Gromacs - Bug #1719
severe performance regression on Piledriver

04/28/2015 03:07 AM - Szilárd Páll

| Status: | Closed |
| Priority: | Normal |
| Assignee: | |
| Category: | core library |
| Target version: | |
| Affected version: | 5.1-beta1 |
| Affected version: | 5.0.4 |

Description
I measure 20-30% performance regression in the non-bonded kernels on AMD Piledriver. The bonded kernels seem to have regressed too, but the effect here is only 4-8%.

The former has barely changed in 5.1. The bonded performance has improved in 5.1, but the source of the original issue may have simply been masked by unrelated improvements (in reduction and RB dihedrals).

Associated revisions
Revision ce772452 - 04/28/2015 01:08 PM - Berk Hess
Re-enabled FMA for AVX-128-FMA

All FMA instructions for AVX-128-FMA were not renamed during a SIMD macro name change, which effectively removed FMA support for AMD.
Fixes #1719.

Change-Id: I855a379d2974d37c586794a191606a360a89c5f

History
#1 - 04/28/2015 11:29 AM - Berk Hess
- Status changed from New to In Progress

For a water box with PME I get 88 sec in nbnxn kernel with 4.6 and 140 sec with 5.1!
The only difference I found in the log files is that -Wno-strict-overflow -fomit-frame-pointer have been removed. Adding those gives 102 sec, so an enormous difference, but still 15% slower than 4.6.

#2 - 04/28/2015 12:15 PM - Gerrit Code Review Bot
Gerrit received a related patchset ‘1’ for Issue #1719.
Uploader: Berk Hess (hess@kth.se)
Change-Id: I855a379d2974d37c586794a191606a360a89c5f
Gerrit URL: https://gerrit.gromacs.org/4533

#3 - 04/29/2015 02:05 PM - Mark Abraham
- Status changed from In Progress to Fix uploaded

Did that fix resolve the full issue?
Mark Abraham wrote:

Did that fix resolve the full issue?

Yes, it has (that's what I meant by verify +1).

#5 - 04/29/2015 02:44 PM - Mark Abraham

- Status changed from Fix uploaded to Closed

ok thanks

Files

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