GROMACS - Task #2535

Feature # 2054 (Accepted): PME on GPU

Task # 2453 (Resolved): PME OpenCL porting effort

consider compiling opencl fft kernels once

05/31/2018 12:04 PM - Mark Abraham

Status:	New	
Priority:	Normal	
Assignee:		
Category:	core library	
Target version:		
Difficulty:	hard	

Description

In https://gerrit.gromacs.org/#/c/7837/, TODOs were noted that we should consider

- lazy pre-compilation of FFT kernels for PME running on OpenCL
- thread-safe RAII-style management of (at least) the underlying clfft library setup and tear down

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 f8443e2b - 09/02/2019 11:44 PM - Mark Abraham

Move initialization of clFFT

Gave ClfftInitializer the responsibility for mutual exclusion, which means the initialization is now convenient to do alongside other PME-on-GPU initialization tasks. This simplifies the code.

Removed mention of lazy initialization, which was not implemented at all.

Refs #2535

Change-Id: I429767b059ddc3b4f16f2f4a8830b54ed1f49fab

History

#1 - 05/31/2018 01:09 PM - Mark Abraham

The compilation of such kernels do depend on the FFT grid size, which may or may not be known until after the PME module is set up (because a user may have used fourierspacing), and might also be subject to auto-tuning. Not needing to re-compile if auto-tuning returns to a previous grid size would be an advantage, but that's a different consideration from pre-compilation.

#2 - 05/31/2018 01:33 PM - Aleksei Iupinov

clFFT clearly has some mentions of caching in its code. I would think that properly storing all grid-related data of PME (such as FFT plan instances) in a map, using grid dimensions as a key, instead of deleting all the old stuff on each reinit, would already achieve this. One would still have to watch out for resource exhaustion, of course, and try to delete old stuff if really needed.