

GROMACS - Bug #1650

Adding "-nsteps" option to gmx tune_pme command line breaks tuning

12/03/2014 11:33 AM - Carsten Kutzner

Status:	Closed	
Priority:	Normal	
Assignee:	Carsten Kutzner	
Category:	analysis tools	
Target version:	5.0.3	
Affected version - extra info:		Difficulty: uncategorized
Affected version:	5.0.2	

Description

All command line arguments that tune_pme does not understand are passed on to the mdrun command line. The latter is used for a quick sanity check whether runs can be executed at all. To make that check quick the option "-nsteps 1" is added to the command line, leading to a double nsteps argument.

Associated revisions

Revision 7025864f - 12/09/2014 01:20 PM - Carsten Kutzner

Make tune_pme understand the "-nsteps" option. Fixes #1650

All command line arguments that tune_pme does not understand are passed over to mdrun. For a quick sanity check the mdrun options are used together with the additional option "-nsteps 1", which then appears twice on the command line.

The solution is to let tune_pme understand the "-nsteps" argument, so that it only occurs on the mdrun command line at launch time. The option for that was already there but before called "-simsteps".

Change-Id: I8362ced75e67b0e28b4a5e1bd427ae6ae4e0e758

History

#1 - 12/03/2014 11:41 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#1650](#).

Uploader: Carsten Kutzner (ckutzne@gwdg.de)

Change-Id: I8362ced75e67b0e28b4a5e1bd427ae6ae4e0e758

Gerrit URL: <https://gerrit.gromacs.org/4263>

#2 - 12/09/2014 04:18 PM - Mark Abraham

- Status changed from New to Closed