GROMACS - Bug #3296

multi run with >1 rank per simulation exits with MPI_ABORT

01/13/2020 08:20 PM - Szilárd Páll

<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>Berk Hess</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version:</td>
<td>2020.1</td>
</tr>
<tr>
<td>Affected version - extra info:</td>
<td>Difficulty: uncategorized</td>
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<tr>
<td>Affected version:</td>
<td>2020</td>
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</tbody>
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Description

$ mpirun --mca mpi_abort_print_stack 1 -np 4 $gmx_mpi mdrun -v -multidir repl_{001..002} -nsteps 0 -s topol

GROMACS: gmx mdrun, version 2020.1-dev-20200110-4879d39
Executable: /nethome/pszilard-projects/gromacs/gromacs-20/build_AVX2_256_gcc8_cuda10.1_ompi400/bin/gmx_mpi
Data prefix: /nethome/pszilard/projects/gromacs/gromacs-20 (source tree)
Working dir: /nethome/pszilard-projects/gromacs/bench/LUMI-bench/agp Ensemble/test_repl-128
Command line:
  gmx_mpi mdrun -v -multidir repl_001 repl_002 -nsteps 0 -s topol

Back Off! I just backed up md.log to ./#md.log.11#
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Compiled SIMD: AVX2_256, but for this host/run AVX_512 might be better (see log).
Reading file topol.tpr, VERSION 2020.1-dev-20200108-e05cc33 (single precision)
Overriding nsteps with value passed on the command line: 0 steps, 0 ps
Overriding nsteps with value passed on the command line: 0 steps, 0 ps
Changing nstlist from 40 to 100, rlist from 1.2 to 1.287

[dev-purley01:30476] *** An error occurred in MPI_Allreduce
[dev-purley01:30476] *** reported by process [566165505,3]
[dev-purley01:30476] *** on communicator MPI_COMM_WORLD
[dev-purley01:30476] *** MPI_Comm: invalid communicator
[dev-purley01:30476] *** MPI_ERRORS_ARE_FATAL (processes in this communicator will now abort,
[dev-purley01:30476] *** and potentially your MPI job)

Associated revisions

Revision 4d60bf59 - 01/16/2020 08:44 PM - Berk Hess
Correct fixed redmine issue id from 3297 to 3296
Recent commit 36a65816 said it fixed issue 3297, but this should have been issue 3296.
Refs #3296
Change-Id: i85a95e818d3cda816211dc2aa8dd32e9e0c69d4

History

#1 - 01/13/2020 08:41 PM - Szilárd Páll

(gdb) bt
#0 0x00007ff8f49ac6bd0 in PMPI_Allreduce () from /opt/tcbsys/openmpi/4.0.0/lib/libmpi.so.40
#1 0x0000000000010e7106 in gmx_sumi_sim (nr=1, r=0x7ffdb99c8abc, ms=0x37f1670) at /nethome/pszilard/projects/gm
The issue is that gmx_multisim_t (and specifically mpi_comm_masters) is used in GpuTaskAssignmentsBuilder::build() in countOverAllRanks() whereas the multisim data is only initialized later with simulatorBuilder.build().