Gromacs - Bug #1126

ICC 11 fails regression tests

01/21/2013 10:21 PM - Roland Schulz

<table>
<thead>
<tr>
<th>Status</th>
<th>Closed</th>
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<tbody>
<tr>
<td>Priority</td>
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</tr>
<tr>
<td>Assignee</td>
<td>Roland Schulz</td>
</tr>
<tr>
<td>Category</td>
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<tr>
<td>Target version</td>
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<td>Affected version</td>
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<td>extra info</td>
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</tr>
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**Description**

icc (ICC) 11.1 20100414

1 failed test: nb_kernel_ElecCSTab_VdwCSTab_GeomW4W4. It fails with SSE4_1. It is OK with Acceleration SSE2 or None.

It is ok with icc 12 on the same machine. Is this a reason to blacklist ICC 11?

```c
f[ 36] ( 1.06046e+03 -3.78918e+02 -2.22384e+02) - ( 9.61060e+02 -5.53853e+02 -8.02258e+01)
 f[ 37] (-1.68256e+02  9.08493e+01 -3.12895e+01) - ( 2.27906e+02 -1.11561e+01 -3.48740e+01)
 f[ 40] (-4.41078e+02 -1.12324e+03 -5.13136e+02) - (-4.63392e+02 -1.20941e+03 -4.08784e+02)
 f[ 41] (-4.22774e+01  5.93652e+02  4.11376e+02) - ( 1.25182e+01  3.52427e+02  3.81509e+02)
 f[ 44] (-3.28924e+02 -5.91344e+02  2.79622e+02) - (-5.10715e+01 -4.70265e+02  3.02135e+02)
 f[ 45] ( 4.96087e+01 -6.61228e+01 -8.32026e+01) - (-6.75656e+00 -1.55283e+00 -1.69959e+02)
 f[ 46] ( 1.55255e+02  6.69600e+02 -1.02909e+02) - ( 2.03064e+02  6.90433e+02 -9.90349e+01)
 f[ 48] (-1.79745e+02  9.15839e+02 -1.75282e+02) - (-4.90734e+01  9.27426e+02 -5.30883e+01)
```

**Associated revisions**

Revision c5ac1409 - 02/18/2013 10:15 PM - Roland Schulz

Issue errors/warnings for ICC before 12.0.0

ICC 11.1 with SSE4.1 gives incorrect results, so CMake will refuse to build with that minor version. Given that we currently don't know anything specific and 11 is old, we warn with any version older than 12.0.0. If more information is available later, this warning can be made more specific.

Fixes #1126

Change-Id: l3c37844c69ce34769187f288c43cd8aef4086c53

Revision de9be0d6 - 06/13/2013 09:45 AM - Roland Schulz

Issue errors/warnings for ICC before 12.0.0

ICC 11.1 with SSE4.1 gives incorrect results, so CMake will refuse to build with that minor version. Given that we currently don't know anything specific and 11 is old, we warn with any version older than 12.0.0. If more information is available later, this warning can be made more specific.

Fixes #1126
History

#1 - 01/21/2013 10:37 PM - Erik Lindahl
There are later patches of icc 11 - at least 11.2

However, I'm not going to put any work into debugging a 3-year old compiler when later versions work fine, so if you don't have access to test those a warning might be in place.

#2 - 01/22/2013 12:05 AM - Roland Schulz
- Status changed from New to In Progress
- Assignee changed from Erik Lindahl to Roland Schulz

https://gerrit.gromacs.org/#/c/2111/

No I don't have any other 11 version. I agree one shouldn't use such an old version and it doesn't make sense to invest time. I only compiled with ICC 11 because one user reported on the gmx-users list problems with ICC 11 (and GB - so I'm not sure it is related) and so I thought it would be good to test. I added the warning.

#3 - 01/22/2013 03:29 PM - Mark Abraham
Confirmed with icc 11.1 20100806, also.

#4 - 04/29/2013 07:53 PM - Mark Abraham
- Status changed from In Progress to Resolved
- Affected version set to 4.6

#5 - 06/10/2013 08:13 PM - Mark Abraham
Sorry, posted on wrong issue

#6 - 06/13/2013 09:55 AM - Roland Schulz
- % Done changed from 0 to 100

Applied in changeset de9be0d6838e9b8cb66f5370da0d8dece38eacb.

#7 - 12/16/2013 05:38 PM - Rossen Apostolov
- Status changed from Resolved to Closed