GROMACS - Bug #2242
PME LJ tests fail with SIMD with an fp exception
09/07/2017 02:25 AM - Roland Schulz

Status: Closed
Priority: Normal
Assignee: Berk Hess
Category: mdrun
Target version: 2016.5
Affected version:
Difficulty: uncategorized

Description
On KNL in debug mode multiple of the the tests fail because of FPE. It seems that not the whole SIMD width is initialized and thus the exp overflows. They pass in release mode.

With reference implementation and GCC 5.4 on HSW (-DGMX_SIMD=Reference -DGMX_SIMD_REF_FLOAT_WIDTH=16 -DGMX_SIMD_REF_DOUBLE_WIDTH=8 -DCMAKE_BUILD_TYPE=Debug) the same tests also produce the FPE. In addition multiple other tests fails with "Reference data item [] not found".

Related issues:
Related to GROMACS - Bug #2234: PME solving test missing reference data failu...

Associated revisions
Revision 16f9979f - 09/12/2017 11:59 AM - Berk Hess
Fix exception in SIMD LJ PME solve
Clear SIMD padding elements in solve helper arrays to avoid, otherwise harmless, fp overflow exceptions.
Fixes #2242
Change-Id: I97e67c4fcc2ef361f54d1627fd0dab4621f4bd33

History
#1 - 09/07/2017 02:12 PM - Aleksei Iupinov
I'm not really knowledgeable in SIMD layer. It seems pme-solve.cpp:98 allocates work for GMX_SIMD_REAL_WIDTH, which comes from impl_x86_avx2_256_definitions.h and is defined as 8. Hence the second part of simdInternal is garbage, causing ldexp overflow. Berk, any ideas on fixing this?

The rest of the failures likely have to do with the arbitrary GMX_FLOAT_MIN cut-off for the reference data, as in #2234. I might have to adjust input coefficients once more, as such small grid values are not meaningful/realistic anyway.

#2 - 09/08/2017 02:06 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2242.
Uploader: Berk Hess (hess@kth.se)
Change-Id: gromacs~release-2016~I131008190dedfdecf8770fe547346d64f399a9f
Gerrit URL: https://gerrit.gromacs.org/6909

#3 - 09/08/2017 02:09 PM - Berk Hess
- Category set to mdrun
- Status changed from New to Fix uploaded
- Assignee changed from Aleksei Iupinov to Berk Hess
- Target version set to 2016.4

No, GMX_SIMD_REAL_WIDTH comes from the file for the appropriate architecture, so 16 for float with KNL. This issue does not seem to be specific for KNL.

#4 - 09/08/2017 03:36 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2242.
Uploader: Berk Hess (hess@kth.se)
Change-ID: gromacs~release-2016~I97e67c4fccc2ef361f54d1627fd0dab46214fd33
Gerrit URL: https://gerrit.gromacs.org/6911

#5 - 09/08/2017 03:52 PM - Berk Hess
- Subject changed from PME tests fail with SIMD width 16 to PME LJ tests fail with SIMD with an fp exception

#6 - 09/08/2017 04:46 PM - Aleksei lupinov
- Related to Bug #2234: PME solving test missing reference data failures on various configurations added

#7 - 09/08/2017 08:17 PM - Roland Schulz
Should we create a separate bug for the reference data issue? Otherwise we shouldn't set the status to "Fix uploaded" until both problems are resolved.

#8 - 09/09/2017 12:07 PM - Aleksei lupinov
I reopened the other one (#2234) which already deals with same problem.

#9 - 09/12/2017 11:57 AM - Mark Abraham
- Target version changed from 2016.4 to 2016.5

Are we happy with behaviour of the 2016 branch? Setting target to 2016.5 for now, but I assume there's no work to do

#10 - 09/12/2017 12:00 PM - Berk Hess
- Status changed from Fix uploaded to Resolved

Applied in changeset 16f9979fb325ca898e2d26b2ae0244908e761fb5.

#11 - 12/11/2017 12:11 PM - Erik Lindahl
- Status changed from Resolved to Closed