**Gromacs - Bug #1553**

**g_hbond segfaults with smooth option**

07/03/2014 07:23 PM - Michael Brunsteiner

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<tr>
<td>Assignee:</td>
<td>David van der Spoel</td>
</tr>
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<td>analysis tools</td>
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**Affected version - extra info:**

**Description**

Hi,

i found that using `g_hbond` as in:

```
g_hbond -f traj.xtc -s topol.tpr -n index.ndx -ac -smooth 1
```

gives me a seg-fault (see for example the stdout below)
i did not include/upload any input files because the files i used tend
to be huge. However this should be reproducible anyway as it seems to be a general issue:
I get the same error for a number of widely different systems, e.g., a polymer blend or
a protein in aqueous solution ...

this happens both with single and double precision (both for the
g_hbond and the trajectory versions) and also for both
g_hbond from gmx-4.6.5 and gmx-5.0-beta2 (the latter with single prec
i seem to recall ... gmx -h wouldn't tell me ...)

if i do not use the smooth option but leave everything else
the same then the segfault goes away ...

cheers,
michael

below a typical stdout of `g_hbond -f traj.xtc -s topol.tpr -n index.ndx -ac -smooth 1`

```
[...]
Select a group: 1
Selected 1: 'Protein'
Select a group: 20
Selected 20: 'Water'
Checking for overlap in atoms between Protein and Water
Calculating hydrogen bonds between Protein (4899 atoms) and Water (23835 atoms)
Found 8389 donors and 8833 acceptors
Making hbmap structure...done.
Reading frame 0 time 0.000
Will do grid-seach on 15x15x15 grid, rcut=0.35
Frame loop parallelized with OpenMP using 8 threads.
Last frame 5000 time 2000.000
Found 88942 different hydrogen bonds in trajectory
Found 181742 different atom-pairs within hydrogen bonding distance
Merging hbonds with Acceptor and Donor swapped
8389/8389
- Reduced number of hbonds from 88942 to 83886
- Reduced number of distances from 181742 to 181742
Back Off! I just backed up hbnun.xvg to ./#hbnun.xvg.1#
Average number of hbonds per timeframe 578.545 out of 3.705e+07 possible
```
Doing autocorrelation according to the theory of Luzar and Chandler.

Normalization for $c(t) = 0.00172792$ for $gh(t) = 3.45631e-07$

WARNING: Correlation function is probably not long enough
because the standard deviation in the tail of $C(t) > 0.001$
Tail value (average $C(t)$ over second half of acf): $0.0786273 +/- 0.00446663$
Segmentation fault (core dumped)

Associated revisions
Revision 3ccedc2d - 06/23/2015 02:24 PM - Erik Lindahl
Removed buggy -smooth hack in hbond module

As discussed in redmine #1553, this was a hack added a while ago, but apparently it leads to segfaults. We should avoid hacks in the first place, and since nobody has been interested in fixing it for the last year it's time to kill it.

Fixes #1553.

Change-Id: I94faa3c543bcca4c729753c8b56cdaf5a5775d0ff

History
#1 - 07/03/2014 10:17 PM - Mark Abraham
- Description updated

#2 - 07/11/2014 11:11 AM - Erik Lindahl
- Assignee set to David van der Spoel

#3 - 07/28/2014 02:41 PM - David van der Spoel
Michael, have you tried to run this without the smooth option? This is some kind of hack that I implemented at one point in time, but which is unnecessary once correlation functions are computed properly (which we are working on https://gerrit.gromacs.org/#/c/3471/). So rather than "fixing" an old hack I would suggest you run without the smooth option for now and try the new version of code once it is finished.

#4 - 07/28/2014 02:57 PM - Michael Brunsteiner
ok, thanks for the feed back, i'll wait ...

BTW ... when i use g_hbond to analyze h-bond dynamics i keep getting a warning "Correlation function is probably not long enough"
i guess this is not surprising as i look at H-bond dynamics in a polymer blend which is very SLOW ... however, i do observe quite a number of switches (bonded<>non-bonded), on average dozens to hundreds per H-bond ... and if i understood that correctly the algorithm you discuss in the paper that is cited by g_hbond (see below) was originally designed to deal with RARE events ... do have any idea how rare an event can be for this to still converge?
The warning message comes from a rather crude analysis where the second half of the ACF (presumed to be the tail) is averaged and it is assumed it should go to zero. If it does not the warning is printed. However, due to the way in which the ACF is computed, the convergence is not as good as it should be, this is why I started to rewrite the code.

ok, thanks ... i'll keep an eye on https://gerrit.gromacs.org/#/c/3471/ ...
cheers,
michael

- Target version changed from 5.0 to 5.x

Gerrit received a related patchset ‘1’ for Issue #1553.
Uploader: Erik Lindahl (erik.lindahl@gmail.com)
Change-Id: I94faa3c543bcca4c729753d8b5cdaf5a5775d0ff
Gerrit URL: https://gerrit.gromacs.org/4757

Status changed from New to Fix uploaded

Status changed from Fix uploaded to Resolved

Status changed from Resolved to Closed