GROMACS - Bug #2403
Multidir sim with #mpiranks = 2*#sim fails
02/06/2018 09:55 PM - Christoph Junghans

Running a twofold multidir sim on 4 mpi ranks - something like:

```bash
mpirun -np 4 /usr/lib64/openmpi/bin/mdrun_openmpi_d -s topol.tpr -c confout.gro -o traj.trr -x traj.xtc -multidir sim1 sim2 -nsteps 500 -v
```

fails with

```text
*** An error occurred in MPI_Barrier
```

while

```bash
mpirun -np 2 /usr/lib64/openmpi/bin/mdrun_openmpi_d -s topol.tpr -c confout.gro -o traj.trr -x traj.xtc -multidir sim1 sim2 -nsteps 500 -v
```

works!
(Note: Using same tpr files for all sims for testing)

Additionally, it prints the following confusing message:

```text
No option -multi
```

I believe all of this worked before the -multi option was removed.

Related issues:

- Related to GROMACS - Task #2425: testing multisim with multiple ranks per sim...
  New
- Has duplicate GROMACS - Bug #2414: -multidir not working due to erroneous use...
  Closed

Associated revisions

Revision fa3593ec - 02/16/2018 02:51 PM - Berk Hess
Correct multisim MPI barrier

An MPI barrier used with multisim was called on incorrect ranks and a barrier was missing.

Fixes #2403

Change-Id: I06a66167afc8dca9cdd4ca9b4f9a806984a6ec7a

Revision 6358ce73 - 03/01/2018 09:44 AM - Berk Hess
Fix mdrun multisim with separate PME ranks

When running multiple simulations using separate PME ranks, mdrun would call MPI_Barrier with MPI_COMM_NULL on some ranks. Note: no new release note needed, since this fixes a fix.
Refs #2403
Fixes #2431
Fixes #2432

Change-Id: i7fe96a15b5030dea3e093d12850f89f00ccc9f48

History

#1 - 02/06/2018 10:15 PM - Mark Abraham
The -multi option is still present in 2018. The print issue is fixed in release-2018 already. I don't know whether your case works, but an almost identical integration test does run, using -multi. That case has been ported to -multisim in master, so I don't know why this might arise.

#2 - 02/07/2018 11:04 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2403.
Uploader: Berk Hess (hess@kth.se)
Change-Id: gromacs~release-2018~I06a66167afc8dca9cdd4ca9b4f9a806984a6ec7a
Gerrit URL: https://gerrit.gromacs.org/7549

#3 - 02/07/2018 04:58 PM - Christoph Junghans
Mark Abraham wrote:

The -multi option is still present in 2018. The print issue is fixed in release-2018 already.

Thanks, it was #2377.

#4 - 02/07/2018 05:16 PM - Mark Abraham
Mark Abraham wrote:

I don't know whether your case works, but an almost identical integration test does run, using -multi. That case has been ported to -multisim in master, so I don't know why this might arise.

Those tests use a single rank per simulation, so didn't hit the barrier in the problematic case. I am working on better test coverage for master branch.

#5 - 02/07/2018 05:16 PM - Mark Abraham
- Status changed from New to In Progress

#6 - 02/08/2018 10:26 AM - Berk Hess
- Category set to mdrun
- Status changed from In Progress to Fix uploaded
- Target version set to 2018.1

#7 - 02/16/2018 03:00 PM - Berk Hess
- Status changed from Fix uploaded to Resolved

Applied in changeset fa3593ec6b33ee61eaa5193891dad6495a0534.

#8 - 02/16/2018 03:27 PM - Mark Abraham
- Has duplicate Bug #2414: -multidir not working due to erroneous use of MPI_Comm_create added

#9 - 02/16/2018 03:28 PM - Mark Abraham
- Status changed from Resolved to Closed

#10 - 02/27/2018 04:43 PM - Mark Abraham
- Related to Task #2425: testing multisim with multiple ranks per simulation added

#11 - 03/01/2018 09:33 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2403.
Uploader: Berk Hess (hess@kth.se)
Change-Id: gromacs~release-2018~i7fe96a15b5030dea3e093d12850f89f00ccc9f48
Gerrit URL: https://gerrit.gromacs.org/7692