

## GROMACS - Task #2475

### make OpenCL 1st class-citizen in the build system

04/10/2018 03:55 PM - Szilárd Páll

<b>Status:</b>	New
<b>Priority:</b>	Normal
<b>Assignee:</b>	
<b>Category:</b>	mdrun
<b>Target version:</b>	2021
<b>Difficulty:</b>	uncategorized
<b>Description</b>	
<p>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.</p>	
<b>TODOs</b>	
<ul style="list-style-type: none"><li>• make GMX_GPU multi-value instead of requiring an additional option to switch OpenCL on</li><li>• tweak detection so GMX_GPU_AUTO and related code (see gmxManageGPU.cmake) is not NVIDIA-centric</li><li>• change recommendation message gmxManageGPU.cmake that recommends "native GPU acceleration on NVIDIA hardware" with CUDA.</li></ul>	

#### History

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**#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

**#3 - 12/20/2019 12:14 PM - Paul Bauer**

- Target version changed from 2020 to 2021