**GROMACS - Bug #2734**

**regressiontests/kernel core dumps on ppc64le**

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

<table>
<thead>
<tr>
<th>Status</th>
<th>In Progress</th>
</tr>
</thead>
<tbody>
<tr>
<td>Priority</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee</td>
<td>Paul Bauer</td>
</tr>
<tr>
<td>Category</td>
<td>testing</td>
</tr>
<tr>
<td>Target version</td>
<td>future</td>
</tr>
<tr>
<td>Affected version</td>
<td>2019.3</td>
</tr>
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</table>

**Description**

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 > mdrun.out 2>&1
```

Abnormal return value for `gmx_d mdrun -nb cpu -notunepme >mdrun.out 2>&1` was -1

FAILED. Check mdrun.out, md.log file(s) in nb_kernel_ElecEwSh_VdwLJSh_GeomW4P1 for nb_kernel_ElecEwSh_VdwLJSh_GeomW4P1

1 out of 142 kernel tests FAILED

Details here: [https://koji.fedoraproject.org/koji/taskinfo?taskID=30691834](https://koji.fedoraproject.org/koji/taskinfo?taskID=30691834)

**Related issues:**

- Related to GROMACS - Bug #2746: regressiontests/freeenergy coulandvdwsequenti... - Closed
- Related to GROMACS - Bug #2747: nb_kernel_ElecEwSh_VdwBhamSw_GeomW4W4 regress... - Closed
- Related to GROMACS - Task #3057: re-enable fusion on Power8/9 - New
- Related to GROMACS - Bug #3116: regressiontests/freeenergy core dumps on ppc64le - 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 - 11/07/2018 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  
Double: 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 regression tests, 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 regression test 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)
Change-Id: gromacs~release-2019~f5650e54dbc47f4e30c42488f4c4f79ac474518a
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)
Change-Id: gromacs~release-2018~f5650e54dbc47f4e30c42488f4c4f79ac474518a
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 Feedback wanted to Resolved
- 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
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

Files

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<tr>
<th>File</th>
<th>Size</th>
<th>Date</th>
<th>Author</th>
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<tbody>
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<td>build.log</td>
<td>6.6 MB</td>
<td>06/15/2019</td>
<td>Christoph Junghans</td>
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