**Gromacs - Bug #1266**

**Affinity setting not supported on Cray XK7**

05/28/2013 12:52 AM - Szilárd Páll

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
</tr>
</thead>
<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>4.6.3</td>
</tr>
<tr>
<td>Affected version</td>
<td>4.6.1</td>
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**Description**

The Cray programming environment (xt-asyncpe) somewhere between the version 5.17(5.18?) and 5.20 versions broke mdrun-s affinity setting capabilities - at least that's what the warning message appearing in the stderr and log suggests.

The behavior was observed on Toedi, the Cray XK7 at CSCS.

Note that by default aprun sets thread affinites (the default is -cc cpu), but this results in poor performance. Previously, the -cc none setting has been used to disable the aprun-set affinities and rely on the affinity set by mdrun.

**Related issues:**

Duplicates Gromacs - Bug #1270: affinity setting broken with MPI

**History**

#1 - 05/28/2013 02:11 AM - Szilárd Páll

Note that based on performance observed earlier, I suspect that already Cray runtimes preceding xt-asyncpe 5.17 were perhaps silently ignoring affinity settings. I'm not entirely sure, I'll have to dig up some old log files and redo the runs with affinities set through aprun which seems to work; e.g. for a Cray XK7 with a single Interlagos CPU per rank, running 4 ranks with 4 threads each getting the otherwise default mdrun affinity requires aprun -cc 0,1,2,3:4,5,6,7:8,9,10,11:12,13,14,15.

#2 - 05/31/2013 07:44 PM - Szilárd Páll

Actually this is a duplicate of #1270. Is it not possible to mark it as such?

#3 - 06/03/2013 02:31 PM - Rossen Apostolov

Marked as such.

When a related issue is added there is a dropdown list that has "duplicate" in it.

#4 - 06/04/2013 11:47 PM - Szilárd Páll

Rossen Apostolov wrote:

  Marked as such.

  When a related issue is added there is a dropdown list that has "duplicate" in it.

Thanks.
#5 - 06/26/2013 01:26 AM - Mark Abraham
- Status changed from New to Fix uploaded
- Target version set to 4.6.3

#6 - 07/05/2013 06:28 PM - Mark Abraham
- Status changed from Fix uploaded to Resolved

#7 - 09/18/2013 06:08 PM - Szilárd Páll
- Status changed from Resolved to Closed