### GROMACS - Bug #1259

gcc-4.6.1 is buggy for AVX_256

05/21/2013 02:39 PM - Mark Abraham

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Mark Abraham</td>
</tr>
<tr>
<td>Category:</td>
<td></td>
</tr>
<tr>
<td>Target version:</td>
<td>4.6.x</td>
</tr>
<tr>
<td>Affected version - extra info:</td>
<td></td>
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<tr>
<td>Affected version:</td>
<td>4.6.1</td>
</tr>
<tr>
<td>Difficulty:</td>
<td>uncategorized</td>
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</tbody>
</table>

**Description**

User reported problem on mailing list with the above combination. SSE4.1 worked on his hardware. Likely [http://gcc.gnu.org/bugzilla/show_bug.cgi?id=49002](http://gcc.gnu.org/bugzilla/show_bug.cgi?id=49002) is to blame, fixed in gcc-4.6.2.

Hopefully Vishar will report back that he succeeded with AVX_256 and a more recent compiler, and we can prevent this build combination.

**Associated revisions**

Revision 310d6352 - 05/13/2014 04:16 PM - Mark Abraham

Prohibit AVX_256 with buggy gcc 4.6.1

Fixes #1259

Change-id: I7c523a90c9d0dd83d61c9d2029194429e22a27ab5d

**History**

#1 - 06/26/2013 12:31 AM - Mark Abraham
- Target version changed from 4.6.3 to 4.6.x

#2 - 08/13/2013 11:49 PM - Mark Abraham
- Status changed from New to Blocked, need info

#3 - 05/13/2014 02:26 PM - Rossen Apostolov
- Subject changed from gcc-4.6.1 probably buggy for AVX_256 to gcc-4.6.1 is buggy for AVX_256
- Status changed from Blocked, need info to Accepted

I can confirm that indeed gromacs-4.6.5 works with gcc-4.6.2, but fails with 4.6.1:

Gromacs version: VERSION 4.6.5
Precision: single
Memory model: 64 bit
MPI library: thread_mpi
OpenMP support: enabled
GPU support: disabled
invsqrt routine: gmx_software_invsqrt(x)
CPU acceleration: AVX_256
FFT library: fftpack (built-in)
Large file support: enabled
RDTSCP usage: enabled
Built on: Tue May 13 13:12 CEST 2014
Built by: rossen@harreleve.pdc.kth.se [CMAKE]
Build OS/arch: Linux 2.6.32-358.23.2.el6.x86_64 x86_64
Build CPU vendor: GenuineIntel
Build CPU brand: Intel(R) Xeon(R) CPU E3-1285 v3 @ 3.60GHz
Build CPU family: 6 Model: 60 Stepping: 3
Build CPU features: aes apic avx avx2 cmov cx8 cx16 f16c fma hlt lahf_lm mmx msr nonstop_tsc pclmulqdq pdcm pdpe1gb popcnt pse rdimm rdtscp sse2 sse3 sse4.1 sse4.2 ssse3 tdx x2apic
C compiler: /afs/pdc.kth.se/home/r/rossen/vo00/local/gcc-4.6.1/bin/gcc GNU gcc (GCC) 4.6.1

04/05/2020

#4 - 05/13/2014 04:17 PM - Gerrit Code Review Bot
Gerrit received a related patchset ‘1’ for Issue #1259.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: I7c523a90ccd8dd8fd3df6cb1914429e22a27ab5d
Gerrit URL: https://gerrit.gromacs.org/3436

#5 - 05/13/2014 08:45 PM - Mark Abraham
- Status changed from Accepted to Resolved
- % Done changed from 0 to 100

Applied in changeset 310d6352bc58c8f073d773c119a579b588828e9e.

#6 - 05/13/2014 09:03 PM - Rossen Apostolov
- Status changed from Resolved to Closed