

GROMACS - Bug #2775

number of ranks reporting was wrong

11/22/2018 10:22 AM - Mark Abraham

Status: Closed	
Priority: Normal	
Assignee:	
Category: mdrun	
Target version: 2019	
Affected version - extra info: many versions	Difficulty: uncategorized
Affected version: 2019-beta2	
Description	
The first part of md.log reported	
<pre>Log file opened on Wed Nov 21 13:55:49 2018 Host: bs-gpu01 pid: 3038 rank ID: 0 number of ranks: 1 :-) GROMACS - gmX mdrun, 2019-beta3-dev-20181119-de71ffa (-:</pre>	
the rank count was not 1, there were two thread mpi ranks launched later. I think the second line is superseded by the later output (we report the node name later, the PID is not particularly useful, and the rank stuff isn't valid until thread-MPI has launched ranks, and is anyway reported later)	
Related issues:	
Related to GROMACS - Bug #2794: Release build fails in PDB2GMX google tests	Closed

Associated revisions

Revision 367d0031 - 11/26/2018 11:23 AM - Mark Abraham

Clean up initial log output

The rank count was incorrect when thread-MPI has not yet spawned threads. It could only be fixed if we would have made that choice before we open the log file, but we want to be able to report problems to the log file from hardware detection or tpr reading which occur before rank choice.

Host name, rank count and rank ID are all reported later, alongside other such information, so there is no need to duplicate and complicate our code.

PID is now reported later alongside other similar information. The log file output looks reasonable, aligned, etc.

Noted TODO for future clean up.

Fixes #2775

Change-Id: Ifda6c44bfe28628934f4614e20eeef436d80707

Revision 515ea06d - 12/10/2018 10:24 AM - Mark Abraham

Make only mdrun report process ID

Recent change 367d003106 changed where mdrun reported the process ID, but in so doing changed various tools to also report the process ID. This made pdb2gmX tests non-reproducible.

Since the process ID is probably only of minor value to the user, and probably only of value to users of mdrun, this change adds support for allowing tools to choose to print the process ID while defaulting to not reporting it.

Fixes #2794

Refs #2775

History

#1 - 11/22/2018 01:37 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2775](#).
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~release-2019~lfda6c44bfe28628934f4614e20eeef436d80707
Gerrit URL: <https://gerrit.gromacs.org/8741>

#2 - 11/26/2018 11:45 AM - Mark Abraham

- Status changed from New to Resolved

Applied in changeset [367d0031064d59ebf7ee650927f4516352be7a38](#).

#3 - 11/28/2018 02:56 PM - Paul Bauer

- Status changed from Resolved to Closed

#4 - 11/28/2018 03:44 PM - Mark Abraham

- Target version set to 2019

#5 - 12/10/2018 02:52 AM - Mark Abraham

- Related to Bug #2794: Release build fails in PDB2GMX google tests added

#6 - 12/10/2018 03:05 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2775](#).
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~release-2019~lcb6e97d4d7502f12e74cbaa2c1f1a969ba99b917
Gerrit URL: <https://gerrit.gromacs.org/8799>