GROMACS - Feature #1078

Improve stderr output

12/19/2012 07:42 PM - Erik Lindahl

Status:	Closed	
Priority:	Normal	
Assignee:	Mark Abraham	
Category:	mdrun	
Target version:	4.6	
Difficulty:	uncategorized	

Description
With the -multi option we write way too much repeated information. It would also be good to add a 1-line CPU info to mdrun output before the GPU detection output. We are duplicating the messages about # of tMPI threads started

Associated revisions

Revision 69e15959 - 01/16/2013 02:16 AM - Mark Abraham

Quiet stderr output, particularly for multi-simulations

- removed printing of DD info to stderr
- printed multi-simulation information only once in places where repetition is clearly redundant (Some repetition remains, but only from each simulation master.)
- add option to not print result of multi-simulation check if it passed, so that we don't have to print things to stderr/stdout just because the .log file is not yet open
- printing of diagnostics about the number of MPI processes present when mdrun starts only goes (once) to each debug file, and not to stderr
- reduced printing of diagnostics about the number of OpenMP threads; now goes to stderr only on SIMMASTER, or once to each debug file
- clarified errors and informational messages about selecting the number of OpenMP threads

Fixes #1078, refs #1083

Change-Id: If782259bcd62ddd9be325393930080b70c5cfb4e

History

#1 - 12/31/2012 08:09 AM - Roland Schulz

Another stderr output which is annoying for large number of MPI ranks, is the NODEID and NNODES which is printed once per rank. Can we remove those or are they important for something?

#2 - 01/02/2013 07:12 AM - Szilárd Páll

I'd add that the long-term major annoyance of all GROMACS programs printing help and usage info by default, without the user requesting it, could be also addressed here.

#3 - 01/02/2013 08:05 AM - Erik Lindahl

Let's separate the two issues. Printing NODEID and NNODES for thousands of processes is a bug that needs to be fixed before 4.6, but it's too late in the release cycle to change the way all Gromacs programs print to stdout.

#4 - 01/02/2013 07:19 PM - Roland Schulz

Should NODEID and NNODES be completely removed or should it still be shown in some cases (e.g. with -v, or env-variable, or debug, or <100 nodes)?

#5 - 01/02/2013 07:21 PM - Erik Lindahl

Showing it with -debug if there are less than 100 nodes makes sense - I can't remember any time where it has helped solve any real bugs.

#6 - 01/07/2013 01:36 PM - Mark Abraham

- Category set to mdrun

- Assignee set to Mark Abraham

The NODEID and NNODES output has been useful on gmx-users to help users work out that they failed to configure with MPI, but the new header information about the execution context replaces that.

I'll take care of this one when I see if [#1024](#) is working

#7 - 01/12/2013 01:36 PM - Mark Abraham

https://gerrit.gromacs.org/#/c/2028/ addresses most of these issues and one or two things I noticed on the way.

Erik, not sure what you want for the one-line CPU info in the original description. Do you want to patch that separately?

#8 - 01/14/2013 12:28 AM - Mark Abraham

- Status changed from New to In Progress

#9 - 01/14/2013 03:11 AM - Erik Lindahl

As we discussed in the patch about adding hardware info, I think the important part is to have all hardware info in the log, and since we have it there it should be fine.

If we keep adding info to stdout, we are just encouraging the user to mention some of their config and guess the rest, instead of properly attaching their logfile to an error message.

#10 - 01/18/2013 03:38 PM - Erik Lindahl

- Status changed from In Progress to Closed