GROMACS - Task #2249

Clarify rounding of SIMD round

09/15/2017 03:44 AM - Roland Schulz

Status:	Closed	
Priority:	Normal	
Assignee:		
Category:		
Target version:	2018-beta3	
Difficulty:	uncategorized	

Description

Adding

```
GMX_EXPECT_SIMD_REAL_EQ(setSimdRealFrom1R(3), round(setSimdRealFrom1R(2.5)));
```

to SimdFloatingpointTest,round fails on AVX. The doxygen of round should specify what happens with ties (to zero (like c++), to even (like IEEE), depending on rounding mode set by user (like current AVX implementation), or undefined). And there should be a test which checks for ties (unless undefined).

Associated revisions

Revision 41531c0f - 12/06/2017 01:57 PM - Roland Schulz

Added doxygen note to clarify rounding mode of SIMD

Also moved unit test of rounding mode into own test to make obvious that rounding mode is independent of ldexp.

Fixes #2249

Change-Id: Iae66e080de141ace7f2b1298f94fdb867f8632fe

History

#1 - 11/30/2017 11:52 PM - Erik Lindahl

I don't think we can (or at least want to) require a specific rounding mode.

While the vast majority uses IEEE, there have been some platforms (IBM Power with VMX or VSX SIMD) that used non-standard rounding either for round() or the float-to-integer-conversions. For this reason (and our exp() implementations, the only thing we require is that those to two rounding functionalities use the same rounding mode - which will make sure the algorithms produce correct results.

The main concern is that the float-to-integer conversion is needed for tables in the most performance-sensitive loop of the entire program, and requiring any rounding mode that isn't natively supported on a specific platform could lead to a very large performance hit.

#2 - 12/03/2017 12:27 PM - Mark Abraham

Sounds like we should test that those conversions are consistent, and document that the behaviour of our round() wrapper (and perhaps the conversions?) is implementation-defined.

#3 - 12/06/2017 12:31 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #2249.
Uploader: Roland Schulz (roland.schulz@intel.com)
Change-Id: gromacs~release-2018~Iae66e080de141ace7f2b1298f94fdb867f8632fe
Gerrit URL: https://gerrit.gromacs.org/7294

#4 - 12/06/2017 01:11 AM - Roland Schulz

- Status changed from New to Fix uploaded

#5 - 12/06/2017 02:34 AM - Szilárd Páll

- Target version set to 2018-beta3

Set target to beta3 as proposed implementation does not have approval yet.

#6 - 12/06/2017 04:09 PM - Roland Schulz

- Status changed from Fix uploaded to Resolved

Applied in changeset [41531c0fa92a6ee491f9df83b9570c307c2cd67d](#).

#7 - 12/06/2017 09:57 PM - Roland Schulz

- Status changed from Resolved to Closed