GROMACS - Bug #2876

2019.1 make check fails on AVX and AVX2 (Intel 2018u3)

03/05/2019 02:50 PM - Stefan Becuwe

Status:	New		
Priority:	Normal		
Assignee:	Erik Lindahl		
Category:			
Target version:			
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:	2019.1		

Description

Hello

make check fails in 2019.1 on two different platforms. In both cases I used Intel 2018 update 3 compilers.

- on AVX, 3 SIMD tests fail, but only in single precision
- on AVX2, 1 MdrunNonIntegratorTests test (and consequently MdrunMpiTests) fails, but only in double precision

I attach for both cases the log file from the error, as well as the output from gmx* -version

FYI: I used the same Intel compiler with GROMACS 2018.3 without problem. On AVX, I had to add "-no-ftz" as a compiler flag to pass the tests.

Kind regards
Stefan

Related issues:

Related to GROMACS - Bug #2883: essentialdynamics fail with Intel MPI	**New**

History

#1 - 03/05/2019 04:43 PM - Erik Lindahl

These look very benign, so it's likely just a matter of allowing a bit more freedom in the tests for the Intel compiler.

#2 - 03/05/2019 04:44 PM - Erik Lindahl

- Assignee set to Erik Lindahl

#3 - 03/07/2019 01:34 PM - Stefan Becuwe

- File regression-avx-2019.1-intel-2019u2.txt added

- File regression-avx2-2019.1-intel-2019u2.txt added

Hello Erik

Update: I also tried the Intel 2019 update 2 compilers. Adding the '-no-ftz' flag on the AVX machine, all tests pass on both platforms!

I also tried the regression tests with Intel 2019 update 2. I found one case that goes wrong on both AVX and AVX2 in both single and double precision, and one extra case that fails on AVX2. See attachment for used flags and errors.

Kind regards
Stefan

#4 - 03/08/2019 03:11 AM - Roland Schulz

The freeenergy error with ICC19u2 with AVX2 I can't reproduce. Could you please attach the mdrun.out, md.log files for those failing freeenergy tests?
The essentialdynamics error I can reproduce. Thanks for the report. The error is in the testing harness not in GROMACS. So you don't have to worry about the error. I crated #2883 for this bug.

#5 - 03/08/2019 03:12 AM - Roland Schulz

- Related to Bug #2883: essentialdynamics fail with Intel MPI added

#6 - 03/08/2019 10:32 AM - Stefan Becuwe

- File freeenergy.tgz added

- File gmx-avx2-interactive-logfile added

Hello Roland

It seems those two specific tests (expanded and simtemp) from freeenergy are influenced by the environment in one way or another.
If I login directly to a compute node or login node, all regression tests pass.
If I start an interactive job (qsub -I -lnodes=1:ppn=28 (all cores)) and run the regression tests, those two tests fail. I reproduced this situation twice.
Let's hope this is useful information.

Kind regards
Stefan

Files

gmx-2019-1-version-variant-1-avx-info.txt	2.7 KB	03/05/2019	Stefan Becuwe
gmx-2019-1-version-variant-1-avx-log.txt	28.8 KB	03/05/2019	Stefan Becuwe
gmx-2019-1-version-variant-2-avx2-info.txt	2.78 KB	03/05/2019	Stefan Becuwe
gmx-2019-1-version-variant-2-avx2-log.txt	264 KB	03/05/2019	Stefan Becuwe
regression-avx-2019.1-intel-2019u2.txt	1.75 KB	03/07/2019	Stefan Becuwe
regression-avx2-2019.1-intel-2019u2.txt	2.45 KB	03/07/2019	Stefan Becuwe
freeenergy.tgz	6.19 KB	03/08/2019	Stefan Becuwe
gmx-avx2-interactive-logfile	4.21 KB	03/08/2019	Stefan Becuwe