

# GROMACS - Bug #2734

## regressiontests/kernel core dumps on ppc64le

11/05/2018 07:09 PM - Christoph Junghans

<b>Status:</b> In Progress	
<b>Priority:</b> Normal	
<b>Assignee:</b> Paul Bauer	
<b>Category:</b> testing	
<b>Target version:</b> future	
<b>Affected version - extra info:</b>	<b>Difficulty:</b> uncategorized
<b>Affected version:</b> 2019.3	
<b>Description</b>	
<pre>GROMACS:      gmx mdrun, version 2018.3 (double precision) Executable:    /builddir/build/BUILD/gromacs-2018.3/serial_d/bin/gmx_d Data prefix:   /builddir/build/BUILD/gromacs-2018.3 (source tree) Working dir:   /builddir/build/BUILD/gromacs-2018.3/serial_d/tests Command line:   gmx_d mdrun -h Thanx for Using GROMACS - Have a Nice Day sh: line 1:  833 Aborted                (core dumped) gmx_d mdrun -nb cpu -notunepme &gt; mdrun.out 2&gt;&amp;1 Abnormal return value for ' gmx_d mdrun      -nb cpu      -notunepme &gt;mdrun.out 2&gt;&amp;1' was -1 FAILED. Check mdrun.out, md.log file(s) in nb_kernel_ElecEwSh_VdwLJSh_GeomW4P1 for nb_kernel_ElecE wSh_VdwLJSh_GeomW4P1 1 out of 142 kernel tests FAILED</pre>	
Details here: <a href="https://koji.fedoraproject.org/koji/taskinfo?taskID=30691834">https://koji.fedoraproject.org/koji/taskinfo?taskID=30691834</a>	
<b>Related issues:</b>	
Related to GROMACS - Bug #2746: regressiontests/freeenergy coulandvdwsequenti...	<b>Closed</b>
Related to GROMACS - Bug #2747: nb_kernel_ElecEwSw_VdwBhamSw_GeomW4W4 regress...	<b>Closed</b>
Related to GROMACS - Task #3057: re-enable fusion on Power8/9	<b>New</b>
Related to GROMACS - Bug #3116: regressiontests/freeenergy core dumps on ppc64le	<b>New</b>

### 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 - 11/07/2018 11:05 AM - Paul Bauer

I added some information for the build, could you try to run the failing test on its own to see where it crashes? Thanks!

Compiler: gcc-8.2.1  
BLAS: openblas  
LAPACK: openblas  
SIMD: None  
Doulbe: ON  
fftw: 3.3.8

**#2 - 11/07/2018 01:55 PM - Christoph Junghans**

Interestingly with work with `GMX_SIMD=IBM_VSX` on ppc64le.

As this is inside an non-interactive rpm build, what exactly do I need to run?

**#3 - 11/07/2018 02:13 PM - Paul Bauer**

Very interesting, indeed.

Best would be running only the failing test in a memory checker, but I don't think this is possible if you can't go physically on the machine. Will check with people here if someone can try to reproduce this.

**#4 - 11/07/2018 04:18 PM - Christoph Junghans**

Yeah, no interactive mode, sorry!

**#5 - 11/07/2018 09:35 PM - Dominik Mierzejewski**

Paul Bauer wrote:

Very interesting, indeed.

Best would be running only the failing test in a memory checker, but I don't think this is possible if you can't go physically on the machine. Will check with people here if someone can try to reproduce this.

I have a ppc64le VM if anyone wants to debug this hands-on. Just send me your public ssh key.

**#6 - 11/08/2018 02:25 PM - Paul Bauer**

I tried reproducing this on the VM that Dominik helpfully provided, with the current head of release-2018, using the same cmake instructions. Running in valgrind shows some invalid reads when running the code, but it didn't crash for me so far.

**#7 - 11/08/2018 02:43 PM - Paul Bauer**

Ok, tried more things but can't get the test to crash. The invalid reads where because I didn't load the correct libgromacs for each build, and don't show up when done correctly. This was now again with the current head of release-2018.

**#8 - 11/08/2018 04:29 PM - Paul Bauer**

- Status changed from New to Feedback wanted

- Target version changed from 2018.4 to 2019

I'll retarget this on 2019, because I was unable to reproduce the issue on the similar VM with the build configuration used during the package build.

**#9 - 11/09/2018 06:36 PM - Szilárd Páll**

I can't repro crashes on Power8 either, but I did produce a bunch of failing regressiontests, see [#2746](#), [#2747](#). There may be something here that sometimes causes only wrong results and occasionally crashes too.

@Christoph: have the runs been repeated in the fedora system, do you see incorrect results in some cases?

**#10 - 11/09/2018 08:03 PM - Christoph Junghans**

I was just trying to build the rpm package and this issue came up in the ``%check`` block. Maybe Dominik has another idea.

**#11 - 12/17/2018 02:36 PM - Paul Bauer**

- Target version changed from 2019 to 2020

this is very likely to be postponed, because it is not clear what the actual issue is

**#12 - 01/03/2019 11:09 AM - Mark Abraham**

- Related to Bug [#2746](#): regressiontests/freeenergy coulandvdwsequential\_vdw failing on Power8 added

**#13 - 01/03/2019 11:09 AM - Mark Abraham**

- Related to Bug #2747: [nb\\_kernel\\_ElecEwSw\\_VdwBhamSw\\_GeomW4W4 regressiontest failing on Power8 added](#)

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

Gerrit received a related patchset '1' for Issue [#2734](#).  
Uploader: Szilárd Páll ([pall.szilard@gmail.com](mailto:pall.szilard@gmail.com))  
Change-Id: gromacs~release-2019~156f50e54db47f4fe30c42488f4c4f79ac474518a  
Gerrit URL: <https://gerrit.gromacs.org/9104>

**#15 - 02/07/2019 02:19 PM - Gerrit Code Review Bot**

Gerrit received a related patchset '1' for Issue [#2734](#).  
Uploader: Szilárd Páll ([pall.szilard@gmail.com](mailto:pall.szilard@gmail.com))  
Change-Id: gromacs~release-2018~156f50e54db47f4fe30c42488f4c4f79ac474518a  
Gerrit URL: <https://gerrit.gromacs.org/9105>

**#16 - 02/08/2019 06:55 AM - Mark Abraham**

- Status changed from Feedback wanted to Fix uploaded  
- Target version changed from 2020 to 2019.1

**#17 - 02/11/2019 01:26 PM - Szilárd Páll**

- Status changed from Fix uploaded to Feedback wanted

@Christoph: can you check if the change uploaded fixes the failing tests?

**#18 - 02/11/2019 02:35 PM - Christoph Junghans**

Can I test this in 2019.1, the rpm already has too many patches in it?

**#19 - 02/12/2019 08:28 AM - Mark Abraham**

Christoph Junghans wrote:

Can I test this in 2019.1, the rpm already has too many patches in it?

Sure, that sounds great.

**#20 - 02/13/2019 05:00 PM - Szilárd Páll**

- Status changed from Feedback wanted to Resolved

Applied in changeset [4a7281ef0020d0ff454608a3ee98b9984a6ac11e](#).

**#21 - 02/13/2019 05:14 PM - Paul Bauer**

- Status changed from Resolved to Closed

**#22 - 02/13/2019 08:08 PM - Szilárd Páll**

Not really ready to close until we get feedback whether the issue is solved, but I guess leaving it on "Feedback wanted" will mean it remains a release blocker?

**#23 - 02/14/2019 02:44 PM - Mark Abraham**

- Status changed from Closed to Feedback wanted  
- Target version changed from 2019.1 to 2019.2

Good idea. Postponed

**#24 - 02/19/2019 06:45 PM - Szilárd Páll**

- Status changed from Feedback wanted to Resolved

Applied in changeset [1ce795fe5693e9790eb7c33896f47d4953867127](#).

**#25 - 04/01/2019 01:13 PM - Paul Bauer**

- Status changed from Resolved to Closed

#### #26 - 06/15/2019 04:12 PM - Christoph Junghans

- File *build.log* added

- Status changed from Closed to In Progress

- Target version changed from 2019.2 to future

- Affected version changed from 2018.3 to 2019.3

It is back in 2019.3:

```
GROMACS:      gmx mdrun, version 2019.3
Executable:   /builddir/build/BUILD/gromacs-2019.3/serial/bin/gmx
Data prefix:  /builddir/build/BUILD/gromacs-2019.3 (source tree)
Working dir:  /builddir/build/BUILD/gromacs-2019.3/serial/tests
Command line:
  gmx mdrun -h
Thanx for Using GROMACS - Have a Nice Day
sh: line 1: 16588 Aborted                (core dumped) gmx mdrun -nb cpu -notunepme > mdrun.out 2>&1
Abnormal return value for ' gmx mdrun -nb cpu -notunepme >mdrun.out 2>&1' was -1
FAILED. Check mdrun.out, md.log file(s) in nb_kernel_ElecEwSw_VdwBhamSw_GeomW4W4 for nb_kernel_ElecEwSw_VdwBhamSw_GeomW4W4
1 out of 142 kernel tests FAILED
```

See <https://koji.fedoraproject.org/koji/taskinfo?taskID=35545387> and attached build.log

#### #27 - 08/12/2019 11:41 AM - Szilárd Páll

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

#### #28 - 10/03/2019 10:31 PM - Christoph Junghans

- Related to Bug #3116: regressiontests/freeenergy core dumps on ppc64le added

#### Files

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build.log	6.6 MB	06/15/2019	Christoph Junghans
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