The attached system (testosterone in a stacked lipid bilayer system with little water) crashes on step 0 when using OpenCL, but works with CUDA or -pme cpu -nb cpu. I'm attaching tpr and log files.

Associated revisions
Revision 23398921 - 02/26/2020 04:08 PM - Szilárd Pál
Document NVIDIA OpenCL broken on Volta and Turing
Refs #3125
Change-id: ld200c1092b279d45a97b98c6fe1d03c2ff14fb0

History
#1 - 10/09/2019 05:26 PM - Berk Hess
It runs fine for me with OpenCL on Nvidia.

#2 - 10/09/2019 07:32 PM - Magnus Lundborg
It works on my computer at home as well (I cannot get cmake to identify the correct opencl versions on my machine at work regardless of cuda version and proper cuda libraries), but I got the error on the threadripper-gpu01 machine. It's probably some hardware/software problem. But the fact that it compiles and then crashes is a bit worrying.

#3 - 10/10/2019 05:39 PM - Szilárd Páll
Magnus Lundborg wrote:

It works on my computer at home as well (I cannot get cmake to identify the correct opencl versions on my machine at work regardless of cuda version and proper cuda libraries), but I got the error on the threadripper-gpu01 machine. It's probably some hardware/software problem. But the fact that it compiles and then crashes is a bit worrying.

That's likely due to the broken NVIDIA Volta (possibly Turing) support. Please try threadripper-gpu02 (has Pascal GPUs) just to confirm.

#4 - 10/10/2019 05:44 PM - Magnus Lundborg
I didn't know Volta was broken. Is it only OpenCL that's the problem? I'll try threadripper-gpu02 and report (possibly tomorrow). But related to that (I'm trying to understand why FEP PME on GPU fails in OpenCL), do you know if there is a problem with Kepler as well?

#5 - 10/10/2019 06:19 PM - Magnus Lundborg
It worked on threadripper-gpu02. So, should this be closed then?

#6 - 10/11/2019 12:02 AM - Szilárd Páll

- Subject changed from Too many LINCS warnings step 0 when using OpenCL to OpenCL on Volta borken

Magnus Lundborg wrote:

I didn't know Volta was broken. Is it only OpenCL that's the problem? I'll try threadripper-gpu02 and report (possibly tomorrow). But related to that (I'm trying to understand why FEP PME on GPU fails in OpenCL), do you know if there is a problem with Kepler as well?
I know of no issues on Kepler.

Magnus Lundborg wrote:

It worked on threadripper-gpu02. So, should this be closed then?

Perhaps we should give the issue a more descriptive title and keep a record of it. It would be good if NVIDIA looked into it.

#7 - 10/11/2019 09:07 AM - Berk Hess

Perhaps we should give the issue a more descriptive title and keep a record of it. It would be good if NVIDIA looked into it.

I like the "borken" though!

Can we detect the Nvidia architecture in OpenCL? If so, we should disable it, since this is dangerous for the user and sucks up time of developers in testing.

#8 - 10/11/2019 09:14 AM - Magnus Lundborg

Szilárd Páll wrote:

Magnus Lundborg wrote:

I didn't know Volta was broken. Is it only OpenCL that's the problem? I'll try threadripper-gpu02 and report (possibly tomorrow). But related to that (I'm trying to understand why FEP PME on GPU fails in OpenCL), do you know if there is a problem with Kepler as well?

I know of no issues on Kepler.

The FEP with PME on GPU did not work (forces, energies and the virial were wrong - contents of grid[0].d_fractShiftsTable and grid[0].d_gridlineIndicesTable were lost when using two grids) on Kepler (with CUDA 9.2). I'll see if I can can CUDA 10 to work and see if that was the problem. It works on threadripper-gpu02 and seemingly in the Jenkins tests.

So, I agree with Berk's suggestions that we should, if possible, disable OpenCL on architectures that are not proven to work or at least on architectures proven not to work.

#9 - 10/11/2019 09:56 PM - Roland Schulz

Comparing the clinfo output from Volta and Pascal should quickly show whether there is any info you can use.

#10 - 10/12/2019 08:45 PM - Szilárd Páll

Berk Hess wrote:

Perhaps we should give the issue a more descriptive title and keep a record of it. It would be good if NVIDIA looked into it.

I like the "borken" though!

Can we detect the Nvidia architecture in OpenCL?

clinfo does print NVIDIA specific information IIRC, so we can likely detect it.

If so, we should disable it, since this is dangerous for the user and sucks up time of developers in testing.

I agree.

Sorry I ran into the issue before (and IIRC raised the issue with some NVIDIA people), but never filed a redmine or tried to look deeper into it. In hindsight, I should have at least filed an issue and added a note in the user guide's "known issues/limitations" section.

I will certainly not have time before beta2, but at some later point I can try to look into it.

#11 - 10/12/2019 08:47 PM - Szilárd Páll

Here's the relevant clinfo code that we should adopt:

https://github.com/Oblomov/clinfo/blob/master/src/clinfo.c#L1502
CC 7.0 is what we'd blacklist.

#12 - 10/13/2019 11:37 PM - Szilárd Páll
- Subject changed from OpenCL on Volta borken to OpenCL on Volta and Turing borken

Szilárd Páll wrote:

Here's the relevant clinfo code that we should adopt:
https://github.com/Oblomov/clinfo/blob/master/src/clinfo.c#L1502

CC 7.0 is what we'd blacklist.

also CC 7.5

#13 - 10/13/2019 11:46 PM - Magnus Lundborg

Szilárd Páll wrote:

Szilárd Páll wrote:

Here's the relevant clinfo code that we should adopt:
https://github.com/Oblomov/clinfo/blob/master/src/clinfo.c#L1502

CC 7.0 is what we'd blacklist.

also CC 7.5

CC 3.0 is the version that lost the contents of d_fractShiftsTable and d_gridlineIndicesTable when using more than one grid.

#14 - 11/01/2019 03:22 PM - Paul Bauer
- Target version changed from 2020-beta2 to 2020-beta3

bump

#15 - 11/04/2019 11:37 AM - Magnus Lundborg

With the latest version of FEP PME on GPU (https://gerrit.gromacs.org/c/gromacs/+/13382) CC 3.0 works since there is only one copy of d_fractShiftsTable and d_gridlineIndicesTable even if there are two grids. So, it's only CC 7.0 and 7.5 that we need to care about now.

#16 - 12/02/2019 01:13 PM - Paul Bauer
- Target version changed from 2020-beta3 to 2020-rc1

bump

#17 - 12/20/2019 08:20 AM - Paul Bauer
- Target version changed from 2020-rc1 to 2020

what is the status here? This needs fixing for 2020!

#18 - 12/20/2019 09:21 AM - Magnus Lundborg

No change I think. I guess we still need to blacklist NVIDIA CC 7.0 and 7.5.

#19 - 12/27/2019 04:19 PM - Paul Bauer
- Target version changed from 2020 to 2020.1

No one has worked on this

#20 - 01/27/2020 04:43 PM - Szilárd Páll

Jon, are you still planning to look into this? If not, I propose that we announce Volta and later as broken in the "known issue" section and close this issue.

#21 - 01/27/2020 04:48 PM - Jonathan Vincent
Szilárd Páll wrote:

Jon, are you still planning to look into this? If not, I propose that we announce Volta and later as broken in the "known issue" section and close this issue.

No this it not on my things to look at right now.

#22 - 02/26/2020 02:46 PM - Szilárd Páll
Jonathan Vincent wrote:

Szilárd Páll wrote:

Jon, are you still planning to look into this? If not, I propose that we announce Volta and later as broken in the "known issue" section and close this issue.

No this it not on my things to look at right now.

OK, we will mark OpenCL broken on Volta and later in the release notes.

#23 - 02/26/2020 04:24 PM - Szilárd Páll

- Status changed from New to Resolved

"Resolving" by documenting the deficiency of the NVIDIA compilers.

#24 - 02/27/2020 11:01 AM - Paul Bauer

- Category deleted (mdrun)
- Target version changed from 2020.1 to 2020.2
- Difficulty deleted (uncategorized)

ok, will bump issue itself

Files

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