

## GROMACS - Bug #2420

### OpenCL implementation not doing device sanity checks

02/23/2018 06:29 PM - Aleksei lupinov

|   |                                  |
|---|----------------------------------|
| <b>Status:</b> Closed   |                                  |
| <b>Priority:</b> Normal   |                                  |
| <b>Assignee:</b>  |                                  |
| <b>Category:</b> core library   |                                  |
| <b>Target version:</b> 2019   |                                  |
| <b>Affected version - extra info:</b> probably all versions before that as well   | <b>Difficulty:</b> uncategorized |
| <b>Affected version:</b> 2018   |                                  |
| <b>Description</b><br>is_gmx_supported_gpu_id() calls do_sanity_checks() in CUDA implementation, even launching a dummy GPU kernel, but does nothing of the kind in OpenCL, only looking at device vendor and OS version.<br><br>Therefore, disabling devices with "sudo nvidia-smi -c 2" causes OpenCL mdrun to fail with CL_DEVICE_NOT_AVAILABLE on context creation. |                                  |
| <b>Related issues:</b><br>Related to GROMACS - Bug #2405: improve gpu_utils-test <b>Closed</b><br>Related to GROMACS - Task #2515: cIFFT RocM compatibility problem <b>Closed</b>   |                                  |

#### Associated revisions

##### Revision 383240b1 - 12/22/2018 02:40 AM - Aleksei lupinov

Add a sanity check for OpenCL devices

Introduced some type traits to support RAII types for OpenCL handles, so that we can safely free resources when responding to OpenCL API error codes, and do so with usefully descriptive error messages.

The new infrastructure is used to implement a check that an OpenCL GPU can execute a dummy kernel.

Fixed some broken docs, and updated some function naming for new style.

Fixes #2420

Change-Id: Id99786d24f77b4b56669b5cfd3a39aa0116cfca

#### History

##### #1 - 02/23/2018 06:29 PM - Aleksei lupinov

- Related to Bug #2405: improve gpu\_utils-test added

##### #2 - 02/27/2018 02:18 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2420](#).

Uploader: Aleksei lupinov ([a.yupinov@gmail.com](mailto:a.yupinov@gmail.com))

Change-Id: gromacs~master~17f234e67787bc1815973027621abdc162501d6fe

Gerrit URL: <https://gerrit.gromacs.org/7626>

##### #3 - 04/24/2018 09:29 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2420](#).

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

Change-Id: gromacs~master~Id99786d24f77b4b56669b5cfd3a39aa0116cfca

Gerrit URL: <https://gerrit.gromacs.org/7786>

##### #4 - 05/23/2018 11:47 AM - Aleksei lupinov

- Related to Task #2515: cIFFT RocM compatibility problem added

**#5 - 06/12/2018 10:48 PM - Mark Abraham**

- Target version changed from 2018.2 to 2018.3

The two fixes waiting in gerrit for follow up are on master branch, so I don't know offhand where we might fix this. It might not be important enough for release-2018.

**#6 - 07/30/2018 02:40 PM - Szilárd Páll**

- Target version changed from 2018.3 to 2019

Mark Abraham wrote:

The two fixes waiting in gerrit for follow up are on master branch, so I don't know offhand where we might fix this. It might not be important enough for release-2018.

Agreed, if we find an easy-to-backport solution we can consider, but otherwise, it's only an improvement in terms of mdrun robustness that doesn't greatly affect its functionality.

**#7 - 12/17/2018 07:53 PM - Gerrit Code Review Bot**

Gerrit received a related patchset '1' for Issue [#2420](#).

Uploader: Szilárd Páll ([pall.szilard@gmail.com](mailto:pall.szilard@gmail.com))

Change-Id: gromacs~release-2019~Id99786d24f77b4b56669b5cfd3a39aa0116cfca

Gerrit URL: <https://gerrit.gromacs.org/8839>

**#8 - 12/17/2018 10:47 PM - Szilárd Páll**

- Status changed from New to In Progress

**#9 - 12/22/2018 02:45 AM - Aleksei lupinov**

- Status changed from In Progress to Resolved

Applied in changeset [383240b164d6a53162fad4f3a2da914328f5f94b](#).

**#10 - 12/22/2018 12:59 PM - Paul Bauer**

- Status changed from Resolved to Closed