investigate whether clang 3.0 really is buggy for the 4.6 group kernels

11/20/2012 06:11 PM - Mark Abraham

Status: Rejected
Priority: Low
Assignee: Mark Abraham
Category: build system
Target version: 4.6.x

Description
Erik's testing of group kernels on clang 3.0 exposed erroneous behaviour that was not seen in clang 3.1, so we suppose there is a compiler bug. We haven't had time to track anything down, so for the time being we have disallowed GROMACS builds for clang 3.0 in https://gerrit.gromacs.org/#/c/1720/.

It would be good to find out why, in case it's a real bug in either GROMACS or clang that is not actually resolved correctly. Even if we can do a bisection on clang, or scan its change log for something that leaps out at us, we don't have time to deal with this now, and perhaps not before 4.6.

Associated revisions
Revision bc34c5f9 - 11/29/2012 11:37 AM - Mark Abraham
Refuse to build with clang 3.0

The 3.0 compiler is definitely buggy for the group kernels, so we refuse to build with this version at all. The test works for both C and C++, and correctly detects (say) Apple clang 4.1 as clang based on the LLVM 3.0 back end, like everybody else seems to base their numbering on!

Refs #1039
Change-Id: I259fab3c022e0cf94c06ff34d2f3af38663d1d7b7

History
#1 - 11/22/2012 01:26 AM - Szilárd Páll

Just tried with "Ubuntu clang version 3.0-6ubuntu3 (tags/RELEASE_30/final) (based on LLVM 3.0)" and with this version I get a bunch of errors, among others the nbnxn_pme and nbnxn_vsite tests also fail which indicates that the NxN PME kernels are also messed up. This is surprising because we had no problem with the Apple clang 3.0 which AFAIK was from upstream 3.0svn (unless Apple fixed bugs in their version and didn't contribute them back upstream).

All 16 simple tests PASSED
FAILED. Check checkpot.out (10 errors), checkforce.out (2072 errors) files in fe_test
FAILED. Check checkpot.out (58 errors), checkforce.out (1123 errors) files in nacl
FAILED. Check checkpot.out (6 errors), checkforce.out (2347 errors) files in nbnxn_pme
FAILED. Check checkpot.out (8 errors), checkforce.out (1762 errors) files in nbnxn_vsite
FAILED. Check checkpot.out (42 errors), checkforce.out (1052 errors) files in tip4p
FAILED. Check checkpot.out (32 errors), checkforce.out (524 errors) files in tip4p_continue
FAILED. Check checkpot.out (86 errors), checkforce.out (3124 errors) files in tip4pflex
7 out of 19 complex tests FAILED
FAILED. Check checkpot.out (4 errors), checkforce.out (6 errors) files in nb_kernel_ElecEw_VdwBham_GeomP1P1
FAILED. Check checkpot.out (4 errors), checkforce.out (857 errors) files in nb_kernel_ElecEw_VdwBham_GeomW3P1
FAILED. Check checkpot.out (4 errors), checkforce.out (1260 errors) files in nb_kernel_ElecEw_VdwBham_GeomW3W3
FAILED. Check checkpot.out (4 errors), checkforce.out (724 errors) files in nb_kernel_ElecEw_VdwBham_GeomW4P1
FAILED. Check checkpot.out (4 errors), checkforce.out (1326 errors) files in nb_kernel_ElecEw_VdwBham_GeomW4W4
FAILED. Check checkpot.out (4 errors), checkforce.out (6 errors) files in nb_kernel_{ElecEw_VdwCSTab_GeomP1P1}
FAILED. Check checkpot.out (4 errors), checkforce.out (648 errors) files in nb_kernel_{ElecEw_VdwCSTab_GeomW3P1}
FAILED. Check checkpot.out (4 errors), checkforce.out (1245 errors) files in nb_kernel_{ElecEw_VdwCSTab_GeomW3W3}
FAILED. Check checkpot.out (2 errors), checkforce.out (693 errors) files in nb_kernel_{ElecEw_VdwCSTab_GeomW4P1}
FAILED. Check checkpot.out (4 errors), checkforce.out (1299 errors) files in nb_kernel_{ElecEw_VdwCSTab_GeomW4W4}
FAILED. Check checkpot.out (4 errors), checkforce.out (6 errors) files in nb_kernel_{ElecEw_VdwLJ_GeomP1P1}
FAILED. Check checkpot.out (4 errors), checkforce.out (648 errors) files in nb_kernel_{ElecEw_VdwLJ_GeomW3P1}
FAILED. Check checkpot.out (2 errors), checkforce.out (693 errors) files in nb_kernel_{ElecEw_VdwLJ_GeomW4P1}
FAILED. Check checkpot.out (4 errors), checkforce.out (1299 errors) files in nb_kernel_{ElecEw_VdwLJ_GeomW4W4}
FAILED. Check checkpot.out (4 errors), checkforce.out (1770 errors) files in nb_kernel_{ElecEw_VdwNone_GeomP1P1}
FAILED. Check checkpot.out (4 errors), checkforce.out (657 errors) files in nb_kernel_{ElecEw_VdwNone_GeomW3P1}
FAILED. Check checkpot.out (4 errors), checkforce.out (1263 errors) files in nb_kernel_{ElecEw_VdwNone_GeomW3W3}
FAILED. Check checkpot.out (2 errors), checkforce.out (633 errors) files in nb_kernel_{ElecEw_VdwNone_GeomW4P1}
FAILED. Check checkpot.out (4 errors), checkforce.out (651 errors) files in nb_kernel_{ElecEwSh_VdwBhamSh_GeomP1P1}
FAILED. Check checkpot.out (4 errors), checkforce.out (651 errors) files in nb_kernel_{ElecEwSh_VdwBhamSh_GeomW3P1}
FAILED. Check checkpot.out (4 errors), checkforce.out (688 errors) files in nb_kernel_{ElecEwSh_VdwBhamSh_GeomW3W3}
FAILED. Check checkpot.out (6 errors), checkforce.out (727 errors) files in nb_kernel_{ElecEwSh_VdwBhamSh_GeomW4P1}
FAILED. Check checkpot.out (4 errors), checkforce.out (1683 errors) files in nb_kernel_{ElecEwSh_VdwBhamSh_GeomW4W4}
FAILED. Check checkpot.out (4 errors), checkforce.out (6 errors) files in nb_kernel_{ElecEwSh_VdwLJSh_GeomP1P1}
FAILED. Check checkpot.out (4 errors), checkforce.out (642 errors) files in nb_kernel_{ElecEwSh_VdwLJSh_GeomW3P1}
FAILED. Check checkpot.out (4 errors), checkforce.out (1668 errors) files in nb_kernel_{ElecEwSh_VdwLJSh_GeomW3W3}
FAILED. Check checkpot.out (4 errors), checkforce.out (681 errors) files in nb_kernel_{ElecEwSh_VdwLJSh_GeomW4P1}
FAILED. Check checkpot.out (4 errors), checkforce.out (1668 errors) files in nb_kernel_{ElecEwSh_VdwLJSh_GeomW4W4}
FAILED. Check checkpot.out (4 errors), checkforce.out (1779 errors) files in nb_kernel_{ElecEwSh_VdwNone_GeomP1P1}
FAILED. Check checkpot.out (4 errors), checkforce.out (642 errors) files in nb_kernel_{ElecEwSh_VdwNone_GeomW3P1}
FAILED. Check checkpot.out (4 errors), checkforce.out (1557 errors) files in nb_kernel_{ElecEwSh_VdwNone_GeomW3W3}
FAILED. Check checkpot.out (4 errors), checkforce.out (630 errors) files in nb_kernel_{ElecEwSh_VdwNone_GeomW4P1}
FAILED. Check checkpot.out (4 errors), checkforce.out (1638 errors) files in nb_kernel_{ElecEwSh_VdwNone_GeomW4W4}
FAILED. Check checkpot.out (4 errors), checkforce.out (48 errors) files in nb_kernel_{ElecEwSw_VdwBhamSw_GeomP1P1}
FAILED. Check checkpot.out (4 errors), checkforce.out (723 errors) files in nb_kernel_{ElecEwSw_VdwBhamSw_GeomW3P1}
FAILED. Check checkpot.out (4 errors), checkforce.out (1758 errors) files in nb_kernel_{ElecEwSw_VdwBhamSw_GeomW3W3}
FAILED. Check checkpot.out (4 errors), checkforce.out (1734 errors) files in nb_kernel_{ElecEwSw_VdwBhamSw_GeomW4P1}
FAILED. Check checkpot.out (4 errors), checkforce.out (717 errors) files in nb_kernel_{ElecEwSw_VdwBhamSw_GeomW4W4}
FAILED. Check checkpot.out (4 errors), checkforce.out (48 errors) files in nb_kernel_{ElecEwSw_VdwLJSw_GeomP1P1}
FAILED. Check checkpot.out (4 errors), checkforce.out (1755 errors) files in nb_kernel_{ElecEwSw_VdwLJSw_GeomW3P1}
FAILED. Check checkpot.out (2 errors), checkforce.out (765 errors) files in nb_kernel_{ElecEwSw_VdwLJSw_GeomW3W3}
FAILED. Check checkpot.out (4 errors), checkforce.out (1737 errors) files in nb_kernel_{ElecEwSw_VdwLJSw_GeomW4P1}
FAILED. Check checkpot.out (4 errors), checkforce.out (1860 errors) files in nb_kernel_{ElecEwSw_VdwNone_GeomP1P1}
FAILED. Check checkpot.out (4 errors), checkforce.out (654 errors) files in nb_kernel_{ElecEwSw_VdwNone_GeomW3P1}
FAILED. Check checkpot.out (4 errors), checkforce.out (1482 errors) files in nb_kernel_{ElecEwSw_VdwNone_GeomW3W3}
FAILED. Check checkpot.out (4 errors), checkforce.out (642 errors) files in nb_kernel_{ElecEwSw_VdwNone_GeomW4P1}
FAILED. Check checkpot.out (2 errors), checkforce.out (1527 errors) files in nb_kernel_{ElecEwSw_VdwNone_GeomW4W4}
50 out of 147 kernel tests FAILED
FAILED. Check checkpot.out (237 errors) files in coulandvdwsequential_coul
FAILED. Check checkpot.out (122 errors) files in coulandvdwsequential_vdw
FAILED. Check checkpot.out (279 errors) files in coulandvdwtogether
FAILED. Check checkpot.out (82 errors) files in relative
FAILED. Check checkpot.out (139 errors) files in restraints
FAILED. Check checkpot.out (14 errors), checkforce.out (3234 errors) files in vdwalone
6 out of 9 freeenergy tests FAILED
All 42 pdb2gmx tests PASSED

11/20/2015 2/3
Just did another batch of simple checking using the aforementioned vanilla clang 3.0:
- I get pretty much the same errors (same tests failing) with O3, O2, and O1.
- The code doesn't even compile with O0:

fatal error: error in backend: Cannot select: intrinsic %llvm.x86.avx.vextractf128.ps.256

If anybody can do further checking using Apple clang 3.0 (which is some obscure 3.0 svn version + who know how many/what kind of Apple patches), feel free to do so. I consider clang 3.0 useless for GROMACS (it's ridiculously fast, though :).