

GROMACS - Bug #345

gmxcpp incorrect path behavior

09/18/2009 12:24 PM - Berk Hess

Status: Closed	
Priority: Normal	
Assignee: David van der Spoel	
Category: mdrun	
Target version: 4.0	
Affected version - extra info:	Difficulty: uncategorized
Affected version:	
Description	
<p>The Gromacs cpp code does not change the search path when parsing an included file that is not in the current directory. The current directory should be changed to the one where the file currently parsed resides.</p> <p>The attached file gives an example of this problem. But I guess that currently we also have the incorrect behavior that gmxcpp will search also in the work directory for files included from files in, for instance, the share/top directory.</p> <p>Berk</p>	

History

#1 - 09/18/2009 12:25 PM - Berk Hess

Created an attachment (id=387)
example system

Added example.

#2 - 09/18/2009 06:01 PM - David van der Spoel

I think I've fixed it in the git master. I hope the chdir is portable enough. Please test. The example did not contain a conf.gro though. The debug output (grompp -debug 1) shows the chdir commands (search for GMXCPP).

#3 - 09/21/2009 09:16 AM - Berk Hess

My test case now work and it also, correctly, gives an error when I include a file present only in the original dir from an itp file in the subdir.

We will need this to reorganize the force field files such that each force field has its own subdir.

Berk

#4 - 09/21/2009 09:19 AM - Berk Hess

Ah, forgot to say that you should also commit this fix in the 4.0 release branch.

(If you are lucky you can use git cherry-pick)

Berk

Files

cpp_subdir.tar	20 KB	09/18/2009	Berk Hess
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