**GROMACS - Bug #2348**

**mdrun can oversubscribe the cores with GPUs, thread-MPI and only -ntomp**

12/12/2017 04:08 PM - Berk Hess

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
</tr>
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<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Berk Hess</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version:</td>
<td>2016.5</td>
</tr>
<tr>
<td>Affected version - extra info:</td>
<td>any version with GPU sharing</td>
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<td>Affected version:</td>
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</tr>
<tr>
<td>Difficulty:</td>
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**Description**

The code for deciding the number of thread-MPI threads did not (correctly) take into account that the number of OpenMP threads my have been set (by either the user of something in the scheduling). This could lead to oversubscribing the number of hardware threads.

Since in general there is no unique way to decide the number of thread-MPI ranks given the number of OpenMP threads, the number of hardware threads and the number of GPUs, we should not allow to specify -ntomp without -ntmpi.

For the CPU case there is a unique solution, so we do not need to change that (and we should not in a release branch).

**Associated revisions**

Revision f10d33f1 - 12/14/2017 10:59 AM - Berk Hess

Require -ntmpi with setting -ntomp with GPUs

With GPUs and thread-MPI, setting only -ntomp could lead to oversubscription of the hardware threads.

Now with GPUs and thread-MPI the user is required to set -ntmpi when using -ntomp. Here we chose that to also require -ntmpi when the user specified both -nt and -ntomp; here we could infer the number of ranks, but it's safer to ask the user to explicitly set -ntmpi.

Note that specifying both -ntmpi and -nt has always worked correctly.

Fixes #2348

Change-Id: lad380721807f5c53b8c70808cea75c5f29341a8f

**History**

#1 - 12/12/2017 04:11 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #2348.
Uploader: Berk Hess (hess@kth.se)
Change-Id: gromacs~release-2016~lad380721807f5c53b8c70808cea75c5f29341a8f
Gerrit URL: https://gerrit.gromacs.org/7337

#2 - 12/14/2017 01:11 PM - Berk Hess

- Status changed from In Progress to Resolved

Applied in changeset f10d33f1efaece61a3691bb1b7941a8565d2a8cf.

#3 - 12/14/2017 04:16 PM - Erik Lindahl

- Status changed from Resolved to Closed