GROMACS - Bug #1387

Wrong return value in topsort.c

11/22/2013 11:57 AM - Manuel Luitz

Status: Closed
Priority: Normal
Assignee: Berk Hess
Category: mdrun
Target version: 4.6.5
Affected version - extra info:
Affected version: 4.6

Difficulty: uncategorized

Description

Function gmx_bool gmx_mtop_bondeds_free_energy(const gmx_mtop_t *mtop) in src/gmxlib/topsort.c returns always true. I think the correct return statement should be

return (bPert ? ilsortUNKNOWN : ilsortNO_FE);

instead. Please comment.

Associated revisions

Revision 99f228b0 - 11/26/2013 11:22 PM - Berk Hess
Fixed return value of gmx_mtop_bondeds_free_energy

The return value was always true, which was harmless, since it could only cause a small performance hit of useless sorting.

Fixes #1387

Change-Id: i088a37473747b03517fbb5e416e791bd542bd49fed2

History

#1 - 11/22/2013 12:00 PM - Manuel Luitz
Typo,
return bPert;
should be the correct return statement

#2 - 11/23/2013 01:43 AM - Mark Abraham
- Category set to mdrun
- Status changed from New to Accepted
- Assignee set to Berk Hess
- Target version changed from 4.6.x to 4.6.5

Yes, that looks like a bug introduced in ec5d23831a6217a92ac4a3dc36d75e93be5236a9 in http://redmine.gromacs.org/projects/gromacs/repository/revisions/ec5d23831a6217a92ac4a3dc36d75e93be5236a9/diff/src/gmxlib/topsort.c

#3 - 11/25/2013 05:56 PM - Berk Hess
- Status changed from Accepted to Fix uploaded
- Priority changed from High to Normal

I uploaded the fix to gerrit.
But this was a harmless issue, since it only caused systems with free-energy on, but no perturbed bondeds to sort the bondeds, without any effect on the order, only a little effect on performance.
#4 - 11/28/2013 06:45 PM - Berk Hess
- Status changed from Fix uploaded to Resolved
- % Done changed from 0 to 100

Applied in changeset 99f228b04707e025a0fd60518c575c1e974ed162.

#5 - 11/28/2013 07:52 PM - Mark Abraham
- Status changed from Resolved to Closed