

GROMACS - Bug #406

g_morph broken in Gromacs 4

04/22/2010 04:26 PM - jim pfaendtner

Status: Closed	
Priority: Normal	
Assignee: Erik Lindahl	
Category: mdrun	
Target version: 4.0	
Affected version - extra info:	Difficulty: uncategorized
Affected version:	
Description	
Created an attachment (id=447) associated files for demonstrating g_morph bug	
Hello,	
I am not able to use g_morph in gromacs 4.0.4 or 4.0.7. This bug has been verified on two separate mac laptops and also a Cray XT5. The version on the cray was compiled by me and also the cray admins.	
I am attaching the files I am using (they worked for g_morph in gromacs 3). This is my error message:	
ftp2fn: No filetype .???	

Program g_morph, VERSION 4.0.7 Source code file: trxio.c, line: 243	
Fatal error: Sorry, write_trxframe_indexed can not write tpa	

I have attached a collection of files with README in the attached tgz. It contains the commands I used to run the g_morph attempt as well as the error message (which is repeated universally everywhere I try).	

History

#1 - 06/02/2010 07:47 PM - David van der Spoel

Fixed typo in gmx_morph.c: efTRO -> efTRX which lead to bug 406

Files

bug.tgz	92.3 KB	04/22/2010	jim pfaendtner
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