GROMACS - Bug #1712

bug(?) with -multidir and single directory

04/01/2015 04:49 PM - Viveca Lindahl

Status: Closed
Priority: Normal
Assignee: Erik Lindahl

Description

'mdrun -multidir my_directory' behaves the same as simply 'mdrun', i.e. starts to look for a tpr in the current directory. A better behavior in my opinion would be to either 1) start running in "my_directory" or 2) give an error.

Associated revisions

Revision 4107b6ba - 06/20/2015 07:30 PM - Erik Lindahl

Handle multidir/multisim with single argument correctly

Mdrun would only initialize the multi option correctly with more than one argument, which caused mdrun to fail in strange ways since it looked for topol.tpr in the current directory instead.

Fixes #1712.

Change-Id: Ib89860fdff5f8523eee6c2f5a068390b8d4e3c8d

History

#1 - 06/18/2015 06:53 PM - Erik Lindahl
- Status changed from New to Accepted

#2 - 06/18/2015 06:53 PM - Erik Lindahl
- Assignee set to Erik Lindahl

#3 - 06/18/2015 07:28 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1712.
Uploader: Erik Lindahl (erik.lindahl@gmail.com)
Change-Id: lb89860fdff5f8523eee6c2f5a068390b8d4e3c8d
Gerrit URL: https://gerrit.gromacs.org/4741

#4 - 06/18/2015 07:29 PM - Erik Lindahl
- Status changed from Accepted to Fix uploaded

#5 - 06/22/2015 12:33 PM - Rossen Apostolov
- Status changed from Fix uploaded to Closed