Gromacs - Bug #1613
Problem with 4.6.x MPI, thread affinity, slurm and node-uneven task spread
10/02/2014 04:45 PM - Åke Sandgren

Status: Closed
Priority: Low
Assignee: mdrun
Category: mdrun
Target version: 5.0.5
Affected version - extra info: 
Affected version: 4.6.x

Description
Just managed to pin down a weird problem which is caused by uneven spread of tasks over nodes and thread affinity causing jobs to hang in gmx_set_thread_affinity.

This happens on our 48-core nodes using a 100 task job that when submitted through slurm (without specifying distribution manually) gets distributed over 3 nodes with 6+47+47 tasks.
We are also using cgroups to allow for multiple jobs per node, so the node with 6 tasks has an affinity mask set for only the 6 cores on a single NUMA. The nodes with 47 tasks have the whole node allocated and thus gets a full 48-core affinity mask.
(Actually due to a bug(/feature?) in slurm the tasks on the node with only 6 cores allocated actually get a single-core per task affinity, but that's not relevant here.)

Anyway, when the code gets to line 1629 in runner.c (this is 4.6.7) and the call to gmx_check_thread_affinity_set we start having problems.

The loop to set bAllSet ends up setting bAllSet to TRUE for the tasks on the two fully allocated nodes and FALSE on the tasks on the third node.
This in turn changes hw_opt->thread_affinity to threadaffOFF on those 6 tasks, but leaves it at threadaffAUTO for the other 2x47 tasks.
gmx_set_thread_affinity then promptly returns for those poor 6 tasks and tries in vain to do a MPI_Comm_split with 6 tasks missing from the equation...

I suggest to gather the bAllSet result from all nodes in gmx_check_thread_affinity_set and make sure all tasks have the same view of the world...

Suggested patch;
gmx_bool bAllSet_All;
MPI_Allreduce(&bAllSet, &bAllSet_All, 1, MPI_INT, MPI_LAND, MPI_COMM_WORLD);
bAllSet = bAllSet_All;

Related issues:
Related to Gromacs - Bug #1614: thread-MPI has broken support for operations ...

Associated revisions
Revision 93a5a180 - 11/26/2014 11:22 AM - Åke Sandgren
Fix problem with mixed affinity mask on different nodes.

If task distribution (with slurm for instance) causes both fully allocated and not-fully allocated nodes to be assigned to the job then there may be tasks with a all-cores affinity mask and tasks with a not-all-cores affinity masks.

Fixes #1613
Change-Id: I71c0daa43a5dd42da57bfd09037806ce1d9334b5

11/19/2015
Your suggested patch seems reasonable! FYI our code review system is open for anyone to submit patches, so you could upload the suggested three-liner it straight to gerrit.gromacs.org. (the 3 steps instructions are here: http://www.gromacs.org/Developer_Zone/Git/Gerrit#Getting_started)

Ok, trying that then :-)
#5 - 10/02/2014 10:28 PM - Mark Abraham
- Related to Bug #1614: thread-MPI has broken support for operations on MPI_INT added

#6 - 04/20/2015 02:23 PM - Mark Abraham
- Category set to mdrun
- Status changed from New to Resolved

#7 - 04/20/2015 02:41 PM - Mark Abraham
- Status changed from Resolved to Closed
- Target version set to 5.0.5