

GROMACS - Task #2475

make OpenCL 1st class-citizen in the build system

04/10/2018 03:55 PM - Szilárd Páll

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|------------------------|---------------|
| Status: | New |
| Priority: | Normal |
| Assignee: | |
| Category: | mdrun |
| Target version: | 2020 |
| Difficulty: | uncategorized |

Description

At the moment the implementation of the GPU support in the build system is rather NVIDIA/CUDA centric and would require a few tweaks to make OpenCL a first-class citizen -- in particular as we're aiming for i) feature parity ii) OpenCL for backward-compatibility with older hardware.

TODOs

- make GMX_GPU multi-value instead of requiring an additional option to switch OpenCL on
- tweak detection so GMX_GPU_AUTO and related code (see gmxBuildGPU.cmake) is not NVIDIA-centric
- change recommendation message gmxBuildGPU.cmake that recommends "native GPU acceleration on NVIDIA hardware" with CUDA.

History

#1 - 04/10/2018 04:03 PM - Mark Abraham

Sounds good, but we should finish dealing with <https://gerrit.gromacs.org/#/c/5586/> first, please.

#2 - 10/30/2018 12:01 PM - Mark Abraham

- Target version changed from 2019 to 2020