BUILD_OWN_FFTW fails regression tests

06/02/2018 12:08 AM - Erik Lindahl

Status: Closed
Priority: High
Assignee: build system
Category: build system
Target version: 2018.2

Description
Ubuntu-18.04, default compilers, and default builds.

If fftw-3.3.5 is downloaded manually and compiled, all regression tests pass.

With -DBUILD_OWN_FFTW=ON, the fft/correlationfunctions tests fail.

Associated revisions
Revision c17474b3 - 06/06/2018 09:48 AM - Erik Lindahl
Bump GMX_BUILD_OWN_FFTW to 3.3.8 to avoid bugs

FFTW-3.3.8 seems to fix build errors with AVX-512, and as reported on the FFTW web page it also removes the -ffast-math flag which results in errors with gcc-8.

Fixes #2541.

Change-Id: Ibe4ef0040986e4b83f92f0bb404c72fa1b5e11ea

History
#1 - 06/04/2018 02:54 PM - Szilárd Páll

The FFT unit tests fail too. The funny thing is that it does not fail on a Threadripper machine, but it does fail on a Xeon Silver CPU. Even more fun is that running with relative path (i.e. bin/fft-test) passes, but not with absolute path as invoked by ctest:

```c
#0 0x00000007fff7787c82 in t1fv_3 () from /tmp/gromacs-18/build/bin/../../lib/libgromacs.so.3
#1 0x00000007fff77ba29b in apply () from /tmp/gromacs-18/build/bin/../../lib/libgromacs.so.3
#2 0x00000007fff74bbdb0 in apply () from /tmp/gromacs-18/build/bin/../../lib/libgromacs.so.3
#3 0x00000007fff77bb5b07 in apply_dit () from /tmp/gromacs-18/build/bin/../../lib/libgromacs.so.3
#4 0x00000007fff74bbdb0 in apply () from /tmp/gromacs-18/build/bin/../../lib/libgromacs.so.3
#5 0x00000007fff73eb954 in gmx_fft_1d (fft=0x55555587bac0, dir=GMX_FFT_FORWARD, in_data=0x555555861ae0, out_data=0x555555862270) at /tmp/gromacs-18/src/gromacs/fft/fft_fftw3.cpp:457
#6 0x00000007fff73eb989 in gmx_fft_many_1d (fft=0x55555587bac0, dir=GMX_FFT_FORWARD, in_data=0x555555861ae0, out_data=0x555555862270) at /tmp/gromacs-18/src/gromacs/fft/fft_fftw3.cpp:470
#7 0x00000005555557e86 in (anonymous namespace)::ManyFFTTest_Complex1DLength48Multi5Test::TestBody (this=0x555555841020) at /tmp/gromacs-18/src/gromacs/fft/tests/fft.cpp:457
#8 0x0000000555555d35ca in testing::internal::HandleSehExceptionsInMethodIfSupported<testing::Test, void> (objcet=0x555555841020, method=virtual testing::Test::TestBody(), location=0x555555563df3 "the test body") at /tmp/gromacs-18/src/external/gmock-1.7.0/gtest/src/gtest.cc:2076
#9 0x0000000555555dec27 in testing::internal::HandleExceptionsInMethodIfSupported<testing::Test, void> (object=0x555555841020, method=virtual testing::Test::TestBody(), location=0x555555563df3 "the test body") at /tmp/gromacs-18/src/external/gmock-1.7.0/gtest/src/gtest.cc:2076
```

02/22/2020
Both Complex1DLength48Multi5Test fw/bw seems to segv. Can't add much more.

#2 - 06/04/2018 03:39 PM - Szilárd Páll
Removing the --enable-avx512 flag also eliminates the issue: [http://termbin.com/vbu5](http://termbin.com/vbu5)

I've had a quick look at the perf scan I did on FFTW 3.3.7 and while the data was awfully noisy, I did saw a few cases where the builds with sse+avx+avx2+avx512 did seems to be faster, but in most cases the sse+avx+avx2+avx512 runs faster.

As a side-note, the current code seems heavy-handed with adding the AVX512 flag; it uses it for compiling FFTW when any flavor of AVX is used. In the current setup, as we already use conditionality, and given that a single FFTW AVX512 kernel might throttle the CPU by another 10-15% (and result in performance loss in other parts of the code build explicitly with AVX2), we should change the condition on line 70 to:

```
elseif(${GMX_SIMD_ACTIVE} MATCHES "^(AVX512)"
```

#3 - 06/04/2018 08:03 PM - Erik Lindahl
I just had a look at the FFTW page, and apparently FFTW-3.3.7 in combination with GCC-8 results in broken builds due to -ffast-math, so it seems prudent that we also upgrade to use FFTW-3.3.8 before GCC-8 becomes widespread.

#4 - 06/05/2018 11:58 AM - Erik Lindahl
FFTW-3.3.8 seems to fix this problem too, so I'll push a change where we simply bump the version for now.

#5 - 06/05/2018 11:58 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2541.
Uploader: Erik Lindahl (erik.lindahl@gmail.com)
Change-Id: gromacs~release-2018~Ibe4ef0040986e4b83f92f0bb404c72fa1b5e11ea
Gerrit URL: [https://gerrit.gromacs.org/7975](https://gerrit.gromacs.org/7975)

#6 - 06/06/2018 10:15 AM - Erik Lindahl
- Status changed from Accepted to Resolved

Applied in changeset c17474b3a82a544b5a145baf73285e7c321495ed.

#7 - 06/07/2018 01:48 AM - Mark Abraham
- Category set to build system
- Status changed from Resolved to Closed
- Target version set to 2018.2