GROMACS - Bug #1662

g_hbond not running

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

Status: Closed
Priority: Normal
Assignee: Erik Marklund
Category: analysis tools
Target version: 5.0.5
Affected version - extra info:
Affected version: 5.x

Difficulty: uncategorized

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 wont 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: Ice934285784ac8b8fd95942a089fb1b65b9ecb51
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