

GROMACS - Bug #2828

Installation issue on Power 9 system with SIMD support

01/12/2019 03:59 AM - Mayank Vats

Status: Feedback wanted	
Priority: Normal	
Assignee:	
Category:	
Target version:	
Affected version - extra info:	Difficulty: uncategorized
Affected version: 2019	

Description

Installed okay with

```
-DGMX_SIMD=None
```

However, after FFTW installation with

```
./configure --prefix=/gpfs/u/home/MMBS/MMBSvats/barn-shared/BGQ_MV/SIMD/fftw3 --enable-shared --enable-threads --enable-openmp --disable-fortran --enable-float *--enable-vsx*
```

and

```
cmake .. -DCMAKE_INSTALL_PREFIX=/gpfs/u/home/MMBS/MMBSvats/barn-shared/BGQ_MV/SIMD/gromacs/ -DCMAKE_PREFIX_PATH=/gpfs/u/home/MMBS/MMBSvats/barn-shared/BGQ_MV/SIMD/fftw3/ -DGMX_PREFER_STATIC_LIBS=ON
```

completes successfully, followed by

```
make -j16 install
```

I get the following errors:

```
In file included from /gpfs/u/home/MMBS/MMBSvats/barn-shared/BGQ_MV/SIMD/gromacs-2019/src/gromacs/simd/impl_ibm_vsx/impl_ibm_vsx.h:51:0,
                 from /gpfs/u/home/MMBS/MMBSvats/barn-shared/BGQ_MV/SIMD/gromacs-2019/src/gromacs/simd/simd.h:147,
                 from /gpfs/u/home/MMBS/MMBSvats/barn-shared/BGQ_MV/SIMD/gromacs-2019/src/gromacs/pbcutil/pbc-simd.h:51,
                 from /gpfs/u/home/MMBS/MMBSvats/barn-shared/BGQ_MV/SIMD/gromacs-2019/src/gromacs/pbcutil/pbc-simd.cpp:45:
/gpfs/u/home/MMBS/MMBSvats/barn-shared/BGQ_MV/SIMD/gromacs-2019/src/gromacs/simd/impl_ibm_vsx/impl_ibm_vsx_simd_double.h: In function 'void gm::store(int32_t*, gm::SimdDInt32)':
/gpfs/u/home/MMBS/MMBSvats/barn-shared/BGQ_MV/SIMD/gromacs-2019/src/gromacs/simd/impl_ibm_vsx/impl_ibm_vsx_simd_double.h:190:42: sorry, unimplemented: unexpected AST of kind compound_literal_expr
    m[0] = vec_extract(x.simdInternal_, 0);
                                   ^
/gpfs/u/home/MMBS/MMBSvats/barn-shared/BGQ_MV/SIMD/gromacs-2019/src/gromacs/simd/impl_ibm_vsx/impl_ibm_vsx_simd_double.h:190: confused by earlier errors, bailing out
```

```
In file included from /gpfs/u/home/MMBS/MMBSvats/barn-shared/BGQ_MV/SIMD/gromacs-2019/src/gromacs/simd/impl_ibm_vsx/impl_ibm_vsx.h:51:0,
                 from /gpfs/u/home/MMBS/MMBSvats/barn-shared/BGQ_MV/SIMD/gromacs-2019/src/gromacs/simd/simd.h:147,
                 from /gpfs/u/home/MMBS/MMBSvats/barn-shared/BGQ_MV/SIMD/gromacs-2019/src/gromacs/pbcutil/pbc-simd.h:51,
                 from /gpfs/u/home/MMBS/MMBSvats/barn-shared/BGQ_MV/SIMD/gromacs-2019/src/gromacs/pbcutil/pbc-simd.cpp:45:
/gpfs/u/home/MMBS/MMBSvats/barn-shared/BGQ_MV/SIMD/gromacs-2019/src/gromacs/simd/impl_ibm_vsx/impl_ibm_vsx_simd_double.h: In function 'void gm::store(int32_t*, gm::SimdDInt32)':
```

```

/gpfs/u/home/MMBS/MMBSvats/barn-shared/BGQ_MV/SIMD/gromacs-2019/src/gromacs/simd/impl_ibm_vsx/impl
_ibm_vsx_simd_double.h:190:42: sorry, unimplemented: unexpected AST of kind compound_literal_expr
    m[0] = vec_extract(x.simdInternal_, 0);
                ^
/gpfs/u/home/MMBS/MMBSvats/barn-shared/BGQ_MV/SIMD/gromacs-2019/src/gromacs/simd/impl_ibm_vsx/impl
_ibm_vsx_simd_double.h:190: confused by earlier errors, bailing out

In file included from /gpfs/u/home/MMBS/MMBSvats/barn-shared/BGQ_MV/SIMD/gromacs-2019/src/gromacs/
simd/impl_ibm_vsx/impl_ibm_vsx.h:51:0,
    from /gpfs/u/home/MMBS/MMBSvats/barn-shared/BGQ_MV/SIMD/gromacs-2019/src/gromacs/
simd/simd.h:147,
    from /gpfs/u/home/MMBS/MMBSvats/barn-shared/BGQ_MV/SIMD/gromacs-2019/src/gromacs/
tables/cubicsplinetable.h:50,
    from /gpfs/u/home/MMBS/MMBSvats/barn-shared/BGQ_MV/SIMD/gromacs-2019/src/gromacs/
tables/cubicsplinetable.cpp:45:
/gpfs/u/home/MMBS/MMBSvats/barn-shared/BGQ_MV/SIMD/gromacs-2019/src/gromacs/simd/impl_ibm_vsx/impl
_ibm_vsx_simd_double.h: In function 'void gmh::store(int32_t*, gmh::SimdDInt32)':
/gpfs/u/home/MMBS/MMBSvats/barn-shared/BGQ_MV/SIMD/gromacs-2019/src/gromacs/simd/impl_ibm_vsx/impl
_ibm_vsx_simd_double.h:190:42: sorry, unimplemented: unexpected AST of kind compound_literal_expr
    m[0] = vec_extract(x.simdInternal_, 0);
                ^
/gpfs/u/home/MMBS/MMBSvats/barn-shared/BGQ_MV/SIMD/gromacs-2019/src/gromacs/simd/impl_ibm_vsx/impl
_ibm_vsx_simd_double.h:190: confused by earlier errors, bailing out

In file included from /gpfs/u/home/MMBS/MMBSvats/barn-shared/BGQ_MV/SIMD/gromacs-2019/src/gromacs/
simd/impl_ibm_vsx/impl_ibm_vsx.h:51:0,
    from /gpfs/u/home/MMBS/MMBSvats/barn-shared/BGQ_MV/SIMD/gromacs-2019/src/gromacs/
simd/simd.h:147,
    from /gpfs/u/home/MMBS/MMBSvats/barn-shared/BGQ_MV/SIMD/gromacs-2019/src/gromacs/
tables/quadraticsplinetable.h:64,
    from /gpfs/u/home/MMBS/MMBSvats/barn-shared/BGQ_MV/SIMD/gromacs-2019/src/gromacs/
tables/quadraticsplinetable.cpp:45:
/gpfs/u/home/MMBS/MMBSvats/barn-shared/BGQ_MV/SIMD/gromacs-2019/src/gromacs/simd/impl_ibm_vsx/impl
_ibm_vsx_simd_double.h: In function 'void gmh::store(int32_t*, gmh::SimdDInt32)':
/gpfs/u/home/MMBS/MMBSvats/barn-shared/BGQ_MV/SIMD/gromacs-2019/src/gromacs/simd/impl_ibm_vsx/impl
_ibm_vsx_simd_double.h:190:42: sorry, unimplemented: unexpected AST of kind compound_literal_expr
    m[0] = vec_extract(x.simdInternal_, 0);
                ^
/gpfs/u/home/MMBS/MMBSvats/barn-shared/BGQ_MV/SIMD/gromacs-2019/src/gromacs/simd/impl_ibm_vsx/impl
_ibm_vsx_simd_double.h:190: confused by earlier errors, bailing out

Preprocessed source stored into /tmp/cc5eCYfS.out file, please attach this to your bugreport.
Preprocessed source stored into /tmp/cce8lFiY.out file, please attach this to your bugreport.
Preprocessed source stored into /tmp/cciu7u8v.out file, please attach this to your bugreport.
Preprocessed source stored into /tmp/ccQoVrMG.out file, please attach this to your bugreport.

I've attached the .out files and the CMake error and output files.

```

History

#1 - 01/18/2019 11:54 AM - Szilárd Páll

- Category deleted (build system)
- Status changed from New to Feedback wanted

You are using a very old gcc version (4.8 series it seems) which most likely has broken VSX support. Please use something modern, e.g. gcc 7/8.

There is no value in even trying to make such old compilers work as they will anyway produce slower code.

Files

File Name	Size	Date	Author
CMakeError.log	104 KB	01/12/2019	Mayank Vats
CMakeOutput.log	398 KB	01/12/2019	Mayank Vats
cc5eCYfS.out	1.77 MB	01/12/2019	Mayank Vats
cce8lFiY.out	1.43 MB	01/12/2019	Mayank Vats
cciu7u8v.out	1.45 MB	01/12/2019	Mayank Vats

