# GROMACS - Bug #2619

## Segfault in gmx trjconv

08/21/2018 11:07 AM - Michael Brunsteiner

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td></td>
</tr>
<tr>
<td>Category:</td>
<td>core library</td>
</tr>
<tr>
<td>Target version:</td>
<td>2018.3</td>
</tr>
<tr>
<td>Affected version - extra info:</td>
<td></td>
</tr>
<tr>
<td>Affected version:</td>
<td>2018.2</td>
</tr>
<tr>
<td>Difficulty:</td>
<td>uncategorized</td>
</tr>
</tbody>
</table>

### Description

Hi,

this is gmx 2018.2 on:

```
uname -a
Linux rcpetemp1 4.4.0-131-generic #157-Ubuntu SMP Thu Jul 12 15:51:36 UTC 2018 x86_64 x86_64 x86_64 GNU/Linux
```

compiled with:
cmake .. -DGMX_BUILD_OWN_FFTW=ON -DGMX_GPU=on && make && make install

given a pdb file (as included further below as text) i see:

```
prompt> gmx trjconv -f a3.pdb -o a3.trr
                   
 (-) GROMACS - gmx trjconv, 2018.2 (-):
                   
 GROMACS is written by:

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and the project leaders:
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check out http://www.gromacs.org for more information.

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GROMACS:      gmx trjconv, version 2018.2
Executable:   /home/micb/local/gmx-2018.2-bin/bin/gmx
Data prefix:  /home/micb/local/gmx-2018.2-bin
Working dir:  /home/micb/current/A2-JnJ-ASD/ff/apis/05-fogal1
Command line:
  gmx trjconv -f a3.pdb -o a3.trr

Will write trr: Trajectory in portable xdr format
Reading frame  0 time 0.000  Reading frames from pdb file
Precision of a3.pdb is 0.0001 (nm)
  '', 21 atoms  0 time  0.000
example pdb:

ATOM    1  O  ASP    1    2.789    1.249    0.110    0.00    0.00
ATOM    2  C  ASP    1    2.347    0.118    0.242    0.00    0.00
ATOM    3  C  ASP    1    0.887   -0.207    0.351    0.00    0.00
ATOM    4  O  ASP    1    3.087   -1.073    0.270    0.00    0.00
ATOM    5  C  ASP    1    4.497   -1.073    0.131    0.00    0.00
ATOM    6  C  ASP    1    5.282   -0.057    0.686    0.00    0.00
ATOM    7  C  ASP    1    6.668   -0.079    0.525    0.00    0.00
ATOM    8  C  ASP    1    7.278   -1.123   -0.167    0.00    0.00
ATOM    9  C  ASP    1    6.501   -2.158   -0.690    0.00    0.00
ATOM   10  C  ASP    1    5.106   -2.150   -0.534    0.00    0.00
ATOM  11 C  ASP  1  4.364  -3.301  -1.114  0.00  0.00
ATOM  12 O  ASP  1  4.766  -3.924  -2.081  0.00  0.00
ATOM  13 O  ASP  1  3.253  -3.650  -0.431  0.00  0.00
ATOM  14 H  ASP  1  0.721  -0.959   1.127  0.00  0.00
ATOM  15 H  ASP  1  0.517  -0.562  -0.613  0.00  0.00
ATOM  16 H  ASP  1  0.339   0.696   0.638  0.00  0.00
ATOM  17 H  ASP  1  0.723   0.727   0.934  0.00  0.00
ATOM  18 H  ASP  1  8.357  -1.134  -0.298  0.00  0.00
ATOM  19 H  ASP  1  6.989  -2.975  -1.220  0.00  0.00
ATOM  20 H  ASP  1  3.083  -3.100   0.356  0.00  0.00
ATOM  21 H  ASP  1  3.083  -3.100   0.356  0.00  0.00

Associated revisions

Revision 54f9fa9d - 08/22/2018 06:18 PM - Paul Bauer
Fix trjconv when running without a structure file

When running trjconv without a reference structure file, the topology information would be left uninitialized and cause subsequent crashes during the deallocation.

Added tests to cover this behaviour.

Fixes #2619

Change-Id: i501c560ee08afca00bc78f6f1b6841b5a5b57

History

#1 - 08/21/2018 11:43 AM - Paul Bauer
Hello, please upload the PDB file as an attachment here, because the formatting gets changed in the form.
Thanks!

#2 - 08/21/2018 01:10 PM - Paul Bauer
Confirmed with another PDB I had available. The issue seems to be caused by not providing a topology when converting and the automatic routines getting confused.

#3 - 08/21/2018 02:40 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2619.
Uploader: Paul Bauer (paul.bauer.q@gmail.com)
Change-Id: gromacs~release-2018~I6f780075a8077f2cb0a141a777d9f430de21e4c2
Gerrit URL: https://gerrit.gromacs.org/8209

#4 - 08/21/2018 03:09 PM - Paul Bauer
- Status changed from New to Fix uploaded

#5 - 08/21/2018 06:32 PM - Mark Abraham
- Description updated

#6 - 08/22/2018 11:36 AM - Mark Abraham
- Subject changed from Error in 'gmx': munmap_chunk(): invalid pointer ... core dump to Segfault in gmx trjconv

#7 - 08/22/2018 12:02 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2619.
Uploader: Paul Bauer (paul.bauer.q@gmail.com)
Change-Id: gromacs~release-2018~I501c560ee08afca00bc78f6f1b6841b5a5b57
Gerrit URL: https://gerrit.gromacs.org/8217

#8 - 08/22/2018 06:45 PM - Paul Bauer
- Status changed from Fix uploaded to Resolved

Applied in changeset 54f9fa9d9df9b3ce4b0a922a4acdecf1b1614746c6.

#9 - 08/23/2018 10:46 AM - Paul Bauer
- Status changed from Resolved to Closed