GROMACS - Bug #264

g_order not producing order parameters

12/01/2008 07:12 PM - Alan Dodd

Status:	Closed		
Priority:	Normal		
Assignee:	David van der Spoel		
Category:	analysis tools		
Target version:	4.0		
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:			

Description

Created an attachment (id=328)
TAR of input files and script used.

All pre-3.3 files I have can be processed quite happily with a version of g_order from 3.2.1, but I can't seem to get 4.0 (or 3.3.1) to produce the basic order.xvg. I've tried specifying all carbons to be calculated in a single group - order.xvg never gets produced. Specifying each equivalent atom in a different group, as worked for 3.2.1, doesn't work either - it only asks for one group, and even if you specify one group to just give it one type of carbon, that still doesn't produce order.xvg, just sg-ang and sk-dist.

History

#1 - 12/11/2008 03:36 PM - David van der Spoel

I have reproduced the bug. Looking into it.

#2 - 12/18/2008 02:30 PM - David van der Spoel

This has now been fixed in CVS by making the output files for the -Sg and -Sk option optional (ffOPTWR instead of ffWRITE).

Files

bugzilla_order.tar	8.31 MB	12/01/2008	Alan Dodd