

## GROMACS - Task #2500

Feature # 2054 (Accepted): PME on GPU

Task # 2453 (Resolved): PME OpenCL porting effort

### detect and allow linking external cFFFT, or no cFFFT

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

<b>Status:</b>	Closed
<b>Priority:</b>	Normal
<b>Assignee:</b>	Mark Abraham
<b>Category:</b>	build system
<b>Target version:</b>	2019.1
<b>Difficulty:</b>	simple
<b>Description</b>	
<p>When <a href="https://gerrit.gromacs.org/7837">https://gerrit.gromacs.org/7837</a> is getting merged, Gromacs OpenCL builds start always linking to the bundled cFFFT. We should be able and prefer to link to the system cFFFT by default though. That might also later raise questions like what is the minimum version of cFFFT required.</p>	
Tasks:	
<ul style="list-style-type: none"><li>• detect external cFFFT (CMake script available here: <a href="https://github.com/clMathLibraries/cFFFT/blob/master/src/FindcFFFT.cmake">https://github.com/clMathLibraries/cFFFT/blob/master/src/FindcFFFT.cmake</a>, as well as in Gromacs master: src/external/cFFFT/src/FindcFFFT.cmake)</li><li>• implement minimum version req'd</li><li>• implement cFFFT version reporting in the -version header</li></ul>	
<b>Related issues:</b>	
Related to GROMACS - Bug #2208: cuFFT linking	<b>New</b>
Related to GROMACS - Task #2515: cFFFT RocM compatibility problem	<b>Closed</b>
Related to GROMACS - Task #2697: improve FFT library flavor/version reporting	<b>New</b>

### Associated revisions

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

Added the bundled cFFFT 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 cFFFT 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 lupinov

Prefer linking to system cFFFT 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 cFFFT version, which is unlikely to matter until they make the 2.14 release.

Fixes #2500

Change-Id: I43ee95d3066823f2c57a49a23fd6dd027dbcc94

**Revision 887b2c2b - 06/25/2018 10:35 AM - Mark Abraham**

Test both internal and external cFFT build in Jenkins

Chose to test external linking of cFFT 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 cFFT 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: I455f7f713310153f2fdbf5197bb32660332649c

**Revision 8459e202 - 01/14/2019 10:37 PM - Mark Abraham**

Improve portability of PME on GPU code

Refs #2500

Change-Id: Id1069b0ad60a9af18b4882ec56364b073c871ebe

**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: Id16d2ff1bd1033cd23e82687b79409ea8d841131

**Revision 98165006 - 01/18/2019 06:28 PM - Mark Abraham**

Disabled internal cFFT when using MSVC with OpenCL

We require cFFT for OpenCL support, and MSVC 2017. But cFFT only supports MSVC 2010, and a user has reported that that cFFT does not compile. As we have not provided for cFFT 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 cFFT support for modern MSVC is available.

Fixes #2500

Change-Id: I736501234cfd51bc1cee5d8a71cb1fb343ddd100

## History

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**#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 cFFT (whether linked statically or dynamically), right?

**#5 - 05/16/2018 04:24 PM - Szilárd Páll**

- *Subject changed from cFFT dynamic linking to detect and allow linking external cFFT*

- *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: cIFFT 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](mailto:a.yupinov@gmail.com))  
Change-Id: gromacs~master~162d7d66f65e147bde17929ccc30abad36e2373c6  
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 cIFFT, 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 cIFFT as a default is implemented, provide system cIFFT 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>

cIFFT 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](mailto:a.yupinov@gmail.com))  
Change-Id: gromacs~master~1f43ee95d3066823f2c57a49a23fd6dd027dbcc94  
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](mailto:mark.j.abraham@gmail.com))  
Change-Id: gromacs~master~1455f7f7713310153f2fdbf5197bb32660332649c  
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.

**#18 - 05/29/2018 11:11 PM - Mark Abraham**

This call must succeed: <https://github.com/ciMathLibraries/ciFFT/blob/master/src/library/lifetime.cpp#L51> and its implementation requires that `dlopen()` can be called.

**#19 - 05/31/2018 04:00 PM - Aleksei lupinov**

- Status changed from *New* to *Resolved*

Applied in changeset [0f193a44be781828d18b76aae834d4eb55a6640e](https://github.com/ciMathLibraries/ciFFT/commit/0f193a44be781828d18b76aae834d4eb55a6640e).

**#20 - 07/30/2018 12:18 PM - Szilárd Páll**

- Status changed from *Resolved* to *Blocked, need info*

implement `ciFFT` 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.

**#21 - 10/15/2018 12:35 PM - Szilárd Páll**

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

**#22 - 10/15/2018 12:36 PM - Szilárd Páll**

- Status changed from *Blocked, need info* to *Resolved*

Szilárd Páll wrote:

implement `ciFFT` 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.

**#23 - 10/15/2018 05:14 PM - Mark Abraham**

- Status changed from *Resolved* to *Closed*

**#24 - 01/09/2019 05:28 PM - Mark Abraham**

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

- 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.

**#25 - 01/10/2019 09:26 AM - Mark Abraham**

Report from Mirco Wahab at [https://mailman-1.sys.kth.se/pipermail/gromacs.org\\_gmx-users/2019-January/123689.html](https://mailman-1.sys.kth.se/pipermail/gromacs.org_gmx-users/2019-January/123689.html)

**#26 - 01/10/2019 09:57 AM - Gerrit Code Review Bot**

Gerrit received a related patchset '1' for Issue [#2500](#).

Uploader: Mark Abraham ([mark.j.abraham@gmail.com](mailto:mark.j.abraham@gmail.com))

Change-Id: `gromacs~release-2019~Id1069b0ad60a9af18b4882ec56364b073c871ebe`

Gerrit URL: <https://gerrit.gromacs.org/8948>

**#27 - 01/10/2019 10:12 AM - Gerrit Code Review Bot**

Gerrit received a related patchset '1' for Issue [#2500](#).

Uploader: Mark Abraham ([mark.j.abraham@gmail.com](mailto:mark.j.abraham@gmail.com))

Change-Id: `gromacs~release-2019~Id16d2ff1bd1033cd23e82687b79409ea8d841131`

Gerrit URL: <https://gerrit.gromacs.org/8949>

**#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](mailto:mark.j.abraham@gmail.com))

Change-Id: gromacs~release-2019~l736501234cf51bc1cee5d8a71cb1fb343ddd100

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