

GROMACS - Bug #2747

nb_kernel_ElecEwSw_VdwBhamSw_GeomW4W4 regressiontest failing on Power8

11/08/2018 03:53 PM - Szilárd Páll

Status:	Closed	
Priority:	Normal	
Assignee:	Szilárd Páll	
Category:		
Target version:	2019.1	
Affected version - extra info:	2019-beta3-dev-20181108-d536de3	Difficulty: uncategorized
Affected version:	2019-beta2	

Description

```
$ bin/gmx -version
      :-) GROMACS - gmx, 2019-beta3-dev-20181108-d536de3 (-:
```

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check out <http://www.gromacs.org> for more information.

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```
GROMACS:      gmx, version 2019-beta3-dev-20181108-d536de3
Executable:   /home/pszilard/gromacs-19/build_p8_gcc7_fftw-own_double/bin/gmx
Data prefix:  /home/pszilard/gromacs-19 (source tree)
Working dir:  /home/pszilard/gromacs-19/build_p8_gcc7_fftw-own_double
Command line:
  gmx -version
```

```
GROMACS version: 2019-beta3-dev-20181108-d536de3
GIT SHA1 hash:   d536de3b5125b79d4222768e356c4914e0758d5a
Precision:      single
Memory model:   64 bit
MPI library:    thread_mpi
OpenMP support: enabled (GMX_OPENMP_MAX_THREADS = 64)
GPU support:    disabled
SIMD instructions: IBM_VSX
FFT library:    fftw-3.3.8
RDTSCP usage:   disabled
TNG support:    enabled
Hwloc support:  hwloc-1.11.8
Tracing support: disabled
```

```
C compiler: /home/pszilard/programs/gcc/7.3/bin/gcc GNU 7.3.0
C compiler flags: -mcpu=power8 -mpower8-vector -mpower8-fusion -mdirect-move -mvsx -Werror=format-overflow -Wundef -Wextra -Wno-missing-field-initializers -Wno-sign-compare -Wpointer-arith -Wall -Wno-unused -Wunused-value -Wunused-parameter -O3 -DNDEBUG -funroll-all-loops -fexcess-precision=fast -Wno-array-bounds
C++ compiler: /home/pszilard/programs/gcc/7.3/bin/g++ GNU 7.3.0
C++ compiler flags: -mcpu=power8 -mpower8-vector -mpower8-fusion -mdirect-move -mvsx -std=c++11 -Wformat-overflow -Wundef -Wextra -Wno-missing-field-initializers -Wpointer-arith -Wmissing-declarations -Wall -O3 -DNDEBUG -funroll-all-loops -fexcess-precision=fast -Wno-array-bounds
```

Related issues:

Related to GROMACS - Bug #2734: regressiontests/kernel core dumps on ppc64le	In Progress
Related to GROMACS - Bug #2746: regressiontests/freeenergy coulandvdwsequential...	Closed
Related to GROMACS - Task #3057: re-enable fusion on Power8/9	New

Associated revisions

Revision 4a7281ef - 02/13/2019 04:50 PM - Szilárd Páll

Disable instruction fusion on Power8

The `-mpower8-fusion` flag seems to be the source of incorrect code; not confirmed, but likely a codegen issue that also affects Power9 with the similar flag used.

Fixes #2747 #2746 #2734

Change-Id: I56f50e54db47f4fe30c42488f4c4f79ac474518a

Revision 1ce795fe - 02/19/2019 02:17 PM - Szilárd Páll

Disable instruction fusion on Power8

The `-mpower8-fusion` flag seems to be the source of incorrect code; not confirmed, but likely a codegen issue that also affects Power9 with the similar flag used.

Fixes #2747 #2746 #2734

Change-Id: I56f50e54db47f4fe30c42488f4c4f79ac474518a

History

#1 - 01/02/2019 05:46 PM - Erik Lindahl

They passed with gcc-8.2 for me, but instead two of the complex tests failed.

#2 - 01/03/2019 11:09 AM - Mark Abraham

- Target version set to 2019.1

Per [#2746](#), I suggest we stop supporting power8.

Setting a version so that we force ourselves to make a decision.

#3 - 01/03/2019 11:09 AM - Mark Abraham

- Related to Bug #2734: regressiontests/kernel core dumps on ppc64le added

#4 - 01/03/2019 11:10 AM - Mark Abraham

- Related to Bug #2746: regressiontests/freeenergy coulandvdwsequential_vdw failing on Power8 added

#5 - 01/28/2019 01:17 PM - Mark Abraham

- Assignee set to Szilárd Páll

szilard to try to repro any of these that we haven't repro-ed, particularly if they might need a weird toolchain?

#6 - 01/31/2019 07:18 PM - Szilárd Páll

Update: looks like this and possibly [#2746](#) and possibly [#2734](#) may be related to the `"-mpower8-fusion"` flag. If I remove it, I so far could not reproduce any of the previous failures.

We could just yank that flag and move on. However given that it is a recommended flag by IBM for Power8 (likely Power9 too, though I've not seen public optimization guides yet), users or computer centers will sometimes take such recommendations and pass them in CMAKE_CXX_FLAGS and than we're back to failing tests.
Hence, we should consider checking whether there is something "illegal" we do (WIP Erik) or otherwise try to report the issue.

#7 - 02/07/2019 02:14 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2747](#).
Uploader: Szilárd Páll (pall.szilard@gmail.com)
Change-Id: gromacs~release-2019~156f50e54db47f4fe30c42488f4c4f79ac474518a
Gerrit URL: <https://gerrit.gromacs.org/9104>

#8 - 02/07/2019 02:19 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2747](#).
Uploader: Szilárd Páll (pall.szilard@gmail.com)
Change-Id: gromacs~release-2018~156f50e54db47f4fe30c42488f4c4f79ac474518a
Gerrit URL: <https://gerrit.gromacs.org/9105>

#9 - 02/08/2019 06:27 AM - Mark Abraham

- Status changed from New to Fix uploaded

#10 - 02/13/2019 04:49 PM - Mark Abraham

- Status changed from Fix uploaded to Closed

#11 - 08/12/2019 11:41 AM - Szilárd Páll

- Related to Task #3057: re-enable fusion on Power8/9 added

Files

checkforce.out	12.2 KB	11/08/2018	Szilárd Páll
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