

## GROMACS - Bug #2325

### avx512 double precision simd failure

12/04/2017 11:00 AM - Mark Abraham

<b>Status:</b> Closed	
<b>Priority:</b> Normal	
<b>Assignee:</b>	
<b>Category:</b> core library	
<b>Target version:</b> 2018	
<b>Affected version - extra info:</b>	<b>Difficulty:</b> uncategorized
<b>Affected version:</b> 2018-beta2	

#### Description

With gcc 7.1 on dev-purley01 (AVX512) in double precision:

```
[ RUN      ] SimdFloatingpointUtilTest.transposeScatterStoreU3
../src/gromacs/simd/tests/simd_floatingpoint_util.cpp:303: Failure
Value of: mem0_[j]
  Actual: 1001.00000000018564
  Expected: refmem[j]
  Which is: 0.10000000000000223
Difference: 1000.9 (60145924867270031 double-prec. ULPs, rel. 1e+04)
Tolerance: abs. 8.88178e-16, 4 ULPs
../src/gromacs/simd/tests/simd_floatingpoint_util.cpp:303: Failure
Value of: mem0_[j]
  Actual: 1002.0000000000223
  Expected: refmem[j]
  Which is: 0.20000000000000445
Difference: 1001.8 (55651121332905610 double-prec. ULPs, rel. 5.01e+03)
Tolerance: abs. 8.88178e-16, 4 ULPs
../src/gromacs/simd/tests/simd_floatingpoint_util.cpp:303: Failure
Value of: mem0_[j]
  Actual: 4.667261465178151e-62
  Expected: refmem[j]
  Which is: 1.0000000000000222
Difference: 1 (917833604050253824 double-prec. ULPs, rel. 1)
Tolerance: abs. 8.88178e-16, 4 ULPs
../src/gromacs/simd/tests/simd_floatingpoint_util.cpp:303: Failure
Value of: mem0_[j]
  Actual: 1010.00000000018612
  Expected: refmem[j]
  Which is: 1.1000000000000245
...
```

which leads various other things to fail, including the settle unit tests to segfault

```
...
[-----] 24 tests from WithParameters/SettleTest
[ RUN      ] WithParameters/SettleTest.SatisfiesConstraints/0
```

#### Associated revisions

##### Revision 22213935 - 12/14/2017 09:36 AM - Erik Lindahl

Work around AVX-512 issues in gcc-5.4 and 7.1

Fixes compilation issues with mixed and double precision builds using AVX-512 SIMD with gcc-5.4 or gcc-7.1. Also tested with gcc-6.3, and Debug as well as Release builds for all three versions, all of which now pass the simd unit tests.

Fixes #2325.

Change-Id: I59c3ae0467b51412d1ebbb5b57a248534288a5db

#### Revision 80dd3f5b - 12/21/2017 10:54 AM - Mark Abraham

Update double-precision test configurations

These changes improve coverage of double precision, using more release mode, particularly with latest gcc and icc, and using 128-bit SIMD, which have been cases that were buggy recently. The other aspects of the configurations that have been modified have been non-critical. Where appropriate, brief rationales are recorded. This resolves an old TODO item in the post-submit matrix.

Fixed a sign mismatch in initializing an OpenCL variable that didn't need to be initialized.

Noted relevant new TODOs.

Refs #2300, #2325, #2326, #2334, #2335, #2336, #2337, #2338

Change-Id: I131fa1a6776d1e7809799c3f931a1fc8100fcdc9

### History

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#### #1 - 12/04/2017 11:09 AM - Mark Abraham

- Description updated

#### #2 - 12/05/2017 03:33 PM - Paul Bauer

Reproduced with gcc-6 and double prevision with GMX\_SIMD=AVX\_512. Looking into it if I find something obvious

#### #3 - 12/05/2017 05:04 PM - Paul Bauer

When stepping through the simd function in the debugger I noticed that the memory in the base address becomes overwritten with garbage at this point

```
_mm512_i32scatter_pd(base, simdoffset.simdInternal_, v0.simdInternal_, sizeof(double));
```

but I don't understand enough of it to know why. Hope that helps the more knowledgeable people.

#### #4 - 12/05/2017 08:26 PM - Roland Schulz

I can't reproduce this. Both with GCC 6.1 and 7.3 the simd unit tests pass.

In both cases I have failures:

7 - EwaldUnitTests (Failed)

17 - TableUnitTests (Failed)

Both those seem unrelated. Did you add any other flags besides "-DGMX\_SIMD=AVX\_512 -DGMX\_DOUBLE=yes"?

#### #5 - 12/06/2017 10:18 AM - Paul Bauer

I used this as my cmake command line options

```
"-DGMX_DOUBLE=yes -DGMX_SIMD=AVX_512 -DCMAKE_C_COMPILER=gcc-6 -DCMAKE_CXX_COMPILER=g++-6"
```

When building from the latest source I also can no longer reproduce this, strangely enough, and I get the same failures in Ewald and Table tests that seem to be simple precision issues.

#### #6 - 12/07/2017 06:04 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2325](#).

Uploader: Mark Abraham ([mark.j.abraham@gmail.com](mailto:mark.j.abraham@gmail.com))

Change-Id: gromacs~release-2018~I131fa1a6776d1e7809799c3f931a1fc8100fcdc9

Gerrit URL: <https://gerrit.gromacs.org/7303>

#### #7 - 12/10/2017 05:57 PM - Erik Lindahl

- Status changed from New to Rejected

Feel free to reopen if it can be reproduced.

#### #8 - 12/10/2017 05:57 PM - Erik Lindahl

- Status changed from Rejected to Closed

**#9 - 12/11/2017 02:25 AM - Mark Abraham**

On dev-purley01, I can reproduce this with release-2017 HEAD b01a10543dcec1ea87e409a28821c3f668e04b2b with a gcc 7.1 AVX512 double-precision Debug build, but not a Release build. With gcc 6-4, again Debug had an issue and Release did not. (All gave the table error from [#2336](#), too.)

All the failing configs warn about "warning: pointer of type 'void \*\*' used in arithmetic [-Wpointer-arith]" three times in transposeScatterStoreU<3> called from multiple places. Notice how the simd test failure has failed to replace mem0 with the correct values during the scatter. That's clearly a gcc bug (Release works ok, all the pointers we use have a non-void base type, so it seems to be doing an incorrect code transformation). Note that gcc permits void-pointer arithmetic as an extension (but I don't think this is related). I will work on a repro case to file a bug

**#10 - 12/12/2017 12:42 PM - Mark Abraham**

- Status changed from Closed to Blocked, need info
- Affected version changed from 2018-beta1 to 2018-beta2

Still present in 2018-beta2 with gcc 6.4 in Debug, both double and mixed builds.

Reopened so that I have a reminder to report this bug. We also need some further investigation and perhaps some kind of workaround so that people can't use whatever range of compilers and build configurations are vulnerable to it.

**#11 - 12/12/2017 04:08 PM - Gerrit Code Review Bot**

Gerrit received a related patchset '1' for Issue [#2325](#).  
Uploader: Erik Lindahl ([erik.lindahl@gmail.com](mailto:erik.lindahl@gmail.com))  
Change-Id: gromacs~release-2018~l59c3ae0467b51412d1ebbb5b57a248534288a5db  
Gerrit URL: <https://gerrit.gromacs.org/7336>

**#12 - 12/12/2017 04:10 PM - Erik Lindahl**

I think I managed to work around it.

**#13 - 12/12/2017 04:11 PM - Erik Lindahl**

- Status changed from Blocked, need info to Fix uploaded

**#14 - 12/14/2017 10:12 AM - Erik Lindahl**

- Status changed from Fix uploaded to Resolved

Applied in changeset [2221393549638e0164015aad3e6b9ea3eb2a0a10](#).

**#15 - 12/14/2017 10:17 AM - Erik Lindahl**

- Status changed from Resolved to Closed