**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

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
</tr>
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<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Roland Schulz</td>
</tr>
<tr>
<td>Category:</td>
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<tr>
<td>Target version:</td>
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<tr>
<td>Affected version:</td>
<td>4.6.5</td>
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<td>Affected version - extra info:</td>
<td>3.3.3, 4.0.7, 4.5.5, 4.6.1, 4.6.3, 4.6.5 show this behaviour</td>
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<tr>
<td>Difficulty:</td>
<td>uncategorized</td>
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**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 -t0 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: lbd692defcddf175450fc43lf735b774f4446b316

- **Revision fa0aef8b - 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: lb7cf8b56e916c12ffccc5123a6755667b7988ae6e6

**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: ibd692dfecdf175450f43f7f35b774bf4446b316
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: lb7c8655e916c12f8cc51523a67596cc7988e6e6
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 81d10b25fc5a4d5c2c84db7975e492e2284e392b17.

#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: lb7c8655e916c12f8cc51523a67596cc7988e6e6
Gerrit URL: https://gerrit.gromacs.org/3666

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