

GROMACS - Bug #2746

regressiontests/freenenergy coulandvdwsequential_vdw failing on Power8

11/08/2018 03:49 PM - Szilárd Páll

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

Description

FAILED. Check checkforce.out (2 errors) file(s) in coulandvdwsequential_vdw for coulandvdwsequential_vdw

Mdrun cannot use the requested (or automatic) number of ranks, retrying with 8.

```
$ bin/gmx -version
```

```
:-) GROMACS - gmx, 2019-beta3-dev-20181108-d536de3 (-:
```

GROMACS is written by:

Emile Apol	Rossen Apostolov	Paul Bauer	Herman J.C. Berendsen
Par Bjelkmar	Christian Blau	Viacheslav Bolnykh	Kevin Boyd
Aldert van Buuren	Rudi van Drunen	Anton Feenstra	Gerrit Groenhof
Anca Hamuraru	Vincent Hindriksen	M. Eric Irrgang	Aleksei Iupinov
Christoph Junghans	Joe Jordan	Dimitrios Karkoulis	Peter Kasson
Jiri Kraus	Carsten Kutzner	Per Larsson	Justin A. Lemkul
Viveca Lindahl	Magnus Lundborg	Erik Marklund	Pascal Merz
Pieter Meulenhoff	Teemu Murtola	Szilard Pall	Sander Pronk
Roland Schulz	Michael Shirts	Alexey Shvetsov	Alfons Sijbers
Peter Tieleman	Teemu Virolainen	Christian Wennberg	Maarten Wolf

and the project leaders:

Mark Abraham, Berk Hess, Erik Lindahl, and David van der Spoel

Copyright (c) 1991-2000, University of Groningen, The Netherlands.

Copyright (c) 2001-2018, The GROMACS development team at

Uppsala University, Stockholm University and

the Royal Institute of Technology, Sweden.

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

GROMACS is free software; you can redistribute it and/or modify it under the terms of the GNU Lesser General Public License as published by the Free Software Foundation; either version 2.1 of the License, or (at your option) any later version.

GROMACS: gmx, version 2019-beta3-dev-20181108-d536de3

Executable: /home/pszilard/gromacs-19/build_p8_gcc7_fftw337/bin/gmx

Data prefix: /home/pszilard/gromacs-19 (source tree)

Working dir: /home/pszilard/gromacs-19/build_p8_gcc7_fftw337

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 #2747: nb_kernel_ElecEwSw_VdwBhamSw_GeomW4W4 regress...	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 - 11/08/2018 05:34 PM - Szilárd Páll

Possibly related to this or [#2747](#), with gcc 8:

```
FAILED. Check checkpoint.out (2 errors), checkforce.out (1869 errors) file(s) in coulandvdwsequential_coul for coulandvdwsequential_coul
```

```
FAILED. Check checkpoint.out (11 errors), checkforce.out (404 errors) file(s) in expanded for expanded
```

```
$ cat tests/regressiontests-release-2019-51d7202/freeenergy/coulandvdwsequential_coul/checkpoint.out
comparing energy file ./reference_s.edr and ener.edr
```

There are 51 and 52 terms in the energy files

```
enm[12] (- - Conserved En.)
```

There are 10 terms to compare in the energy files

```
Coul. recip.      step 40:      -3352.61,  step 40:      163097
Potential         step 40:      -30117.5,  step 40:      136332
```

Files read successfully

```
$ cat tests/regressiontests-release-2019-51d7202/freeenergy/expanded/checkpoint.out
comparing energy file ./reference_s.edr and ener.edr
```

There are 40 terms in the energy files

There are 11 terms to compare in the energy files

Coul. recip.	step 0:	321.338,	step 0:	336.118
Coul. recip.	step 1:	325.129,	step 1:	325.502
Coul. recip.	step 2:	325.259,	step 2:	325.845
Coul. recip.	step 3:	322.506,	step 3:	323.083
Coul. recip.	step 4:	318.435,	step 4:	318.805
Coul. recip.	step 6:	313.25,	step 6:	312.932
Coul. recip.	step 7:	314.874,	step 7:	314.292
Coul. recip.	step 8:	320.291,	step 8:	319.605
Coul. recip.	step 9:	329.26,	step 9:	328.631
Coul. recip.	step 10:	340.449,	step 10:	339.993
Coul. recip.	step 68:	321.619,	step 68:	321.962

Files read successfully

#2 - 11/09/2018 12:04 AM - Szilárd Pál

Update: several free neergy tests fail intermittently with gcc 8 too, also with GMX_SIMD=None and GMX_FFT_LIBRARY=fftpack, but this time some bonded energy terms are not matching:

```
$ cat tests/regressiontests-release-2019-51d7202/freeenergy/coulandvdwtogether/checkpot.out
comparing energy file ./reference_s.edr and ener.edr
```

There are 49 terms in the energy files

There are 10 terms to compare in the energy files

Angle	step 16:	8.28424,	step 16:	8.33762
Angle	step 17:	7.8723,	step 17:	7.92783
Angle	step 18:	7.31895,	step 18:	7.37155

Files read successfully

```
$ less tests/regressiontests-release-2019-51d7202/freeenergy/coulandvdwsequential_coul/checkpot.out
comparing energy file ./reference_s.edr and ener.edr
```

There are 51 and 52 terms in the energy files

enm[12] (- - Conserved En.)

There are 10 terms to compare in the energy files

Coul. recip.	step 12:	-3356.1,	step 12:	46807.7
Potential	step 12:	-30089.6,	step 12:	20074.2
Coul. recip.	step 20:	-3350.21,	step 20:	-3345.8
Coul. recip.	step 21:	-3349.77,	step 21:	-3344.29
Coul. recip.	step 22:	-3349.32,	step 22:	-3343.03
Potential	step 22:	-30046.6,	step 22:	-30014.8
Coul. recip.	step 23:	-3348.88,	step 23:	-3342.08
Potential	step 23:	-30034.9,	step 23:	-30001.2
Coul. recip.	step 24:	-3348.49,	step 24:	-3341.54
Potential	step 24:	-30025.1,	step 24:	-29991.2
Coul. recip.	step 25:	-3348.19,	step 25:	-3341.42
Potential	step 25:	-30018.2,	step 25:	-29985.7
Coul. recip.	step 26:	-3348.01,	step 26:	-3341.73
Coul. recip.	step 27:	-3348,	step 27:	-3342.43
Coul. recip.	step 28:	-3348.15,	step 28:	-3343.46
Coul. recip.	step 29:	-3348.47,	step 29:	-3344.65
Coul. recip.	step 37:	-3351.75,	step 37:	-3347.99
Coul. recip.	step 38:	-3351.97,	step 38:	-3347.57
Ryckaert-Bell.	step 39:	4.96147,	step 39:	4.91132
Coul. recip.	step 39:	-3352.24,	step 39:	-3347.31
Ryckaert-Bell.	step 40:	5.04869,	step 40:	4.99534
Coul. recip.	step 40:	-3352.61,	step 40:	-3347.35
Potential	step 40:	-30117.5,	step 40:	-30086.2

Files read successfully

#3 - 01/03/2019 11:08 AM - Mark Abraham

- Target version set to 2019.1

I suggest we stop supporting power 8. There's essentially zero HPC usage, so it just isn't a priority.

Setting a target so that we make a decision about the support offered.

#4 - 01/03/2019 11:09 AM - Mark Abraham

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

#5 - 01/03/2019 11:10 AM - Mark Abraham

- Related to Bug #2747: nb_kernel_ElecEwSw_VdwBhamSw_GeomW4W4 regressiontest failing on Power8 added

#6 - 01/03/2019 02:13 PM - Szilárd Páll

Mark Abraham wrote:

I suggest we stop supporting power 8. There's essentially zero HPC usage, so it just isn't a priority.

Setting a target so that we make a decision about the support offered.

None of this is an effort to support Power8 just as our testing on other non-mainstream platforms isn't support for those. With the same reasoning neither ARMv7, even ARMv8, anything 32-bit, anything Intel older Intel Sandy Bridge (or Ivy), let alone Windows should be a priority.

Portability does not mean the code can in theory be ported (and if it happens to not work we claim it is unsupported), but that it actually does work across different platforms that meet the common requirements for the codebase to compile and function correctly. We're using vanilla GNU toolchain on a vanilla ppc64 Linux distribution, so nothing custom or vendor-specific is involved that would point to an effort beyond ensuring portability, hence explicit Power8 platform support is not a concern here, I think.

Of course, if such observations do not reproduce in other cases, we can flag this as a "known issue and consider it solved.

PS: ORNL and other US labs do use Power8 GPU clusters for some testing, e.g. without a live project affiliation AFAIK even to ORNL employees only [Summitdev](#) (Power S822LC, that is Power8 + P100) is available.

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

Gerrit received a related patchset '1' for Issue [#2746](#).

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 [#2746](#).

Uploader: Szilárd Páll (pall.szilard@gmail.com)

Change-Id: gromacs~release-2018~156f50e54db47f4fe30c42488f4c4f79ac474518a

Gerrit URL: <https://gerrit.gromacs.org/9105>

#9 - 02/08/2019 06:50 AM - Mark Abraham

Szilárd Páll wrote:

Mark Abraham wrote:

I suggest we stop supporting power 8. There's essentially zero HPC usage, so it just isn't a priority.

Setting a target so that we make a decision about the support offered.

None of this is an effort to support Power8 just as our testing on other non-mainstream platforms isn't support for those. With the same reasoning neither ARMv7, even ARMv8, anything 32-bit, anything Intel older Intel Sandy Bridge (or Ivy), let alone Windows should be a priority.

Indeed, none of them are priorities. ARMv7 I would drop in a heartbeat except that we happen to have one already. 32-bit was agreed years ago was not supported. Older Intel happens to be even easier to test so unlikely to be dropped. The Windows port is much more about that our code compiles with a different compiler, C++ and C standard library, and has fewer hidden assumptions about POSIX systems - which is sustainable only if it is easy to test.

Portability does not mean the code can in theory be ported

Portable means "able to be ported," not "has been tested and does not require porting." GROMACS is a portable code because we have designed it that way, and also because we have taken care to support a range of platforms.

(and if it happens to not work we claim it is unsupported),

Was that a constructive thing to say?

but that it actually does work across different platforms

For us to claim that it "actually does work" requires that we've spent the time to test it, which is one of the prerequisites for saying something is "supported." How often we prioritise the time to test it depends on how much effort that will cost us compared to the benefit our users derive (directly or indirectly).

that meet the common requirements for the codebase to compile and function correctly.

We're using vanilla GNU toolchain on a vanilla ppc64 Linux distribution, so nothing custom or vendor-specific is involved that would point to an effort beyond ensuring portability, hence explicit Power8 platform support is not a concern here, I think.

Of course, if such observations do not reproduce in other cases, we can flag this as a "known issue and consider it solved."

PS: ORNL and other US labs do use Power8 GPU clusters for some testing, e.g. without a live project affiliation AFAIK even to ORNL employees only [Summitdev](#) (Power S822LC, that is Power8 + P100) is available.

Good to know. Hopefully the comment about "Initial access to the summitdev system will be limited to the OLCF CAAR teams" is now out of date.

#10 - 02/08/2019 06:50 AM - Mark Abraham

- Status changed from New to Fix uploaded

#11 - 02/13/2019 04:50 PM - Mark Abraham

- Status changed from Fix uploaded to Resolved

#12 - 02/13/2019 04:51 PM - Mark Abraham

- Status changed from Resolved to Closed

#13 - 08/12/2019 11:41 AM - Szilárd Páll

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

Files

checkforce.out	390 KB	11/08/2018	Szilárd Páll
----------------	--------	------------	--------------