GROMACS - Bug #84

g_order tool does not produce deut. order parameters

05/31/2006 06:50 AM - Arneh Babakhani

Status:	Closed			
Priority:	High			
Assignee:	David van der Spoel			
Category:	analysis tools			
Target version:	3.3.1			
Affected version - extra info:		**Difficulty:**	uncategorized	
Affected version:				

Description

This problem was first noted by Sukit Leekumjorn <leekumjo@vt.edu> , as described in his/her posting to the GMX user-list:

"I have encounter some problem with g_order in Gromacs3.3.1. I noticed that tetrahedral order parameter has been added to the new version and for some reason, the program seems to call for calc_tetra_order_parm loop rather than calculate regular tail order parameter. For Gromacs3.3, the order parameter calculates normally. Below is the run from g_order in 3.3.1. It stops at "Select a group" and nothing proceed afterward when it should have picked the listed atoms (group 0 to 17) and started the calculation. I did put group 0 and the program started to calculate and it gave sg-ang.xvg and sk-dist.xvg as the outputs. " (it does not give an output for the deuterium order parameters)

Prof. Van Der Spoel then suggested to remedy the problem by replacing (at lines 579 and 580, of gmx_order.c) the calls to opt2fn by opt2fn_null.

But even after doing this, recompiling and reinstalling GROMACS, the problem persists (no change).

Thanks,

Arneh Babakhani

History

#1 - 06/03/2006 11:56 AM - David van der Spoel

Created an attachment (id=42)
patch to gmx_order.c

his fix by Paul van Maaren might do the trick

#2 - 06/04/2006 11:10 AM - Paul van

Created an attachment (id=43)
gmx_order.c patch against gromacs-3.3.1

The previous patch was against CVS release-3-3-patches, this one is against gromacs-3.3.1.tgz from www.gromacs.org

#3 - 06/05/2006 09:06 AM - Arneh Babakhani

Yep, this patch seems to do the trick, thanks!

(In reply to comment #2)

> Created an attachment (id=43) [edit]
> gmx_order.c patch against gromacs-3.3.1
>
> The previous patch was against CVS release-3-3-patches, this one is against
> gromacs-3.3.1.tgz from www.gromacs.org

Files

gmx_order.patch	1.62 KB	06/03/2006	David van der Spoel
gmx_order.patch-3.1.1	1.81 KB	06/04/2006	Paul van