## GROMACS - Bug #1270

**affinity setting broken with MPI**

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<tbody>
<tr>
<td>Priority:</td>
<td>High</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Sander Pronk</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version:</td>
<td>4.6.3</td>
</tr>
<tr>
<td>Affected version - extra info:</td>
<td></td>
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<tr>
<td>Affected version:</td>
<td>4.6.2</td>
</tr>
<tr>
<td>Difficulty:</td>
<td>uncategorized</td>
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### 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
  - Closed 09/13/2013
- Has duplicate GROMACS - Bug #1266: Affinity setting not supported on Cray XK7
  - Closed 05/28/2013

### 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: i236e81923324d7873f3d8633889b91c7c02a7843

### 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 78569369348e07a300a03f90e667e61879f58025.

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

Sander Pronk wrote:

Applied in changeset 78569369348e07a300a03f90e667e61879f58025.

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