

GROMACS - Feature #1204

multi simulations should report that they are multi simulations

03/19/2013 06:50 PM - Mark Abraham

Status:	Closed
Priority:	Normal
Assignee:	Erik Lindahl
Category:	mdrun
Target version:	5.0
Difficulty:	uncategorized
Description	
The .log files for an 8-simulation system on a 32-core machine running 4 OpenMP threads per MPI process report	
Using 1 MPI process Using 4 OpenMP threads	
which is fine, but there should also be a diagnostic that -multi is working the way the user intended it.	

Associated revisions

Revision 424e3bb0 - 06/24/2014 01:59 PM - Erik Lindahl

Added multisimulation info to log/output

mdrun now reports that it is part of a multisimulation setup, how many simulations there are, and that the detailed MPI/OpenMP data applies to the individual simulation.

Fixes #1204.

Change-Id: I04f1edf9a7fd1eda202b83713bdd877807242dca

History

#1 - 05/22/2013 04:55 AM - Mark Abraham

- Target version changed from 4.6.2 to future
- Affected version set to 4.6.1

#2 - 05/22/2013 05:43 AM - Mark Abraham

- Target version changed from future to 4.6.x

#3 - 09/10/2013 03:53 PM - Mark Abraham

Also, non-REMD multi simulations do not check for .tpr consistency, e.g. with number of simulation steps. Not sure if that's a feature or a bug. md_support.c tries to check the number of steps, but the code is broken (e.g. use of MASTER, not SIMMASTER; and/or subsequent use of gmx_bcast, which only functions within a simulation)

#4 - 06/18/2014 02:25 PM - Mark Abraham

- Tracker changed from Bug to Feature
- Subject changed from multi simulations do not report that they are multi simulations to multi simulations should report that they are multi simulations
- Target version changed from 4.6.x to 5.x

#5 - 06/23/2014 11:08 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#1204](#).
Uploader: Erik Lindahl (erik@kth.se)
Change-Id: I04f1edf9a7fd1eda202b83713bdd877807242dca
Gerrit URL: <https://gerrit.gromacs.org/3669>

#6 - 06/23/2014 11:08 PM - Erik Lindahl

- Status changed from New to Fix uploaded

#7 - 06/24/2014 08:29 PM - Erik Lindahl

- Status changed from *Fix uploaded* to *Resolved*

#8 - 06/24/2014 08:29 PM - Erik Lindahl

- Status changed from *Resolved* to *Closed*

#9 - 07/15/2014 06:39 AM - Teemu Murtola

- Category set to *mdrun*

- Assignee set to *Erik Lindahl*

- Target version changed from *5.x* to *5.0*

#10 - 04/27/2015 09:37 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#1204](#).

Uploader: Mark Abraham (mark.j.abraham@gmail.com)

Change-Id: I6857eea3a705ac9db1fa8964b2105820526b9a23

Gerrit URL: <https://gerrit.gromacs.org/4532>