

GROMACS - Task #2515

Feature # 2054 (Accepted): PME on GPU

Task # 2453 (Resolved): PME OpenCL porting effort

clFFT RocM compatibility problem

05/23/2018 11:47 AM - Aleksei lupinov

Status:	Closed	
Priority:	High	
Assignee:	Szilárd Páll	
Category:	core library	
Target version:	2019	
Difficulty:	uncategorized	
Description		
<p>PME with OpenCL uses 3D FFT as implemented in the external clFFT library. As of May 2018, the current RocM stack (1.8.0) is known to compile clFFT badly: https://github.com/clMathLibraries/clFFT/issues/218 The PME OpenCL kernels do work with RocM (Ewald unit tests pass), but PmeTest in mdrun tests fails, as some iterations use -pmefft gpu/auto. (Additionally, clFFT kernel compilation with rocm even outputs a few warnings during the execution). clFFT is known to work at least with recent AMDGPU-PRO drivers 17.50 and 18.10, with all supported CUDA OpenCL versions, and with whatever runtime the "old" AMD build config has (fglrx 15.something?). With this in mind, if situation doesn't improve before release 2019 (by improvements in RocM OpenCL runtime, clFFT, or even the unlikely alternative path of using rocFFT library: https://github.com/RadeonOpenCompute/ROCm-OpenCL-Runtime/issues/53), an OpenCL compiler version check should be implemented in our device sanity checks. I assume one can detect RocM compiler, whether in host or device code, and disallow PmeRunMode::GPU accordingly (still allowing PmeRunMode::Mixed).</p>		
Related issues:		
Related to GROMACS - Task #2500: detect and allow linking external clFFT, or ...		Closed
Related to GROMACS - Bug #2420: OpenCL implementation not doing device sanity...		Closed

Associated revisions

Revision a41344a0 - 05/31/2018 01:13 PM - Aleksei lupinov

Added the bundled clFFT into OpenCL builds

Used an object library, since we have no need of a real library, to have or to install, whether shared or static. Checked for the availability of dynamic loading, and made it available portably to libgromacs.

Clfft initialization class is added and used in mdrunner to initialize/tear down clFFT library resources in a thread-safe manner, and only on ranks that require such setup. Noted TODOs for future work.

Noted a useful style for explicit listing of source files.

Refs #2500
Refs #2515
Refs #2535

Change-Id: I62d7d66f65e147bde17929ccc30abad36e2373c6

History

#1 - 05/23/2018 11:47 AM - Aleksei lupinov

- Related to Task #2500: detect and allow linking external clFFT, or no clFFT added

#2 - 05/23/2018 11:47 AM - Aleksei lupinov

- Related to Bug #2420: OpenCL implementation not doing device sanity checks added

#3 - 05/23/2018 12:32 PM - Gerrit Code Review Bot

Gerrit received a related patchset '9' for Issue [#2515](#).
Uploader: Aleksei lupinov (a.yupinov@gmail.com)
Change-Id: gromacs~master~162d7d66f65e147bde17929ccc30abad36e2373c6
Gerrit URL: <https://gerrit.gromacs.org/7837>

#4 - 09/20/2018 05:53 PM - Szilárd Páll

- Status changed from New to In Progress
- Assignee set to Szilárd Páll

Update: our reports and push have paid back, ROCm 1.9 compiles and all unit clFFT tests pass that we care about (only four DP tests fail, but we have no DP GPU support, so that's not an issue). GROMACS unit- and regressiontests pass too.

I'm in the process of verifying that this Fiji/Baffin and will update this redmine accordingly.

#5 - 09/21/2018 03:28 PM - Szilárd Páll

Looks like only double precision FFT kernel tests fail on Fiji too, so I'm cautiously going to state: ROCm + clFFT is likely safe to use on these AMD architectures.

Issues filed against ROCm-OpenCL-Driver on github:
<https://github.com/RadeonOpenCompute/ROCm-OpenCL-Driver/issues/72>

Will keep testing future ROCm releases; for reference, this is the procedure:

```
https://github.com/clMathLibraries/clFFT.git
mkdir build_clFFT
# set up fftw for cmake detection
cmake ../clFFT/src -DBUILD_TEST=ON && make &&\
  LD_LIBRARY_PATH=$PWD/library staging/Test 2>&1 | tee test-${HOSTNAME}.log
```

#6 - 09/21/2018 03:28 PM - Szilárd Páll

- Status changed from In Progress to Resolved

#7 - 10/12/2018 02:34 PM - Mark Abraham

- Status changed from Resolved to Closed