

GROMACS - Bug #3127

mdrun-mpi-test -ntmpi 2 runs out of memory with OpenCL on Nvidia

10/09/2019 05:33 PM - Berk Hess

Status: New	
Priority: Normal	
Assignee:	
Category:	
Target version:	
Affected version - extra info:	Difficulty: uncategorized
Affected version: 2020-beta1	
Description	
A debug build with opencl on Nvidia hardware always has mdrun-mpi-test run out of memory when using 2 MPI ranks:	
Program: mdrun-mpi-test, version 2020-beta1-dev-20191009-000599bc12	
Source file: src/gromacs/nbnxm/opencl/nbnxm_ocl_data_mgmt.cpp (line 537)	
MPI rank: 0 (out of 2)	
Fatal error:	
On rank 0 failed to create context for GPU #GeForce GTX 1070:	
OpenCL error -6: CL_OUT_OF_HOST_MEMORY	