**GROMACS - Bug #2466**

**Compile error on Mac with CUDA support**

03/26/2018 12:44 AM - Scott Calabrese Barton

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<tbody>
<tr>
<td>Priority:</td>
<td>Low</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Szilárd Páll</td>
</tr>
<tr>
<td>Category:</td>
<td>build system</td>
</tr>
<tr>
<td>Target version:</td>
<td></td>
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<tr>
<td>Affected version - extra info:</td>
<td></td>
</tr>
<tr>
<td>Affected version:</td>
<td>2018.1</td>
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**Description**

I'm unable to compile 2018 or 2018.1 on Mac with CUDA support. I am using macOS 10.13.3 with Xcode 9.2 and CUDA Toolkit 9.1. fftw is installed via HomeBrew.

I am able to compile and run GROMACS 2016.5 using the following cmake command:

```
$ cmake .. -DGMX_GPU=on -DCMAKE_INSTALL_PREFIX=/usr/local/gromacs -DGMX_OPENMP=ON
```

However, when I try this approach with 2018 or 2018.1, I get the following error using the make command:

```
/Users/scb/desktop/build/gromacs-2018.1/src/gromacs/mdlib/nbnxn_cuda/nbnxn_cuda_kernel_pruneonly.cu(41): error: explicit instantiation definition directive for __global__ functions with clang host compiler is not yet supported
/Users/scb/desktop/build/gromacs-2018.1/src/gromacs/mdlib/nbnxn_cuda/nbnxn_cuda_kernel_pruneonly.cu(42): error: explicit instantiation definition directive for __global__ functions with clang host compiler is not yet supported
2 errors detected in the compilation of "/var/folders/6g/304ssmh94nqfs4dnb0__1fsm0000gp/T//tmpxft_000050c1_000000000-13_nbnxn_cuda.compute_70.cpp1.ii".
```

A transcript of the session is attached.

**History**

#1 - 04/10/2018 07:02 PM - Szilárd Páll

Unfortunately, I do not think we can fix this in the current release. The compiler that CUDA supports simply does not support a feature that is required to compile the code.

#2 - 04/11/2018 09:57 AM - Mark Abraham

Szilárd Páll wrote:

Unfortunately, I do not think we can fix this in the current release. The compiler that CUDA supports simply does not support a feature that is required to compile the code.

I assume the issue is that the global function can't have a template parameter in this case. It would be straightforward to have two global functions nbnxn_kernel_prune_cuda_true and nbnxn_kernel_prune_cuda_false, such that each of them calls the corresponding templated internal function. Would that work?

#3 - 05/31/2018 09:43 AM - Mark Abraham


Hey! Maybe somewhere could help me. I have some problems when I try to compile gromacs on OS X with eGPU:

Hey! Maybe somewhere could help me. I have some problems when I try to compile gromacs on OS X with eGPU:

Copyright (c) 2005-2017 NVIDIA Corporation

Built on Tue_Dec_19_21:36:29_CST_2017

Cuda compilation tools, release 9.1, V9.1.128
when I use clang/clang++ compilers:

clang 

clang version 6.0.0 (tags/RELEASE_600/final)
Target: x86_64-apple-darwin17.5.0
Thread model: posix

InstalledDir: /usr/local/Cellar/llvm/6.0.0/bin

Found CUDA installation: /usr/local/cuda, version unknown

I can found OpenMP:
-- Found OpenMP_C: -fopenmp=libomp (found version "3.1")
-- Found OpenMP_CXX: -fopenmp=libomp (found version "3.1")
-- Found OpenMP: TRUE (found version "3.1")

but:
-- Check for working NVCC/C compiler combination
-- Check for working NVCC/C compiler combination - broken

CMake Error at cmake/gmxManageGPU.cmake:291 (message):

CUDA compiler does not seem to be functional.
-- Configuring incomplete, errors occurred!

when I use llvm-gcc/llvm-g++ or CC/C++ compilers:

c++

Apple LLVM version 9.0.0 (clang-900.0.39.2)
Target: x86_64-apple-darwin17.5.0
Thread model: posix

InstalledDir: /Applications/Xcode.app/Contents/Developer/Toolchains/XcodeDefault.xctoolchain/usr/bin

Found CUDA installation: /usr/local/cuda, version unknown

llvm-gcc

Apple LLVM version 9.0.0 (clang-900.0.39.2)
Target: x86_64-apple-darwin17.5.0
Thread model: posix

InstalledDir: /Applications/Xcode.app/Contents/Developer/Toolchains/XcodeDefault.xctoolchain/usr/bin

Found CUDA installation: /usr/local/cuda, version unknown

I can not find OpenMP:
-- Could NOT find OpenMP_C (missing: OpenMP_C_FLAGS OpenMP_C_LIB_NAMES) (found version "1.0")
-- Could NOT find OpenMP_CXX (missing: OpenMP_CXX_FLAGS OpenMP_CXX_LIB_NAMES) (found version "1.0")

and when I do make:

[ 3%] Building C object src/gromacs/CMakeFiles/tng_io_obj.dir/__/external/tng_io/src/lib/md5.c.o
[ 3%] Built target tng_io_obj
[ 3%] Generating baseversion-gen.c
[ 3%] Building NVCC (Device) object src/gromacs/CMakeFiles/libgromacs.dir/mdlib/nbnxn_cuda/libgromacs_generated_nbnxn_cuda.cu.o
I don't know if it would work and right now I can't prioritize testing this. Next week I can look into it.

CUDA clang may be a good alternative.

Colin Smith wrote:

I am having this same problem. I'm trying to use Gromacs with a classroom full of Macs that have NVIDIA GPUs and am stuck using Gromacs 2016 on them. It would be great if the solution proposed by Mark (or something else) worked.

Scott Calabrese Barton wrote:

I can confirm that 2018.2 compiles well after upgrading CUDA to 9.2. Szilárd's point regarding NVIDIA GPU presence in Macs is well taken, except that external GPUs are now available for Mac, and future Mac support for OpenCL is uncertain at best.

Scott Calabrese Barton wrote:

I can confirm that 2018.2 compiles well after upgrading CUDA to 9.2.
Thanks for the feedback. I assume you did have to turn off testing?

Szilárd's point regarding NVIDIA GPU presence in Macs is well taken, except that external GPUs are now available for Mac,

True, however note: i) NVIDIA GPUs are officially not supported by Apple ii) TB3 has max 4 PCIe lanes available (possibly through the PCH) which will make GPU acceleration inefficient.
(As a side-note, I might not be up-to-date, but IIRC the cost of an eGPU enclosure would cover at least two thirds of the cost of a decent workstation, like a Ryzen 5).

#10 - 08/20/2018 12:04 PM - Szilárd Páll

- Status changed from Feedback wanted to Closed

Switching to "resolved" given that the latest NVIDIA / Apple toolchains eliminates the issue. Feel free to provide further feedback if there are unresolved issues.

Files

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<th>File Name</th>
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<th>Date</th>
<th>Author</th>
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<tr>
<td>gromacs-2018.1-error.txt</td>
<td>15.4 KB</td>
<td>03/25/2018</td>
<td>Scott Calabrese Barton</td>
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