

GROMACS - Bug #2421

EwaldUnitTests and SimdUnitTests fail on ppc64le with gcc-8.0.1

02/25/2018 02:57 AM - Christoph Junghans

Status: Closed	
Priority: Normal	
Assignee: Mark Abraham	
Category: core library	
Target version: future	
Affected version - extra info:	Difficulty: uncategorized
Affected version: 2018	

Description

```
/builddir/build/BUILD/gromacs-2018/src/testutils/refdata.cpp:925: Failure
```

```
  In item: /Forces/[0]/X
```

```
  Actual: -11.769416809082031
```

```
  Reference: -10.129964828491211
```

```
Difference: 1.63945 (1719090 single-prec. ULPs, rel. 0.162)
```

```
Tolerance: abs. 1.43051e-06, 12 ULPs
```

```
Google Test trace:
```

```
/builddir/build/BUILD/gromacs-2018/src/gromacs/ewald/tests/pmegathertest.cpp:413: Testing force gathering with CPU for PME grid size 16 12 14, order 4, 1 atoms, without reduction
```

and

```
/builddir/build/BUILD/gromacs-2018/src/gromacs/simd/tests/bootstrap_loadstore.cpp:112: Failure
```

```
Value of: pCopyDst[i]
```

```
  Actual: 5
```

```
Expected: pCopySrc[i]
```

```
Which is: 6
```

```
SIMD load or store not moving data correctly for element 0
```

Found here: <https://koji.fedoraproject.org/koji/taskinfo?taskID=25294220> (detailed build.log for ppe64le attached)

Associated revisions

Revision e6932745 - 03/19/2018 10:31 AM - Mark Abraham

Fix VSX SIMD with gcc 8

gcc 8 apparently generates different code for the former GROMACS code, which seems buggy. See

https://bugzilla.redhat.com/show_bug.cgi?id=1556989#c3

and https://gcc.gnu.org/bugzilla/show_bug.cgi?id=84907

Fixes #2421

Change-Id: I31492cd582b785cdfb42e8b999a165a7339ce4be

Revision f1712c37 - 03/27/2018 09:31 PM - Mark Abraham

More gcc-8 fixes for POWER

Fixes #2421

Change-Id: I43c13df3a217d0f2154dca0ef215efd9cd27474a

Revision 9ae6059d - 06/13/2018 12:32 AM - Mark Abraham

More fixes to suit gcc 8 for double build

gcc 7 supports the same syntax, but only gcc 8 requires it.

xl code path untested, because we have no access to a working compiler

Fixes #2421

Change-Id: I8f89af4b066be68e07a286a9fa45b8ded3c925f3

History

#1 - 02/25/2018 03:05 AM - Christoph Junghans

I think it is problem with gcc-8 as the same build worked fine on Fedora27 with gcc-7.2.1 (<https://koji.fedoraproject.org/koji/buildinfo?buildID=1019225>)

#2 - 02/25/2018 09:02 PM - Christoph Junghans

And this is with `GMX_SIMD=IBM_VSX`.

#3 - 02/25/2018 09:09 PM - Mark Abraham

gcc 8.0.1 is still pre-release. I don't have access to it anywhere, since my access is all to production login nodes. So I suggest we file a regression report with gcc.

#4 - 02/25/2018 09:41 PM - Christoph Junghans

You could do:

```
$ docker pull fedora:rawhide
$ docker run -it fedora:rawhide /bin/bash
```

#5 - 02/25/2018 10:53 PM - Mark Abraham

Christoph Junghans wrote:

You could do:
[...]

Yes, but that won't work on any machine capable of executing VSX instructions.

#6 - 02/26/2018 03:04 PM - Erik Lindahl

This appears to be bugs in the very basic load/store operations. Unfortunately I've seen those before, and although it might be possible to work around some of them, it indicates severe compiler bugs.

#7 - 03/16/2018 06:47 PM - Christoph Junghans

GCC upstream thinks this is a bug in Gromacs and proposed a patch here: https://bugzilla.redhat.com/show_bug.cgi?id=1556989#c3

```
--- gromacs-2018/src/gromacs/simd/impl_ibm_vsx/impl_ibm_vsx_simd_float.h.jj      2017-12-11 13:44:54.000000000 +
0100
+++ gromacs-2018/src/gromacs/simd/impl_ibm_vsx/impl_ibm_vsx_simd_float.h      2018-03-16 17:02:45.915186989 +010
0
@@ -121,14 +121,14 @@ static inline SimdFloat gmx_simdcall
  simdLoadU(const float *m, SimdFloatTag = {})
  {
-     return {
+         *reinterpret_cast<const __vector float *>(m)
+         vec_xl(0, m)
    };
  }

  static inline void gmx_simdcall
  storeU(float *m, SimdFloat a)
  {
-     *reinterpret_cast<__vector float *>(m) = a.simdInternal_;
+     vec_xst(a.simdInternal_, 0, m);
  }

  static inline SimdFloat gmx_simdcall
@@ -157,14 +157,14 @@ static inline SimdFInt32 gmx_simdcall
  simdLoadU(const std::int32_t *m, SimdFInt32Tag)
  {
-     return {
+         *reinterpret_cast<const __vector int *>(m)
+         vec_xl(0, m)
    };
  }

  static inline void gmx_simdcall
  storeU(std::int32_t * m, SimdFInt32 a)
  {
-     *reinterpret_cast<__vector int *>(m) = a.simdInternal_;
+     vec_xst(a.simdInternal_, 0, m);
  }

  static inline SimdFInt32 gmx_simdcall
--- gromacs-2018/src/gromacs/simd/impl_ibm_vsx/impl_ibm_vsx_simd_double.h.jj  2017-12-11 13:44:54.000000000
+0100
+++ gromacs-2018/src/gromacs/simd/impl_ibm_vsx/impl_ibm_vsx_simd_double.h    2018-03-16 17:05:08.248153217 +01
00
@@ -121,14 +121,14 @@ static inline SimdDouble gmx_simdcall
  simdLoadU(const double *m, SimdDoubleTag = {})
  {
-     return {
+         *reinterpret_cast<const __vector double *>(m)
+         vec_xl(0, m)
    };
  }

  static inline void gmx_simdcall
  storeU(double *m, SimdDouble a)
  {
-     *reinterpret_cast<__vector double *>(m) = a.simdInternal_;
+     vec_xst(a.simdInternal_, 0, m);
  }

  static inline SimdDouble gmx_simdcall
```

#8 - 03/16/2018 07:28 PM - Christoph Junghans

And <http://gcc.gnu.org/PR84907>

#9 - 03/16/2018 10:23 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2421](#).

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

Change-Id: gromacs~release-2018~l31492cd582b785cdfb42e8b999a165a7339ce4be

Gerrit URL: <https://gerrit.gromacs.org/7688>

#10 - 03/17/2018 12:38 AM - Mark Abraham

With and without that patch, gcc 7.2 in release mode is fine. gcc 6.3 without that patch is fine. But with it:

```
FAILED: src/gromacs/simd/tests/CMakeFiles/simd-test.dir/bootstrap_loadstore.cpp.o
/gpfs/software/opt/gcc/6.3.0/bin/g++ -DGMX_DOUBLE=0 -DGTEST_HAS_PTHREAD=1 -DHAVE_CONFIG_H -DTEST_DATA_PATH=\"
src/gromacs/simd/tests\" -DTEST_TEMP_PATH=\"/gpfs/homeb/padc/padc010/git/master/build-cmake-gcc-6.3-release/sr
c/gromacs/simd/tests/Testing/Temporary\" -isystem ../src/external/gmock-1.7.0/gtest/include -isystem ../src/ex
ternal/gmock-1.7.0/include -Isrc -isystem ../src/external/thread_mpi/include -I../src -isystem /gpfs/homeb/pad
c/padc010/progs/include -mcpu=power8 -mpower8-vector -mpower8-fusion -mdirect-move -mvsx -std=c++11 -Wund
ef -Wextra -Wno-missing-field-initializers -Wpointer-arith -Wmissing-declarations -Wall -O3 -DNDEBUG -funroll
-all-loops -fexcess-precision=fast -Wno-array-bounds -Wno-unused-variable -MD -MT src/gromacs/simd/tests/C
MakeFiles/simd-test.dir/bootstrap_loadstore.cpp.o -MF src/gromacs/simd/tests/CMakeFiles/simd-test.dir/bootstra
p_loadstore.cpp.o.d -o src/gromacs/simd/tests/CMakeFiles/simd-test.dir/bootstrap_loadstore.cpp.o -c ../src/gro
macs/simd/tests/bootstrap_loadstore.cpp
../src/gromacs/simd/tests/bootstrap_loadstore.cpp: In member function 'virtual void gmx::test::{anonymous}::Si
mdBootstrapTest_loadUI_Test::TestBody()':
../src/gromacs/simd/tests/bootstrap_loadstore.cpp:183:1: error: unrecognizable insn:
}
^
(insn 66 65 69 3 (set (reg:V4SI 270)
      (vec_select:V4SI (vec_select:V4SI (mem:V4SI (reg:DI 271 [ ivtmp.541 ]) [0 S16 A8])
        (parallel [
          (const_int 3 [0x3])
          (const_int 2 [0x2])
          (const_int 1 [0x1])
          (const_int 0 [0])
        ]))
      (parallel:V4SI [
        (const_int 2 [0x2])
        (const_int 3 [0x3])
        (const_int 0 [0])
        (const_int 1 [0x1])
      ]))) ../src/gromacs/simd/impl_ibm_vsx/impl_ibm_vsx_simd_float.h:161 -1
(expr_list:REG_DEAD (reg:DI 271 [ ivtmp.541 ])
  (expr_list:REG_EQUAL (vec_select:V4SI (vec_select:V4SI (mem:V4SI (reg:DI 234 [ ivtmp.541 ]) [0 S16 A8]
]))
  (parallel [
    (const_int 3 [0x3])
    (const_int 2 [0x2])
    (const_int 1 [0x1])
    (const_int 0 [0])
  ]))
  (parallel:V4SI [
    (const_int 2 [0x2])
    (const_int 3 [0x3])
    (const_int 0 [0])
    (const_int 1 [0x1])
  ]))
  (nil))))
../src/gromacs/simd/tests/bootstrap_loadstore.cpp:183:1: internal compiler error: in extract_insn, at recog.c:
2287
0x107c87f3 _fatal_insn(char const*, rtx_def const*, char const*, int, char const*)
.../gcc-6.3.0/gcc/rtl-error.c:108
0x107c8857 _fatal_insn_not_found(rtx_def const*, char const*, int, char const*)
.../gcc-6.3.0/gcc/rtl-error.c:116
0x1078f447 extract_insn(rtx_insn*)
.../gcc-6.3.0/gcc/recog.c:2287
0x1067607b scan_one_insn
.../gcc-6.3.0/gcc/ira-costs.c:1431
```

```
0x1067607b process_bb_for_costs
  ../../gcc-6.3.0/gcc/ira-costs.c:1592
0x10677727 find_costs_and_classes
  ../../gcc-6.3.0/gcc/ira-costs.c:1699
0x10679117 ira_set_pseudo_classes(bool, _IO_FILE*)
  ../../gcc-6.3.0/gcc/ira-costs.c:2239
0x1069f7cf move_loop_invariants()
  ../../gcc-6.3.0/gcc/loop-invariant.c:2254
0x106999cb execute
  ../../gcc-6.3.0/gcc/loop-init.c:523
Please submit a full bug report,
with preprocessed source if appropriate.
Please include the complete backtrace with any bug report.
See <http://gcc.gnu.org/bugs.html> for instructions.
```

#11 - 03/17/2018 12:53 AM - Erik Lindahl

Based on the IBM feedback, it's only version 8 that will get the ABI change.

I would suggest that we simply add a check for the gcc version and use the old construct for version < 7.

Cheers,

Erik

#12 - 03/19/2018 10:30 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2421](#).
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~master~I31492cd582b785cdfb42e8b999a165a7339ce4be
Gerrit URL: <https://gerrit.gromacs.org/7690>

#13 - 03/19/2018 11:50 AM - Mark Abraham

- Status changed from New to Resolved

#14 - 03/19/2018 11:50 AM - Mark Abraham

- Target version set to 2018.1

#15 - 03/19/2018 12:00 PM - Mark Abraham

Applied in changeset [e693274554dfba67124dbc2769d0a885dae42b08](#).

#16 - 03/20/2018 06:36 AM - Christoph Junghans

- File build.log added

Some of the other tests still fail after patching in https://github.com/gromacs/gromacs/commit/e693274554dfba67124dbc2769d0a885dae42b08_patch

#17 - 03/20/2018 08:40 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2421](#).
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~release-2018~l43c13df3a217d0f2154dca0ef215efd9cd27474a
Gerrit URL: <https://gerrit.gromacs.org/7696>

#18 - 03/20/2018 09:15 AM - Mark Abraham

- Status changed from Resolved to Fix uploaded

#19 - 03/20/2018 02:19 PM - Mark Abraham

Double precision needs some work, too

#20 - 03/20/2018 04:23 PM - Mark Abraham

I think I have double fixed, but will finish it tomorrow

#21 - 03/21/2018 01:01 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2421](#).
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~release-2018~l8f89af4b066be68e07a286a9fa45b8ded3c925f3
Gerrit URL: <https://gerrit.gromacs.org/7710>

#22 - 03/21/2018 04:10 PM - Christoph Junghans

I patched 92d6e21 in, but it is still failing: <https://koji.fedoraproject.org/koji/taskinfo?taskID=25859230>

#23 - 03/21/2018 04:18 PM - Mark Abraham

- Target version changed from 2018.1 to 2018.2

#24 - 03/21/2018 04:20 PM - Mark Abraham

will look further, but am away for ~1 week

#25 - 03/27/2018 10:00 PM - Mark Abraham

- Status changed from Fix uploaded to Resolved

Applied in changeset [f1712c3766eb80b52d1aab55b54d8b22cacfd68b](#).

#26 - 03/28/2018 09:43 AM - Christoph Junghans

Don't we need the 2nd patch set, too?

#27 - 03/28/2018 02:59 PM - Mark Abraham

- Status changed from Resolved to Fix uploaded

probably, that last post is done by a bot

#28 - 06/05/2018 04:44 PM - Mark Abraham

- Category changed from testing to core library
- Status changed from Fix uploaded to Feedback wanted

Christoph With gcc 8.1.0 on POWER9, I can no longer reproduce any issues with @make check (mixed and double; release and debug). Can you resubmit the fedora build and confirm? Thus I assume there is no further need of any fix.

#29 - 06/05/2018 04:46 PM - Mark Abraham

Mark Abraham wrote:

Christoph With gcc 8.1.0 on POWER9, I can no longer reproduce any issues with @make check (mixed and double; release and debug). Can you resubmit the fedora build and confirm? Thus I assume there is no further need of any fix.

Ignore this, I can reproduce the problem. I was mistakenly checking the branch including the fix.

#30 - 06/06/2018 02:06 AM - Christoph Junghans

- File *build.log.txt* added

Still persists with gcc-8.1.1, log attached

#31 - 06/07/2018 01:47 AM - Mark Abraham

Christoph Junghans wrote:

Still persists with gcc-8.1.1, log attached

OK, tests pass for me with gcc 8.1.0 on JURON with <https://gerrit.gromacs.org/#/c/7710/3> - can you try that for us please Christoph?

#32 - 06/07/2018 02:41 PM - Christoph Junghans

- File *build.log.txt* added

Even patching ba13293 in didn't help.

#33 - 06/12/2018 05:38 PM - Christoph Junghans

Mark, I got a confused with all the patch flying around, I added <https://gerrit.gromacs.org/#/c/7710/> (ba13293), do I need <https://gerrit.gromacs.org/#/c/7688/> (e693274) as well?

#34 - 06/12/2018 05:47 PM - Mark Abraham

Christoph Junghans wrote:

Mark, I got a confused with all the patch flying around, I added <https://gerrit.gromacs.org/#/c/7710/> (ba13293), do I need

<https://gerrit.gromacs.org/#/c/7688/> (e693274) as well?

No, the latter is the grandparent patch of the former - see git log

#35 - 06/12/2018 05:50 PM - Mark Abraham

I'll upload some comparable cmake+make logs shortly

#36 - 06/12/2018 10:44 PM - Mark Abraham

- File *tmpi-double.txt* added

- File *marks-build-log.txt* added

- Target version changed from 2018.2 to 2018.3

tmpi-double.txt is cut from Christoph's build.log.txt from comment 32. The only point of interest I can see in these build log diffs is that cmake host SIMD detection looks a bit different. So maybe both our observations are valid on the hardware+software stack we're testing. So I guess we have to defer resolving this issue until we have more information from somewhere.

#37 - 06/13/2018 12:45 AM - Mark Abraham

- Status changed from *Feedback wanted* to *Resolved*

Applied in changeset [9ae6059da61adba8fd4135446cbaa4ff21de682a](#).

#38 - 08/13/2018 04:23 PM - Paul Bauer

Hej, would you consider this one now as fully resolved, or should we still keep it open for the future?

#39 - 08/13/2018 10:57 PM - Christoph Junghans

I think the issue still persists on Fedora, but honestly I lost track, which patches got merged already.

#40 - 08/15/2018 11:55 AM - Paul Bauer

- Target version changed from 2018.3 to *future*

ok, I'll move this to future then, if there are no strong opinions against having it still open if more bugs are found

#41 - 01/03/2019 10:57 AM - Mark Abraham

- Status changed from *Resolved* to *Closed*

Open it when we have an issue. Otherwise we have hundreds of issues whose status is unknown!

Files

build.log	35.2 MB	02/25/2018	Christoph Junghans
build.log	35.1 MB	03/20/2018	Christoph Junghans
build.log.txt	35.6 MB	06/06/2018	Christoph Junghans
build.log.txt	35.6 MB	06/07/2018	Christoph Junghans
marks-build-log.txt	1.48 MB	06/12/2018	Mark Abraham
tmpi-double.txt	6.83 MB	06/12/2018	Mark Abraham