detect and allow linking external clFFT, or no clFFT

05/09/2018 04:09 PM - Aleksei Iupinov

Status: Closed
Priority: Normal
Assignee: Mark Abraham
Category: build system
Target version: 2019.1
Difficulty: simple

Description
When [https://gerrit.gromacs.org/7837](https://gerrit.gromacs.org/7837) is getting merged, Gromacs OpenCL builds start always linking to the bundled clFFT. We should be able and prefer to link to the system clFFT by default though. That might also later raise questions like what is the minimum version of clFFT required.

Tasks:
- detect external clFFT (CMake script available here: [https://github.com/clMathLibraries/clFFT/blob/master/src/FindclFFT.cmake](https://github.com/clMathLibraries/clFFT/blob/master/src/FindclFFT.cmake), as well as in Gromacs master: src/external/clFFT/src/FindclFFT.cmake)
- implement minimum version req'd
- implement clFFT version reporting in the -version header

Related issues:
- Related to GROMACS - Bug #2208: cuFFT linking
- Related to GROMACS - Task #2515: clFFT RocM compatibility problem
- Related to GROMACS - Task #2697: improve FFT library flavor/version reporting

Associated revisions
Revision a41344a0 - 05/31/2018 01:13 PM - Aleksei Iupinov
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

Revision 0f193a44 - 05/31/2018 03:58 PM - Aleksei Iupinov
Prefer linking to system clFFT rather than bundled one

Wrote a new find_package module that works in more modern ways. Updated install guide.

Currently there is no support for checking the clFFT version, which is unlikely to matter until they make the 2.14 release.

 Fixes #2500
Revision 887b2c2b - 06/25/2018 10:35 AM - Mark Abraham
Test both internal and external clFFT build in Jenkins

Chose to test external linking of clFFT in pre-submit because that compiles several minutes faster. Chose to test internal linking in post-submit because rapid throughput is less important there.

The clfft label is used to understand that external linking of clFFT is required for this configuration, much like the fftw, fftpack and mkl labels, however there is no need to explicitly tie the clfft label to the gpu or opencl ones.

Refs #2500

Change-Id: I455f7f7713310153f2f5197bb32660332649c

Revision 8459e202 - 01/14/2019 10:37 PM - Mark Abraham
Improve portability of PME on GPU code

Refs #2500

Change-Id: ld1069b0ad60a9a18b4882ec56364b073c871ebe

Revision 89c9d32f - 01/18/2019 01:51 PM - Mark Abraham
Improve nvcc error reporting

When nvcc fails, tell the user about both standard error and standard output. The former code was broken if _cuda_test_err would be undefined, and reported by a user (see the link at Redmine #2500).

Change-Id: ld16d2ff1bd1033cd23e82ed87b79409ea8d341131

Revision 98165006 - 01/18/2019 06:28 PM - Mark Abraham
Disabled internal clFFT when using MSVC with OpenCL

We require clFFT for OpenCL support, and MSVC 2017. But clFFT only supports MSVC 2010, and a user has reported that that clFFT does not compile. As we have not provided for clFFT support to be disabled at configure time (nor taught mdrun that it might not be able to run PME on an OpenCL GPU in this case), it is simplest to withdraw support for this corner case until clFFT support for modern MSVC is available.

Fixes #2500

Change-Id: I736501234cd51bc1cee5d8a71cb1f343dd100

History

#1 - 05/09/2018 04:09 PM - Aleksei lupinov
- Description updated

#2 - 05/09/2018 04:11 PM - Aleksei lupinov
- Private changed from Yes to No

#3 - 05/09/2018 04:11 PM - Aleksei lupinov
- Related to Bug #2208: cuFFT linking added

#4 - 05/11/2018 06:17 PM - Szilárd Páll
This isn't really about dynamic linking, but more about external clFFT (whether linked statically or dynamically), right?

#5 - 05/16/2018 04:24 PM - Szilárd Páll
- Subject changed from clFFT dynamic linking to detect and allow linking external clFFT
- Description updated
Updated title to better reflect the scope.

#6 - 05/16/2018 04:27 PM - Szilárd Páll
- Target version changed from future to 2019
- Difficulty simple added
- Difficulty deleted (uncategorized)

Given that no opt-out bundling may be a showstopper for distros, I'll target this for 2019.

We should also evaluate what are the needs on the Intel side when the PME port lands and gets tested.

#7 - 05/16/2018 04:59 PM - Aleksei lupinov
- Description updated

Yes, that is correct, thanks

#8 - 05/23/2018 11:47 AM - Aleksei lupinov
- Related to Task #2515: clFFT RocM compatibility problem added

#9 - 05/23/2018 12:32 PM - Gerrit Code Review Bot
Gerrit received a related patchset '9' for Issue #2500.
Uploader: Aleksei lupinov (a.yupinov@gmail.com)
Change-Id: gromacs~master~I62d7d665e147bde17929ccc30abad36e2373c6
Gerrit URL: https://gerrit.gromacs.org/7837

#10 - 05/23/2018 04:26 PM - Mark Abraham
The current icc-18 opencl config takes 4.5 minutes per verify to compile the bundled clFFT, so being able to use an external library would be a useful improvement in throughput times. I am not sure what the best approach should be to do that.

#11 - 05/23/2018 04:43 PM - Aleksei lupinov
Wow, OK.

Once linking to system clFFT as a default is implemented, provide system clFFT in presubmit and none in post-submit? No explicit changes in releng required then, even (explicitness might be better, of course). It's the libclfft-dev package with dependencies in Ubuntu 16.04, likely non-default one.

#12 - 05/23/2018 06:15 PM - Aleksei lupinov
https://packages.ubuntu.com/search?suite=default&section=all&arch=any&keywords=clfft&searchon=names

clFFT not packaged for Ubuntu 14, only 16+...

#13 - 05/23/2018 06:46 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2500.
Uploader: Aleksei lupinov (a.yupinov@gmail.com)
Change-Id: gromacs~master~If43ee95d3066823f2c57a49a23fd6dd027dbcc94
Gerrit URL: https://gerrit.gromacs.org/7939

#14 - 05/28/2018 09:51 PM - Mark Abraham
clfft from AMD has a hard dependency on dynamic loading, which I have now incorporated into the build of the bundled clfft.

#15 - 05/29/2018 12:05 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2500.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~master~I455f7f7713310153f2fdb5197bb32660332649c
Gerrit URL: https://gerrit.gromacs.org/7959

#16 - 05/29/2018 05:47 PM - Roland Schulz
But the dynamic loading dependency is only for timing not for functionality, right?

#17 - 05/29/2018 06:09 PM - Aleksei lupinov
Supposedly yes. I failed to find proper documentation on what this statTimer library does.
This call must succeed: [https://github.com/clMathLibraries/clFFT/blob/master/src/library/lifetime.cpp#L51](https://github.com/clMathLibraries/clFFT/blob/master/src/library/lifetime.cpp#L51) and its implementation requires that dlopen() can be called.

- Status changed from New to Resolved

Applied in changeset 0f193a44be781828d18b76aae834d4eb55a6640e.

- Status changed from Resolved to Blocked, need info

implement clFFT version reporting in the -version header

AFAICT, the above is not implemented yet. Could move it to a separate task as we likely want a more unified GPU FFT version reporting.

- Related to Task #2697: improve FFT library flavor/version reporting added

- Status changed from Blocked, need info to Resolved

Szilárd Páll wrote:

implement clFFT version reporting in the -version header

AFAICT, the above is not implemented yet. Could move it to a separate task as we likely want a more unified GPU FFT version reporting.

Created a more general issue related to FFT library version reporting. AFAICT we can close this.

- Status changed from Resolved to Closed

- Subject changed from detect and allow linking external clFFT to detect and allow linking external clFFT, or no clFFT

- Status changed from Closed to Accepted

- Assignee set to Mark Abraham

- Target version changed from 2019 to 2019.1

If our internal clfft doesn't build on a platform, and there's none found on the system, then that blocks the OpenCL build. Users should be able to get OpenCL support for NB even if there is no way to build clfft.

This does stop a Windows build supporting OpenCL, but the principle is more important than the fact of such a Windows version not working.


Gerrit received a related patchset '1' for Issue #2500.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~release-2019~Id16d2ff1bd1033cd23e82687b79409ea8d841131

Gerrit received a related patchset '1' for Issue #2500.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~release-2019~Id1069b0ad60a9af18b4882ec56364b073c871ebe
Gerrit URL: [https://gerrit.gromacs.org/8948](https://gerrit.gromacs.org/8948)
#28 - 01/10/2019 11:53 AM - Gerrit Code Review Bot
Gerrit received a related patchset ‘1’ for Issue #2500.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~release-2019~I736501234d51bc1cee5d8a71cb1fb343ddd100
Gerrit URL: https://gerrit.gromacs.org/8952

#29 - 01/11/2019 01:32 PM - Mark Abraham
- Status changed from Accepted to Fix uploaded

#30 - 01/18/2019 06:45 PM - Mark Abraham
- Status changed from Fix uploaded to Resolved

Applied in changeset 98165006a4c002b9b14273b2cae994c149e6b439.

#31 - 01/28/2019 11:42 AM - Mark Abraham
- Status changed from Resolved to Closed