GROMACS - Bug #1270

affinity setting broken with MPI

05/31/2013 07:18 PM - Szilárd Páll

Status: Closed
Priority: High
Assignee: Sander Pronk
Category: mdrun
Target version: 4.6.3
Affected version - extra info: Difficulty: uncategorized
Affected version: 4.6.2

Description
With the MPI builds (i.e GMX_MPI=ON) the affinity setting seems to be broken. While affinity setting works with the exact same build and launch configuration when compiling with thread_mpi, with MPI I get the warning suggesting that affinity setting is not supported by the current platform.

This means that tMPI_Thread_setaffinity_support() returns TMPI_SETAFFINITY_SUPPORT_NO which suggests that HAVE_PTHREAD_SETAFFINITY is not defined. I suspect a bug in the build system.

As this bug will result in no affinities set in all MPI runs, it will cause considerable performance regression - especially at high parallelization where OpenMP is used.

Related issues:
Related to GROMACS - Bug #1334: concurrency-related bug with thread-MPI
Has duplicate GROMACS - Bug #1266: Affinity setting not supported on Cray XK7

Associated revisions
Revision 78569369 - 07/01/2013 08:03 PM - Sander Pronk
Comprehensive hwinfo structure concurrency fix.

The hwinfo structure and structures contained therein are inherently global to any mdrun processes/ranks. This patch makes sure that
- The hwinfo structure is shared among all threads
- Only one thread creates a hwinfo structure
- The hwinfo structure is safe to read for all threads after they obtain it

In addition, it fixes the detection for pthread_setaffinity in thread_mpi.

This fixes concurrency issues with thread affinity settings with or without MPI, and makes runner.c slightly easier to read because the concurrency logic is pushed to gmx_detect_hardware.c

Fixes #1270, #1254

Note that #1254 issue 3 seems to be an OpenMPI bug.

Change-Id: I236e81923324d7873f3d889b91c702a7843

History
#1 - 05/31/2013 07:41 PM - Szilárd Páll
The bug was introduced by 972ab1f9 which moved the code that does the HAVE_PTHREAD_SETAFFINITY in to the TMPI_ENABLE macro which is called only with thread_mpi. The solution is moving this check out similarly to the way TMPI_TEST_ATOMICS is done.

#2 - 06/01/2013 08:28 AM - Mark Abraham
Ugh. Thanks for the diagnosis!

#3 - 06/01/2013 08:31 AM - Sander Pronk
- Assignee changed from Berk Hess to Sander Pronk
#4 - 06/03/2013 02:32 PM - Rossen Apostolov
- Status changed from New to Fix uploaded

#5 - 07/05/2013 06:28 PM - Mark Abraham
- Status changed from Fix uploaded to Resolved

#6 - 08/13/2013 08:55 PM - Sander Pronk
- % Done changed from 0 to 100

Applied in changeset `78569369348e07a300a03f90e667e61879858025`.

#7 - 09/18/2013 06:20 PM - Szilárd Páll
- Status changed from Resolved to Closed

Sander Pronk wrote:

Applied in changeset `78569369348e07a300a03f90e667e61879858025`.

Closing this issue, but I wanted to note that the change seems to be causing yet another problem, see #1334.