

GROMACS - Bug #1618

g_protonate segfaults unconditionally

10/06/2014 05:19 PM - Björn Forsberg

Status: In Progress	
Priority: Normal	
Assignee: Erik Lindahl	
Category: preprocessing (pdb2gmx,grompp)	
Target version:	
Affected version - extra info:	Difficulty: uncategorized
Affected version: 5.0.2	

Description

g_protonate segfaults on version 4.6.8 (shown below), but also on 5.0.2. I am unable to attempt it on 5.1 at the moment. Appears to be related to calling protonate(), located in src/kernel/genhydro.c

```
g_protonate -s ref_test.pdb -f test.xtc
```

...

Select group to process:

```
Group 0 ( System) has 398 elements
Group 1 ( Protein) has 398 elements
Group 2 ( Protein-H) has 398 elements
Group 3 ( C-alpha) has 50 elements
Group 4 ( Backbone) has 150 elements
Group 5 ( MainChain) has 200 elements
Group 6 ( MainChain+Cb) has 249 elements
Group 7 ( MainChain+H) has 200 elements
Group 8 ( SideChain) has 198 elements
Group 9 ( SideChain-H) has 198 elements
```

Select a group: 0

Selected 0: 'System'

```
Reading frame 0 time 1.000 Opening force field file /nethome/bjornf/gromacs/./gromacs/share/top/gmx2.ff/aminoacids.hdb
```

```
Opening force field file /nethome/bjornf/gromacs/./gromacs/share/top/gmx2.ff/atomtypes.atp
```

```
Atomtype 1
```

```
Opening force field file /nethome/bjornf/gromacs/./gromacs/share/top/gmx2.ff/aminoacids.n.tdb
```

```
Opening force field file /nethome/bjornf/gromacs/./gromacs/share/top/gmx2.ff/aminoacids.c.tdb
```

```
[1] 30440 segmentation fault (core dumped) ./gromacs/build/src/kernel/g_protonate -s ref_test.pdb -f test.xtc
```

Associated revisions

Revision 0d9d2c84 - 06/29/2015 09:46 AM - Erik Lindahl

Removed gmx protonate tool

This tool appears to have been largely unused, since testing shows it crashes for a normal trajectory all the way back to 4.6. Since it is only relevant for united-atom force fields, we'll reduce the maintenance load by simply removing it for now - it might reappear in the future.

Refs #1618.

Change-Id: If57e250f0ffbe32bcc948d09b54b225db9724c35

Revision 85ea4302 - 08/17/2015 02:11 PM - Mark Abraham

Remove infrastructure for gmx protonate

The front end was removed earlier.

Refs #1618

Change-Id: I0e58d3cb5451a4aabebedf3bc5920c088c1a3923f

History

#1 - 06/20/2015 12:11 PM - Erik Lindahl

- Assignee set to Erik Lindahl

#2 - 06/20/2015 12:11 PM - Erik Lindahl

- Status changed from New to In Progress

#3 - 06/20/2015 06:32 PM - Peter Kasson

You're too fast! :) Was testing this one before I hopped on the flight last night, but I don't have a patch yet. Just got to the reproduce + trace stage. I'll go hunt some other bugs.

#4 - 06/24/2015 10:48 PM - Berk Hess

Could this be related to the hackblock fix that Erik fixed recently (forgot the id's)? Unfortunately there is no stack trace here.

#5 - 06/24/2015 10:55 PM - Erik Lindahl

Unfortunately not, I already tested those fixes here!

Will paste debug session below.

#6 - 06/24/2015 10:56 PM - Erik Lindahl

```
Process 72223 stopped
* thread #1: tid = 0x1a5059, 0x00000001000bfc42 libgromacs.0.0.0.dylib`calc_all_pos(pdba=0x00000001024047b0, x=0x000000010301fa00, nab=0x0000000103011800, ab=0x0000000103007c00, bCheckMissing=0) + 210 at genhydro.c:389, queue = 'com.apple.main-thread', stop reason = EXC_BAD_ACCESS (code=1, address=0x8)
  frame #0: 0x00000001000bfc42 libgromacs.0.0.0.dylib`calc_all_pos(pdba=0x00000001024047b0, x=0x000000010301fa00, nab=0x0000000103011800, ab=0x0000000103007c00, bCheckMissing=0) + 210 at genhydro.c:389
   386             for (j = 0; j < nab[i]; j += ab[i][j].nr)
   387             {
   388                 /* check if we're adding: */
-> 389                 if (ab[i][j].oname == NULL && ab[i][j].tp > 0)
   390                 {
   391                     bFoundAll = TRUE;
   392                     for (m = 0; (m < ab[i][j].nctl && bFoundAll); m++)
(lldb) bt
* thread #1: tid = 0x1a5059, 0x00000001000bfc42 libgromacs.0.0.0.dylib`calc_all_pos(pdba=0x00000001024047b0, x=0x000000010301fa00, nab=0x0000000103011800, ab=0x0000000103007c00, bCheckMissing=0) + 210 at genhydro.c:389, queue = 'com.apple.main-thread', stop reason = EXC_BAD_ACCESS (code=1, address=0x8)
  * frame #0: 0x00000001000bfc42 libgromacs.0.0.0.dylib`calc_all_pos(pdba=0x00000001024047b0, x=0x000000010301fa00, nab=0x0000000103011800, ab=0x0000000103007c00, bCheckMissing=0) + 210 at genhydro.c:389
    frame #1: 0x00000001000be328 libgromacs.0.0.0.dylib`add_h_low(pdbaptr=0x00007fff5fbfd8b0, xptr=0x00007fff5fbfda30, nah=39, ah=0x000000010282a800, nterpairs=1, ntdb=0x0000000102402170, ctdb=0x0000000102402ea0, rN=0x00000000000102402eb0, rC=0x0000000102402ec0, bCheckMissing=0, nabptr=0x00007fff5fbfe708, abptr=0x00007fff5fbfe710, bUpdate_pdba=0, bKeep_old_pdba=1) + 840 at genhydro.c:537
    frame #2: 0x00000001000bdee5 libgromacs.0.0.0.dylib`add_h(pdbaptr=0x00007fff5fbfd8b0, xptr=0x00007fff5fbfda30, nah=39, ah=0x000000010282a800, nterpairs=1, ntdb=0x0000000102402170, ctdb=0x0000000102402ea0, rN=0x00000000000102402eb0, rC=0x0000000102402ec0, bAllowMissing=1, nabptr=0x00007fff5fbfe708, abptr=0x00007fff5fbfe710, bUpdate_pdba=1, bKeep_old_pdba=1) + 261 at genhydro.c:778
    frame #3: 0x00000001000bf6e7 libgromacs.0.0.0.dylib`protonate(atomsptr=0x00007fff5fbfdbf8, xptr=0x00007fff5fbfda30, protdata=0x00007fff5fbfe6f8) + 1191 at genhydro.c:891
    frame #4: 0x00000001000dc93b libgromacs.0.0.0.dylib`gmx_protonate(argc=1, argv=0x00007fff5fbffaf8) + 2507 at protonate.c:200
    frame #5: 0x0000000100149f74 libgromacs.0.0.0.dylib`gmx::(anonymous namespace)::CMainCommandLineModule::run(this=0x0000000102205c50, argc=5, argv=0x00007fff5fbffaf8) + 36 at cmdlinemodulemanager.cpp:119
    frame #6: 0x00000001001492ed libgromacs.0.0.0.dylib`gmx::CommandLineModuleManager::run(this=0x00007fff5fbff9e0, argc=5, argv=0x00007fff5fbffaf8) + 813 at cmdlinemodulemanager.cpp:545
    frame #7: 0x00000001000024f1 gmx`main(argc=6, argv=0x00007fff5fbffaf0) + 433 at gmx.cpp:58
    frame #8: 0x00007fff959f15c9 libdyld.dylib`start + 1
```

#7 - 06/28/2015 02:49 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#1618](#).
Uploader: Erik Lindahl (erik.lindahl@gmail.com)
Change-Id: If57e250f0ffbe32bcc948d09b54b225db9724c35
Gerrit URL: <https://gerrit.gromacs.org/4800>

#8 - 06/28/2015 02:50 PM - Erik Lindahl

While we might be able to fix gmx protonate, this tools appears to have been pretty much unused since the crashes go all the way back to 4.6. Since

nobody has complained, I think it's better that we remove it and focus on a few high-quality tools. It was anyway mostly intended for united atom force fields when written a long time ago, and those are mostly deprecated today.

#9 - 08/17/2015 02:10 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#1618](#).

Uploader: Mark Abraham (mark.j.abraham@gmail.com)

Change-Id: I0e58d3cb5451a4aabebedf3bc5920c088c1a3923f

Gerrit URL: <https://gerrit.gromacs.org/5011>

Files

ref_test.pdb	30.8 KB	10/06/2014	Björn Forsberg
test.xtc	103 KB	10/06/2014	Björn Forsberg