segfaults in three regression tests with NVIDIA OpenCL multi-GPU runs

12/07/2015 07:52 PM - Szilárd Páll

Status: Closed
Priority: Normal
Assignee: mdrun
Category: mdrun
Target version:
Affected version:
Extra info:
Difficulty: uncategorized

Affected version: 5.1.1

Description
The following tests segfault when executed on two GPUs (gmx mdrun -ntmpi 2 -gpu_id 01):

- complex.nbnxn-ljpme-LB-geometric
- complex.nbnxn_rzero
- complex.position-restraints

backtrace:

```
#0 0x000000f7c3d3189f0b in ?? () from /usr/lib/x86_64-linux-gnu/libnvidia-opencl.so.1
#1 0x000000f7c3d3189a2a in ?? () from /usr/lib/x86_64-linux-gnu/libnvidia-opencl.so.1
#2 0x000000f7c3d3184632 in ?? () from /usr/lib/x86_64-linux-gnu/libnvidia-opencl.so.1
#3 0x000000f7c426dbdca in sync_ocl_event (stream=0x7fcd34872d30, ocl_event=0x7fcd340831f0) at /mnt/workspace/Gromacs_Gerrit_5_1-test-opencl-slave/d27c5006/gromacs/src/gromacs/mdlib/nbnxn_ocl/nbnxn_ocl.cpp:331
#4 0x000000f7c426dcf7d in nbnxn_gpu_launch_cpyback (nb=0x7fcd34082db0, nbatom=0x7fcd34081350, flags=1013, alloc=0) at /mnt/workspace/Gromacs_Gerrit_5_1-test-opencl-slave/d27c5006/gromacs/src/gromacs/mdlib/nbnxn_ocl/nbnxn_ocl.cpp:952
#5 0x000000f7c426d4ecccc in do_force_cutsVERLET (fplog=0x0, cr=0x7fcd340071f0, inputrec=0x7fcd34007270, step=0, nrnb=0x7fcd3406bb60, wcycle=0x7fcd3406b640, top=0x7fcd349ce990, groups=0x7fcd340077a0, box=0x7fcd3406bb10, x=0x7fcd349d1580, hist=0x7fcd3497dc40, f=0x7fcd349d7ca0, vir_force=0x7fcd3407f450, mdatoms=0x7fcd34333d90, enerd=0x7fcd3498f730, fcd=0x7fcd34069920, lambda=0x7fcd349884d0, graph=0x0, fr=0x7fcd3406bf30, ic=0x7fcd34082060, vsite=0x0, mu_tot=0x7fcd3407f5f0, t=0, field=0x0, ed=0x0, bBornRadii=1, flags=1013) at /mnt/workspace/Gromacs_Gerrit_5_1-test-opencl-slave/d27c5006/gromacs/src/gromacs/mdlib/sim_util.cpp:1061
#6 0x000000f7c426d4e02 in do_md (fplog=0x0, cr=0x7fcd340071f0, inputrec=0x7fcd34007270, step=0, nrnb=0x7fcd3406bb60, wcycle=0x7fcd3406b640, top=0x7fcd349ce990, groups=0x7fcd340077a0, box=0x7fcd3497db10, x=0x7fcd349d1580, hist=0x7fcd3497dc40, f=0x7fcd349d7ca0, vir_force=0x7fcd3407f450, mdatoms=0x7fcd34333d90, enerd=0x7fcd3498f730, fcd=0x7fcd34069920, lambda=0x7fcd349884d0, graph=0x0, fr=0x7fcd3406bf30, vsite=0x0, mu_tot=0x7fcd3407f5f0, t=0, field=0x0, ed=0x0, bBornRadii=1, flags=1013) at /mnt/workspace/Gromacs_Gerrit_5_1-test-opencl-slave/d27c5006/gromacs/src/gromacs/mdlib/sim_util.cpp:2009
#7 0x000000000004iacb in do_md (fplog=0x0, cr=0x7fcd340071f0, nfile=35, fnm=0x7fcd34005a90, oenv=0x155c7d0, bVerbose=0, bCompact=1, nstglobalcomm=5, vsite=0x0, constr=0x7fcd3497db10, state=0x7fcd34079160, tape=0x7fcd34079160, walltime_accounting=0x7fcd343338d0) at /mnt/workspace/Gromacs_Gerrit_5_1-test-opencl-slave/d27c5006/gromacs/src/programs/mdrun/mdrun.cpp:1078
#8 0x0000000000042835b in mdrunner (hw_opt=0x7fcd3c07f5f0, fplog=0x0, cr=0x7fcd340071f0, nfile=35, fnm=0x7fcd34005a90, oenv=0x155c7d0, bVerbose=0, bCompact=1, nstglobalcomm=1, ddxxyz=0x7fcd3c07f5f0)
```

02/24/2020
c, dd_node_order=1, rdd=0, rconstr=0, dddlb_opt=0x42da2a "auto", dlb_scale=0.800000012, ddcx=0x0, ddcy=0x0, ddcz=0x0, nbpu_opt=0x42da2a "auto", nstlist_cmdline=0, nsteps_cmdline=-2, nstepout=1000, resetstep=-1, nmultisim=0, repl_ex_nst=0, repl_ex_nex=0, repl_ex_seed=-1, pforce=-1, opt_perio=15, max_hours=-1, imdport=0, Flags=7168

at /mnt/workspace/Gromacs_Gerrit_5_1-test-opencl-slave/d27c5006/gromacs/src/programs/mdrun/runner.cpp:1282
#9 0x0000000000042528e in mdrunner_start_fn (arg=0x155ddd0) at /mnt/workspace/Gromacs_Gerrit_5_1-test-opencl-slave/d27c5006/gromacs/src/programs/mdrun/runner.cpp:186
#10 0x00000000000426ea0f6 in tMPI_Thread_starter (arg=0x15cb518) at /mnt/workspace/Gromacs_Gerrit_5_1-test-opencl-slave/d27c5006/gromacs/src/external/thread_mpi/src/tmpi_init.c:397
#11 0x00000000000426e61201 in tMPI_Thread_starter (arg=0x15cc550) at /mnt/workspace/Gromacs_Gerrit_5_1-test-opencl-slave/d27c5006/gromacs/src/external/thread_mpi/src/thread_mpi.c:234
#12 0x00000000000426f07e9a in start_thread (arg=0x7fcd3fc080700) at pthread_create.c:308
#13 0x00000000000426f0438d in clone () at../sysdeps/unix/sysv/linux/x86_64/clone.so:112
#14 0x000000000000000000000 in ?? ()

Related issues:
Related to GROMACS - Bug #1990: LJ-PME unstable with OpenCL

Closed

Associated revisions
Revision ad8209b5 - 12/27/2015 04:54 AM - Mark Abraham
Fix some OpenCL issues
Added routine to convert error codes into more helpful diagnostics. Called it in one place that needed some troubleshooting, but an overhaul of OpenCL error handling is needed (in master branch).

Introduced new OpenCL control variable to indicate when there is a non-local event upon which it is valid to wait, since it is an error to wait upon an ocl_event that was never returned by an API call.

Converted mdrun integration tests to rely on the improved automated resource assignment in 5.1, because that copes better with the limitations of the OpenCL implementation.

Worked around limitation where real MPI + OpenCL can't use more than one GPU on a node, by disabling GPU support for that test case.

Fixed inappropriate use of mdrun -nt, where the number of thread-MPI ranks was intended.

Updated install guide.

Fixes #1871

Change-Id: I11e6b2bdf67f91489f3ec0d671081d99661fa62

History
#1 - 12/08/2015 11:36 PM - Gerrit Code Review Bot
Gerrit received a related patchset '5' for Issue #1871.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: I11e6b2bdf67f91489f3ec0d671081d99661fa62
Gerrit URL: https://gerrit.gromacs.org/5430

#2 - 12/17/2015 08:09 PM - Sziárd Páll
- Status changed from New to In Progress

#3 - 12/28/2015 01:15 AM - Mark Abraham
- Status changed from In Progress to Resolved

Applied in changeset ad8209b537febfa3c39b994ef417b423666da2803.

#4 - 01/12/2016 12:01 PM - Sziárd Páll
- Status changed from Resolved to Closed
- Related to Bug #1990: LJ-PME unstable with OpenCL added