

GROMACS - Bug #1779

OpenCL MD not stable maybe because of Parrinello-Rahman

07/15/2015 03:48 PM - Carlo Camilloni

Status: Closed	
Priority: Normal	
Assignee:	
Category: mdrun	
Target version: 5.1	
Affected version - extra info:	Difficulty: uncategorized
Affected version: 5.1-rc1	
Description	
<p>A simulation with pressure coupling is unstable (lincs warning after ~ 100 steps) when using AMD GPU with OpenCL while it is stable without using GPU (-nb cpu) and is stable as well without pressure coupling and using GPU</p> <p>compiled on os/x with clang-600.0.57, open-mpi 1.6.5 run as</p> <pre>gmx_mpi mdrun -s topol-nvt-nogen.tpr -nsteps 3000 -v</pre> <p>GROMACS version: VERSION 5.1-rc1 Precision: single Memory model: 64 bit MPI library: MPI OpenMP support: disabled GPU support: enabled OpenCL support: enabled invsqrt routine: gmx_software_invsqrt(x) SIMD instructions: AVX_256 FFT library: fftw-3.3.4-sse2 RDTSCP usage: enabled C++11 compilation: disabled TNG support: enabled Tracing support: disabled Built on: Tue 7 Jul 2015 17:11:31 BST Built by: carlo Build OS/arch: Darwin 13.4.0 x86_64 Build CPU vendor: GenuineIntel Build CPU brand: Intel(R) Xeon(R) CPU E5-1650 v2 @ 3.50GHz Build CPU family: 6 Model: 62 Stepping: 4 Build CPU features: aes apic avx clfsb cmov cx8 cx16 f16c htt lahf_lm mmx msr nonstop_tsc pcid pclmuldq pdcm pdpe1gb popcnt pse rdrnd rdtscp sse2 sse3 sse4.1 sse4.2 ssse3 tdt x2apic C compiler: /Applications/Xcode.app/Contents/Developer/Toolchains/XcodeDefault.xctoolchain/usr/bin/cc Clang 6.0.0.6000057 C compiler flags: -mavx -Wall -Wno-unused -Wunused-value -Wunused-parameter -Wno-unknown-pragmas -O3 -DNDEBUG C++ compiler: /Applications/Xcode.app/Contents/Developer/Toolchains/XcodeDefault.xctoolchain/usr/bin/c++ Clang 6.0.0.6000057 C++ compiler flags: -mavx -Wextra -Wno-missing-field-initializers -Wpointer-arith -Wall -Wno-unused-function -Wno-unknown-pragmas -O3 -DNDEBUG Boost version: 1.57.0 (external) OpenCL include dir: /System/Library/Frameworks/OpenCL.framework OpenCL library: /System/Library/Frameworks/OPENCL.framework OpenCL version: 1.2</p>	
History	
#1 - 07/15/2015 05:48 PM - Mark Abraham	
Thanks. What GPU was this?	
#2 - 07/15/2015 07:01 PM - Carlo Camilloni	

it is an

AMD Radeon HD - FirePro D500

#3 - 07/28/2015 12:26 PM - Erik Lindahl

- Status changed from New to Resolved

Unfortunately this is not a Gromacs bug, but bad drivers or compilers in OS X. The only way you can get it working is to upgrade to OS X 10.10.4, or possibly 10.10.3.

#4 - 08/15/2015 07:21 PM - Erik Lindahl

- Status changed from Resolved to Closed

Gromacs-5.1 will not allow OpenCL on AMD devices until OS X 10.10.4.

#5 - 08/16/2015 11:53 AM - Mark Abraham

- Target version set to 5.1

Files

topol-npt-nogen.tpr	851 KB	07/15/2015	Carlo Camilloni
topol-nvt-nogen.tpr	851 KB	07/15/2015	Carlo Camilloni