

## GROMACS - Task #2522

Feature # 2054 (Accepted): PME on GPU

Task # 2453 (Resolved): PME OpenCL porting effort

### OpenCL context duplication

05/25/2018 12:38 PM - Aleksei lupinov

<b>Status:</b>	Resolved
<b>Priority:</b>	Normal
<b>Assignee:</b>	
<b>Category:</b>	
<b>Target version:</b>	future
<b>Difficulty:</b>	uncategorized
<b>Description</b>	
<p>Current PME OpenCL code creates its own <code>cl_context</code> in <code>PmeGpuProgramImpl</code>, based on input <code>gmx_device_info_t*</code>. NB with OpenCL also creates its own OpenCL context. OpenCL contexts can correspond to multiple devices: <a href="https://www.khronos.org/registry/OpenCL/sdk/1.2/docs/man/xhtml/classDiagram.html">https://www.khronos.org/registry/OpenCL/sdk/1.2/docs/man/xhtml/classDiagram.html</a></p> <p>NB and PME not sharing same <code>cl_context</code> on the rank can even be detrimental - it's possible they would not have access to each other's <code>cl_mem</code>'s.</p> <p><code>cl_context</code> management should be taken away from <code>PmeGpuProgramImpl/nbnxn_gpu_create_context()</code> and put into a new class, which would get constructed from a set of <code>gmx_device_info_t*</code>.</p> <p>The instance of this class should get created based on the GPU task assignment.</p> <p>PME/NB still need to store references to this object to get the <code>cl_context/gmx_device_info_t*</code> out of it.</p>	
<b>Related issues:</b>	
Related to GROMACS - Feature #3115: Device stream manager	<b>New</b>

#### Associated revisions

##### Revision b2a95c76 - 05/28/2018 03:11 PM - Aleksei lupinov

Support persistent device context-derived data in PME tests

PME OpenCL will need to not recompile kernels for running each unit test. With this in mind, a persistent `PmeGpuProgram` class is tasked with GPU kernel setup, and passed around, using a typedef. The purpose of the class is to hold the PME program data that should only be set up once and live forever for the given device context. `PmeGpuProgramImpl` structure is now tasked with managing function pointers to the CUDA kernels' instances, and will later be tasked with compiling OpenCL kernels.

Refs #2453, #2522

Change-Id: I85a01bfc92ec3a108825414b14e2be3731433c9a

##### Revision 6975bfd - 03/11/2020 03:59 PM - Artem Zhmurov

Take over management of OpenCL context from PME and NBNXM

This patch set creates the `DeviceContext` in runner and passes it to the consumers (PME and NBNXM). This removes unnecessary management code duplication, makes the device buffers in two modules compatible.

Fixes #2522

Fixes #3315

Refs #3311

Change-Id: I10358cfaced5b5c7dbdddf95679c9a9703f3a2c0

#### History

##### #1 - 05/25/2018 01:51 PM - Aleksei lupinov

- Description updated

##### #2 - 05/28/2018 12:16 PM - Aleksei lupinov

- Description updated

**#3 - 05/28/2018 03:13 PM - Gerrit Code Review Bot**

Gerrit received a related patchset '19' for Issue [#2522](#).  
Uploader: Mark Abraham ([mark.j.abraham@gmail.com](mailto:mark.j.abraham@gmail.com))  
Change-Id: gromacs~master~l85a01bfc92ec3a108825414b14e2be3731433c9a  
Gerrit URL: <https://gerrit.gromacs.org/7818>

**#4 - 10/30/2018 12:07 PM - Mark Abraham**

- Target version changed from 2019 to 2020

**#5 - 10/03/2019 10:47 PM - Szilárd Páll**

- Related to Feature #3115: Device stream manager added

**#6 - 12/20/2019 12:19 PM - Paul Bauer**

- Target version changed from 2020 to future

**#7 - 03/11/2020 04:15 PM - Artem Zhmurov**

- Status changed from New to Resolved

Applied in changeset [6975fbfd22030a08bbe076151a3de69894a4de2f](#).