GROMACS - Bug #1711

gmx x2top seg fault

03/27/2015 02:05 PM - Justin Lemkul

<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>Erik Lindahl</td>
</tr>
<tr>
<td>Category</td>
<td>preprocessing (pdb2gmx,grompp)</td>
</tr>
<tr>
<td>Target version</td>
<td>5.0.7</td>
</tr>
<tr>
<td>Affected version</td>
<td>git master</td>
</tr>
<tr>
<td>Difficulty</td>
<td>uncategorized</td>
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Description

As reported on gmx-users:


gdb backtrace indicates line 1054 (in version 5.0.4, line 1050 in current master) is to blame:

```
Program received signal SIGSEGV, Segmentation fault.
0x00007ffff66be7e0 in gen_pad (nnb=0x7fffffffaf40, atoms=0x6523c0, rtp=0x7fffffff7dd2ac0, plist=0x7fffffff97f0, excsls=0x680120, hb=0x0, bAllowMissing=1) at /home/jalemkul/code/gromacs/gromacs-5.0.4/src/gromacs/gmxpreprocess/gen_ad.c:1054
1054 for (j = 0; j < hbang->nb; j++)
(gdb) bt
#0 0x00007ffff66be7e0 in gen_pad (nnb=0x7fffffffaf40, atoms=0x6523c0, rtp=0x7fffffff7dd2ac0, plist=0x7fffffff97f0, excsls=0x680120, hb=0x0, bAllowMissing=1) at /home/jalemkul/code/gromacs/gromacs-5.0.4/src/gromacs/gmxpreprocess/gen_ad.c:1054
1054 for (j = 0; j < hbang->nb; j++)
(gdb) bt
#0 0x00007ffff66ac889 in gmx_x2top (argc=1, argv=0x7fffffffe240)
   at /home/jalemkul/code/gromacs/gromacs-5.0.4/src/gromacs/gmxpreprocess/x2top.c:589
#1 0x00007ffff66ac889 in gmx_x2top (argc=1, argv=0x7fffffffe240)
   at /home/jalemkul/code/gromacs/gromacs-5.0.4/src/gromacs/gmxpreprocess/x2top.c:589
#2 0x00007ffff671515d in gmx::(anonymous namespace)::CommandLineModule::run (this=0x644610, argc=7, argv=0x7fffffff7ee240)
   at /home/jalemkul/code/gromacs/gromacs-5.0.4/src/gromacs/gmxpreprocess/gen_ad.c:1054
#3 0x00007ffff6717487 in gmx::CommandLineModuleManager::run (this=0x7fffffff7ee120, argc=7, argv=0x7fffffff7ee240)
   at /home/jalemkul/code/gromacs/gromacs-5.0.4/src/gromacs/commandline/cmdlinemodulemanager.cpp:545
#4 0x00008000000040ed9a in main (argc=8, argv=0x7fffffff238) at /home/jalemkul/code/gromacs/gromacs-5.0.4/src/programs/gmx.cpp:58
```

The bug appears to have been introduced in commit 7ba0a841df25e54d36586e31003f9f93bd2588d

Related issues:

Related to GROMACS - Bug #1276: pdb2gmx ignores angles when no bonds are present

Revision fadb3ecb - 06/24/2015 11:09 PM - Erik Lindahl

Avoid accessing hackblocks for x2top

Previous fixes for generating dihedrals would cause us to access the hackblock even when using x2top, which we should not do.

Fixes #1711.

Change-Id: Id0ea6d524d80b87fe257c9f4f1c48cbe828654

History
#1 - 06/17/2015 11:52 AM - Rossen Apostolov
- Related to Bug #1276: pdb2gmx ignores angles when no bonds are present added

#2 - 06/18/2015 06:54 PM - Erik Lindahl
- Status changed from New to Accepted
- Assignee set to Erik Lindahl

#3 - 06/23/2015 10:44 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1711.
Uploader: Erik Lindahl (erik.lindahl@gmail.com)
Change-Id: l0ea6d524d80b87fe257c9fd4f1c48c4be828654
Gerrit URL: https://gerrit.gromacs.org/4773

#4 - 06/23/2015 10:45 PM - Erik Lindahl
- Status changed from Accepted to Fix uploaded

#5 - 06/29/2015 03:22 PM - Erik Lindahl
- Status changed from Fix uploaded to Resolved

#6 - 06/29/2015 03:22 PM - Erik Lindahl
- Status changed from Resolved to Closed

#7 - 07/11/2016 07:41 PM - Mark Abraham
- Target version changed from 5.x to 5.0.7