz</td>
</tr>
<tr>
<td>Category:</td>
<td>core library</td>
</tr>
<tr>
<td>Target version:</td>
<td>4.6.x</td>
</tr>
<tr>
<td>Affected version -</td>
<td>4.6.1, 4.6.3, 4.6.5</td>
</tr>
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<td>extra info:</td>
<td></td>
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<td>Affected version:</td>
<td>4.6.5</td>
</tr>
<tr>
<td>Difficulty:</td>
<td>uncategorized</td>
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Description

I want to extract a section from a .xtc using trjconv -b -e and then reset the time to start at 0.

When I try to do it in a single trjconv step, it does reset the starting time, but it also only print every second step.

For example, I might do this to extract and retime, then check the timing using g_traj:

```
trjconv -f MD.xtc -o out.xtc -b 2 -t0 0
```

echo 0 |g_traj -f out.xtc -s MD.tpr -ob box.xvg

```
rm -f out.xtc
```

The output in box.xvg is:

```
0 2.99635 2.99635 2.99453 0 0 0
0.4 2.99835 2.99835 2.99643 0 0 0
0.8 2.99916 2.99916 2.99691 0 0 0
...```

But if I remove the -t0 flag to trjconv, I get:

```
2 2.99635 2.99635 2.99453 0 0 0
2.2 2.99709 2.99709 2.99581 0 0 0
2.4 2.99835 2.99835 2.99643 0 0 0
```

Note that the workaround is to do the -b and -t0 in two steps.

I suspect that this is related to issue 1405.

I tested 4.6.1-4.6.5, all of which show the issue. When testing 4.5.5, 4.0.7, and 3.3.3, I ran into issue 1405 even with "-b 2" so was unable to be sure how recent this issue is.

Related issues:

Related to GROMACS - Bug #1405: some trjconv -b and -t0 combinations lead to ...

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: lbd692dfeccdf175450fc43f7d35b774bf4446b316

Revision fa0aeff8b - 11/26/2014 06:33 PM - Mark Abraham

Fix trjconv modifying fr.time unnecessarily

03/20/2020
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: ibf7c8655e916c12f8cc51523a67556cc7988ae6e6

History

#1 - 12/13/2013 03:43 AM - Rossen Apostolov
- Related to Bug #1405: some trjconv -b and -t0 combinations lead to a never-ending stream of output to the new xtc added

#2 - 06/14/2014 03:12 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1406.
Uploader: Roland Schulz (roland@rschulz.eu)
Change-Id: lbd692dfeccf175450fc43ff7d5b774bf4446b316
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 #1406.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: lbf7c8655e916c12f8cc51523a67556cc7988ae6e6
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 81d10b25fc5a4cf2c84b7975e492e2284a392b17.

#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 #1406.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: lbf7c8655e916c12f8cc51523a67556cc7988ae6e6
Gerrit URL: https://gerrit.gromacs.org/3666

#8 - 07/15/2014 12:19 PM - Teemu Murtola
- Category set to core library
- Target version set to 4.6.x

Files

skip2.tgz 777 KB 12/12/2013 Chris Neale