

GROMACS - Bug #3101

detect compilation failed

09/20/2019 05:38 PM - Stefano Guglielmo

Status: Blocked, need info	
Priority: Normal	
Assignee: Erik Lindahl	
Category: build system	
Target version:	
Affected version - extra info:	Difficulty: uncategorized
Affected version: 2019.2	

Description

SIMD detection failed upon compiling Gromacs 2019.2 on a workstation equipped with amd threadripper 2990wx cpu.
Cmake invocation was:
-DGMX_BUILD_OWN_FFTW=ON -DREGRESSIONTEST_DOWNLOAD=ON -DGMX_SIMD=AVX2_256 -DGMX_GPU=ON.
In attachment relevant CMake files.

History

#1 - 09/23/2019 07:00 PM - Szilárd Páll

- Category set to build system

#2 - 09/23/2019 07:01 PM - Szilárd Páll

- Status changed from New to Blocked, need info

GMX_SIMD=AVX2_256 in your CMake cache, so this is certainly not a cache file from a failing detection

#3 - 09/23/2019 10:21 PM - Stefano Guglielmo

- File CMakeCache.txt added
- File CMakeError.log added
- File CMakeOutput.log added

Sorry, those were files coming from compilation in which I set -DGMX_SIMD=AVX2_256; even in that case the output of CMake showed the error of detection. Anyway please find in attachment the files coming from compilation with DGMX_SIMD=AUTO.

Thanks again
Stefano

#4 - 09/24/2019 04:57 PM - Szilárd Páll

Stefano Guglielmo wrote:

Sorry, those were files coming from compilation in which I set -DGMX_SIMD=AVX2_256; even in that case the output of CMake showed the error of detection. Anyway please find in attachment the files coming from compilation with DGMX_SIMD=AUTO.

Thanks. Two more things:

- can you please make sure that the issue reproduces with the most recent 2019 release?
- would you be able to test a slightly older cmake version on your machine (I've certainly used 3.12/3.13 successfully).

#5 - 09/24/2019 05:26 PM - Stefano Guglielmo

- File CMakeCache_cmake313.txt added
- File CMakeCache_cmake315.txt added
- File CMakeError_cmake313.log added
- File CMakeError_cmake315.log added
- File CMakeOutput_cmake313.log added
- File CMakeOutput_cmake315.log added

When compiling with CMake-3.15 the same error was encountered with gromacs 2019.3. Using CMake 3.13.5 no error was present for both gromacs versions. I attach the CMake files for version 2019.3 compiled with the two versions of CMake. Please let me know if you need CMake files for successful compilation of gromacs 2019.2 with CMake 3.13.5 as well.

Thanks

#6 - 12/27/2019 10:52 AM - Erik Lindahl

- Assignee set to Erik Lindahl

Files

CMakeError.log	20.9 KB	09/20/2019	Stefano Guglielmo
CMakeCache.txt	69.1 KB	09/20/2019	Stefano Guglielmo
CMakeOutput.log	146 KB	09/20/2019	Stefano Guglielmo
CMakeCache.txt	67.4 KB	09/23/2019	Stefano Guglielmo
CMakeError.log	16.5 KB	09/23/2019	Stefano Guglielmo
CMakeOutput.log	136 KB	09/23/2019	Stefano Guglielmo
CMakeCache_cmake315.txt	67.5 KB	09/24/2019	Stefano Guglielmo
CMakeCache_cmake313.txt	70.3 KB	09/24/2019	Stefano Guglielmo
CMakeError_cmake313.log	20.7 KB	09/24/2019	Stefano Guglielmo
CMakeError_cmake315.log	16.5 KB	09/24/2019	Stefano Guglielmo
CMakeOutput_cmake313.log	147 KB	09/24/2019	Stefano Guglielmo
CMakeOutput_cmake315.log	136 KB	09/24/2019	Stefano Guglielmo