GROMACS - Bug #2779

Error when using a large PME grid on a GPU

11/27/2018 04:16 PM - Grégoire Gschwend

Status: Closed
Priority: Normal
Assignee: mdrun
Category: mdrun
Target version: 2018.5
Affected version - extra info: 2018.2
Affected version: 2018.2

Difficulty: uncategorized

Description
GROMCAS 2018.2 displays the following error message
"Error while launching kernel pme_solve_kernel: invalid argument"
when launching the simulation with the command:
gmx mdrun -v -deffnm nvt -ntmpi 16 -ntomp 2 -npme 1 -pme gpu -nb gpu
however, the simulation works fine with:
gmx mdrun -v -deffnm nvt -ntmpi 16 -ntomp 2
It seems that the error appears with relatively large systems (box of 10 nm x 10 nm x 40 nm). I could not reproduce the error with a system of 3 nm x 3 nm x 9 nm.

Associated revisions
Revision aa2305c1 - 12/05/2018 09:54 AM - Berk Hess
Make large PME grids work on GPU
With PME grids with z size larger than 511 too large blocks could be launched causing a cryptic CUDA error.
Fixes #2779
Change-Id: i0833609f64ad2e0ad6b7a799cd2b693f2dec3939

Revision c15057c7 - 12/11/2018 05:20 AM - Berk Hess
Make large PME grids work on GPU
With PME grids with z size larger than 511 too large blocks could be launched causing a cryptic CUDA or OpenCL error.
Fixes #2779
Change-Id: l92376ae0e9d5a338084df8f3a2cf46ca1b711a6a

History
#1 - 11/28/2018 09:24 AM - Paul Bauer
I can reproduce this on my machine with v2018.2 and with the current HEAD of release 2018

#2 - 11/28/2018 09:24 AM - Paul Bauer
- Status changed from New to Accepted

#3 - 11/28/2018 09:47 AM - Berk Hess
- Status changed from Accepted to In Progress
I suppose this is the threads per block limit issue that is attempted to be fixed by: https://gerrit.gromacs.org/#/c/8709/

#4 - 11/28/2018 10:10 AM - Paul Bauer
Still dies with https://gerrit.gromacs.org/#/c/8709/ and this error

Program: gmx mdrun, version 2019-beta3-dev-20181116-2bdca7b34
Source file: src/gromacs/gpu_utils/cudautils.cuh (line 347)
Function: void launchGpuKernel(void (*)(Args ...), const KernelLaunchConfig&, CommandEvent*, const char*, const std::array<void*, sizeof... (Args)>&) [with Args = {PmeGpuCudaKernelParams}; CommandEvent = void]
MPI rank: 15 (out of 16)

Internal error (bug):
GPU kernel (PME solve) failed to launch: invalid argument

#5 - 11/28/2018 10:53 AM - Berk Hess
Try changing to 32 instead of 16 :)

#6 - 11/28/2018 11:25 AM - Paul Bauer
gmx mdrun -v -deffnm nvt -ntmpi 32 -ntomp 2 -npme 1 -pme gpu -nb gpu
Program: gmx mdrun, version 2019-beta3-dev-20181116-2bdca7b34
Source file: src/gromacs/domdec/domdec_setup.cpp (line 764)
MPI rank: 0 (out of 32)

Fatal error:
The number of ranks you selected (31) contains a large prime factor 31. In most cases this will lead to bad performance. Choose a number with smaller prime factors or set the decomposition (option -dd) manually.

For more information and tips for troubleshooting, please check the GROMACS website at http://www.gromacs.org/Documentation/Errors

#7 - 11/28/2018 01:26 PM - Paul Bauer
So, this also happens with -ntmpi 33, -ntmpi 17, -ntmpi 5, -ntmpi 2.
It also gives the error

Internal error (bug):
GPU kernel (PME solve) failed to launch: invalid argument

#8 - 11/28/2018 01:35 PM - Berk Hess
I meant 32 warps per block instead of the 16 the change set. But I meant it half joking, since this is obviously not a solution. One can always come up with a larger system. Instead we could e.g. launch the kernel multiple times.

#9 - 11/28/2018 01:36 PM - Berk Hess
- Subject changed from Error when using 3dc Ewald with dedicated pme rank on GPU to Error when using a large PME grid on a GPU

I changed the subject to what I think the actual issue is.

#10 - 11/28/2018 01:58 PM - Paul Bauer
Sorry that I misunderstood you there!

#11 - 12/03/2018 10:24 PM - Berk Hess
We are not at all at a block count limit. The issue is that we assign one (or more) grid line to a block, so we can't have more grid points than 32*#warps_per_block along the minor dimension (currently always z, I think).

Is it easy to change this?

#12 - 12/04/2018 11:36 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2779.
Uploader: Berk Hess (hess@kth.se)
Change-Id: gromacs~release-2019~If8c126f0a18fc6291f459d1370c4e834cd46d252
Gerrit URL: https://gerrit.gromacs.org/8778
Gerrit received a related patchset ‘1’ for Issue #2779.
Uploader: Berk Hess (hess@kth.se)
Change-Id: gromacs~release-2018~I9908f7742b80552d4ba29dcf707103f4c5a3efd
Gerrit URL: https://gerrit.gromacs.org/8779

Uploader: Berk Hess
- Category set to mdrun
- Status changed from In Progress to Fix uploaded
- Target version set to 2018.5

I uploaded a fix to release-2018 and release-2019 that adds a check for grid size along Z <= 512.
Without changing the complex kernel indexing, we could increase this limit to 2048, which would cover all practical cases. But optimal performance for small and medium setups with CUDA seems indeed to be at 512 threads per block. So ideally we would only use more threads when needed. This is a bit cumbersome in the current code though.

Gerrit received a related patchset ‘1’ for Issue #2779.
Uploader: Berk Hess (hess@kth.se)
Change-Id: gromacs~release-2019~Ic8f7e08a934db58e47a3eccc52e6a8eec9be3870
Gerrit URL: https://gerrit.gromacs.org/8780

Uploader: Berk Hess
- Status changed from Fix uploaded to Resolved

Applied in changeset aa2305c1ade76cc0c2de9b515ab8d68b6cda26b2.

Applied in changeset c15057c7d8537a1c7c85ee4d50bae585d76a5e3e.

Uploader: Paul Bauer
- Status changed from Resolved to Closed

Files

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