

GROMACS - Bug #2567

make check fails at test 23 SIMD errors

07/09/2018 05:38 PM - Brian Bennion

Status: New	
Priority: Normal	
Assignee:	
Category:	
Target version:	
Affected version - extra info:	Difficulty: uncategorized
Affected version: 2018.1	

Description

build command

```
cmake ../-DCMAKE_C_COMPILER=/usr/tce/packages/intel/intel-18.0.1/bin/icc
-DCMAKE_INSTALL_PREFIX=/usr/gapps/bbs/TOSS-3-Catalyst/
-DCMAKE_CXX_COMPILER=/usr/tce/packages/intel/intel-18.0.1/bin/icc
make -j18 successfully compiles.
```

```
[ PASSED ] 265 tests.
[ FAILED ] 3 tests, listed below:
[ FAILED ] SimdMathTest.exp
[ FAILED ] SimdMathTest.expSingleAccuracy
[ FAILED ] SimdMathTest.expSingleAccuracyUnsafe
3 FAILED TESTS

Start 24: GmxAnaTest
24/33 Test #24: GmxAnaTest ..... Passed 0.23 sec
Start 25: GmxPreprocessTests
25/33 Test #25: GmxPreprocessTests ..... Passed 0.32 sec
Start 26: CorrelationsTest
26/33 Test #26: CorrelationsTest ..... Passed 0.50 sec
Start 27: AnalysisDataUnitTests
27/33 Test #27: AnalysisDataUnitTests ..... Passed 0.19 sec
Start 28: SelectionUnitTests
28/33 Test #28: SelectionUnitTests ..... Passed 0.40 sec
Start 29: TrajectoryAnalysisUnitTests
29/33 Test #29: TrajectoryAnalysisUnitTests ..... Passed 0.78 sec
Start 30: EnergyAnalysisUnitTests
30/33 Test #30: EnergyAnalysisUnitTests ..... Passed 0.25 sec
Start 31: CompatibilityHelpersTests
31/33 Test #31: CompatibilityHelpersTests ..... Passed 0.05 sec
Start 32: MdrunTests
32/33 Test #32: MdrunTests ..... Passed 3.31 sec
Start 33: MdrunMpiTests
33/33 Test #33: MdrunMpiTests ..... Passed 0.12 sec
```

97% tests passed, 1 tests failed out of 33

Label Time Summary:

```
GTest = 9.16 sec (33 tests)
IntegrationTest = 3.66 sec (3 tests)
MpiTest = 0.24 sec (3 tests)
UnitTest = 5.50 sec (30 tests)
```

Total Test time (real) = 9.45 sec

The following tests FAILED:

23 - SimdUnitTests (Failed)

Errors while running CTest

```
make[3]: *** [CMakeFiles/run-ctest-nophys] Error 8
```

```
make[2]: *** [CMakeFiles/run-ctest-nophys.dir/all] Error 2
make[1]: *** [CMakeFiles/check.dir/rule] Error 2
make: *** [check] Error 2
uname -a
Linux catalyst160 3.10.0-862.3.2.1chaos.ch6.x86_64 #1 SMP Tue May 22 08:12:37 PDT 2018 x86_64 x86_
64 x86_64 GNU/Linux
```

History

#1 - 07/09/2018 06:17 PM - Mark Abraham

- Description updated

#2 - 07/09/2018 06:21 PM - Mark Abraham

Thanks for the report. What was the target machine? e.g. what does `gmx version -h` report?

#3 - 07/10/2018 09:35 AM - Mark Abraham

Also what does running the test binary on those tests actually report? e.g. `$build/bin/simd-test --gtest_filter=*exp*`