

## GROMACS - Bug #2892

### Wrong avx-512 support for own fftw build using clang-6

03/13/2019 11:36 AM - Bernd Doser

<b>Status:</b> Closed	
<b>Priority:</b> Normal	
<b>Assignee:</b>	
<b>Category:</b> build system	
<b>Target version:</b> 2019.2	
<b>Affected version - extra info:</b> tested versions 2019.1 and 2018.6	<b>Difficulty:</b> uncategorized
<b>Affected version:</b> 2019	
<b>Description</b>	
Building GROMACS 2019.1 with	
<pre>cmake -DCMAKE_BUILD_TYPE=release -DGMX_BUILD_OWN_FFTW=ON .. make</pre>	
using clang-6, I get following error during fftw build:	
<pre>/work/build/clang/src/external/build-fftw/fftwBuild-prefix/src/fftwBuild/simd-support/simd-avx512.h:48:2: error: "compiling simd-avx512.h without avx-512f support</pre>	
There is no error doing the same with gcc-7.	
Both are using the same optimization flags for FFTW (--enable-sse2;--enable-avx;--enable-avx2;--enable-avx512), whereas used processor is only supporting avx and avx2.	
Best regards, Bernd	

#### Associated revisions

##### Revision 7e1a8b8e - 03/19/2019 10:33 AM - Mark Abraham

Prevented FFTW build errors with clang and AVX-512

FFTW hard-codes the inclusion of files that does not work with its AVX-512 flags when using the clang compiler, so in this case GROMACS should compile without AVX-512 support.

Updated release notes, but didn't update the install guide for this niche case.

Fixes #2892

Change-Id: Iida18fad66e654511937d51ee58f42440de2a321d

#### History

##### #1 - 03/18/2019 12:30 PM - Mark Abraham

- Status changed from New to Feedback wanted

- Target version set to 2019.2

I presume that error is coming from clang-6 being the compiler used to compile FFTW. I can reproduce that with clang-6 and clang-7 if I use CC and CXX environment variables to influence the compiler chosen by the fftw configure call (which the GROMACS build system does not attempt to control). I deduce that FFTW does not support clang on KNL architectures.

Thus if you want to compile GROMACS with clang and use the build-own-fftw feature, then you should set the compilers to use with GROMACS with CMAKE\_C\_COMPILER and CMAKE\_CXX\_COMPILER, and let the FFTW configure find GCC from the environment.

Perhaps we should update our docs accordingly

**#2 - 03/18/2019 12:47 PM - Bernd Doser**

Dear Mark,

thanks for the verification. I was setting the compiler with

```
-DCMAKE_C_COMPILER=clang  
-DCMAKE_CXX_COMPILER=clang++
```

As my processor is not supporting avx512, I would assume the FFTW optimization flags are wrong. If I fix them in src/external/build-fftw/CMakeLists.txt, everything works fine with clang.

Please see <https://github.com/HITS-MCM/gromacs-ramd/commit/52eda180ee9390be43621da10851df60854f63e0>

Best regards,  
Bernd

**#3 - 03/19/2019 10:27 AM - Mark Abraham**

Bernd Doser wrote:

Dear Mark,

thanks for the verification. I was setting the compiler with

```
-DCMAKE_C_COMPILER=clang  
-DCMAKE_CXX_COMPILER=clang++
```

Sure, that controls the compiler used for GROMACS. It does not affect the compiler used for building FFTW in the case at hand.

As my processor is not supporting avx512, I would assume the FFTW optimization flags are wrong. If I fix them in src/external/build-fftw/CMakeLists.txt, everything works fine with clang.

Please see <https://github.com/HITS-MCM/gromacs-ramd/commit/52eda180ee9390be43621da10851df60854f63e0>

OK. Clearly fftw cannot be built by clang with AVX-512 support.

**#4 - 03/19/2019 10:34 AM - Gerrit Code Review Bot**

Gerrit received a related patchset '1' for Issue [#2892](#).  
Uploader: Mark Abraham ([mark.j.abraham@gmail.com](mailto:mark.j.abraham@gmail.com))  
Change-Id: gromacs~release-2019~lda18fad66e654511937d51ee58f42440de2a321d  
Gerrit URL: <https://gerrit.gromacs.org/9331>

**#5 - 03/22/2019 05:00 PM - Mark Abraham**

- Status changed from *Feedback wanted* to *Resolved*

Applied in changeset [7e1a8b8e135f1f5587f9ddcba086a745548ca6ed](#).

**#6 - 03/25/2019 01:38 PM - Paul Bauer**

- Status changed from *Resolved* to *Closed*