

GROMACS - Bug #1002

g_dist lists ndx input as optional but fails if no index file provided

09/11/2012 08:03 PM - Peter Kasson

Status: Closed	
Priority: Normal	
Assignee:	
Category:	
Target version: 4.6	
Affected version - extra info: 4.6, 4.5.x	Difficulty: uncategorized
Affected version:	
Description	
We should either make the index file required or (better yet) offer the default index groups.	
<pre>Option Filename Type Description ----- -f run_start2.gro Input Trajectory: xtc trr trj gro g96 pdb cpt -s run.tpr Input Run input file: tpr tpb tpa -n index.ndx Input, Opt. Index file -o dist.svg Output, Opt. xvgr/xmgr file -lt lifetime.svg Output, Opt. xvgr/xmgr file Option Type Value Description ----- -h bool no Print help info and quit [no]version bool no Print version info and quit -nice int 19 Set the nicelevel -b time 0 First frame (ps) to read from trajectory -e time 0 Last frame (ps) to read from trajectory -dt time 0 Only use frame when t MOD dt = first time (ps) -xvg enum xmgrace xvg plot formatting: xmgrace, xmgr or none [no]intra bool yes Calculate distances without considering periodic boundaries, e.g. intramolecular. -dist real 0 Print all atoms in group 2 closer than dist to the center of mass of group 1 Reading file run.tpr, VERSION 4.0.99_development_20090520 (single precision) ----- Program g_dist, VERSION 4.6-dev-20120910-68140ec Source code file: /Users/kasson/Desktop/Software/gromacs-4.6/src/gmplib/futil.c, line: 531 File input/output error: index.ndx For more information and tips for troubleshooting, please check the GROMACS website at http://www.gromacs.org/Documentation/Errors -----</pre>	

Associated revisions

Revision d5856471 - 10/18/2012 11:27 AM - Alexey Shvetsov

[tools] Allow g_dist to use default index group

This should fix #1002

Change-Id: I93db5821bd2eb333f89c21d84f8f52eabc2a7dc3

Signed-off-by: Alexey Shvetsov <alexxy@omrb.pnpi.spb.ru>

History

#1 - 10/19/2012 04:33 AM - Roland Schulz

- Status changed from *New* to *In Progress*

#2 - 12/29/2012 12:16 AM - Erik Lindahl

- Status changed from *In Progress* to *Closed*

Fixed in revision d5856471.