Gromacs - Bug #1662

**g_hbond not running**

12/17/2014 06:32 PM - Antoni Borysik

<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 Marklund</td>
</tr>
<tr>
<td>Category:</td>
<td>analysis tools</td>
</tr>
<tr>
<td>Target version:</td>
<td>5.0.5</td>
</tr>
<tr>
<td>Affected version:</td>
<td>GROMACS 4.6.7</td>
</tr>
</tbody>
</table>

**Affected version:** 5.x

**Description**

Hi, have run various vacuum simulations with GROMACS 4.6.7. I find I can calculate h-bonds using `g_hbond -f md.trr -s md.tpr` on some simulations just fine while on others the system freezes ‘Frame loop parallelized with OpenMP using 32 threads’ even after leaving > 12 hours there is no progress or error. I have not found this problem on the web nor been able to sort out myself. I have tried various `-nthreads` flags including 1 and it won't budge. I get no error report it just freezes -> any insight would be most appreciated.

**Associated revisions**

Revision aa1cfd57 - 02/14/2015 10:52 AM - Erik Marklund

`gmx hbond` no longer removes PBC when none is present

Fixes #1662

Change-Id: Ice934285784ac8b8fd95942a089fb1b65b9ecb51

**History**

#1 - 01/06/2015 11:00 AM - Erik Marklund

- Assignee changed from Antoni Borysik to Erik Marklund

#2 - 01/06/2015 11:05 AM - Erik Marklund

I think this is related to the absence of pbc and I can reproduce this with other gas-phase trajectories. (Why doesn't `g_hbond` have the `-nopbc` option btw?) Will dig deeper.

#3 - 01/06/2015 04:02 PM - Erik Marklund

- Target version changed from 4.6.8 to 5.0.5
- Affected version changed from 4.6.7 to 5.x

The bug is there in release-5-0. I'll fix it and try to backport to release-4-6.

#4 - 01/06/2015 11:51 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #1662
Uploader: Erik Marklund (e.g.marklund@gmail.com)
Change-Id: lce934285784ac8b8fd95942a089fb1b65b9ecb51
Gerrit URL: https://gerrit.gromacs.org/4350

#5 - 01/08/2015 10:30 AM - Mark Abraham
Subject changed from h_hbond not running to g_hbond not running

#6 - 04/09/2015 10:51 AM - Mark Abraham
- Status changed from New to Closed