### 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: | |
| 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**

```bash
$ 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 0d9d2c64** - 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: I0e58d3cb5451a4aabebdf3bc5920c088c1a3923f
You're too fast! :) I 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.

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

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.i.abraham@gmail.com)
Change-id: i0e58d3cb5451a4aabe6df3bc5920c088c1a3923f
Gerrit URL: https://gerrit.gromacs.org/5011

Files

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