GROMACS - Task #3415

Task # 3272 (New): Port complete CI testing to Gitlab

Port Pre-submit matrix to Gitlab CI

03/09/2020 01:32 PM - Paul Bauer

Status:	New	
Priority:	Normal	
Assignee:	Szilárd Páll	
Category:	testing	
Target version:	2021-refactoring	
Difficulty:	uncategorized	

Description

The different build configurations that are currently in the pre submit matrix for Jenkins need to be ported as configurations for the Gitlab CI.
What is needed is the definition of build and test jobs for different compilers that will duplicate the current pre submit matrix as far as possible.

History

#1 - 03/16/2020 05:46 PM - Paul Bauer

The following configurations need to be available for building GROMACS (testing can be done in more configs)

- cmake-3.13.0 + OpenMPI + Cuda 9.0 + gcc-7
- cmake-3.13.0 + clang-7
- cmake-3.13.0 + gcc-8 + x11
- cmake-3.13.0 + clang-8 + hwloc-1
- cmake-3.13.0 + clang-9 + hwloc-2
- cmake-3.13.0 + gcc-7 + Nvidia OpenCL + clFFT
- cmake-3.14.7 + gcc-9 + AMD OpenCL + clFFT

We can likely condense those into fewer configurations if needed, but this is the basic selection I came up with when condensing the current pre-submit matrix

#2 - 03/20/2020 09:13 AM - Paul Bauer

for 2020 I generated those containers now, and can push them up later

```
gromacs/cmake-3.9.6-gcc-5-cuda-9-mpi:2020
gromacs/cmake-3.15.7-gcc-8-cuda-10.1:2020
gromacs/cmake-3.9.6-gcc-6-cuda-10.1-opencl-clfft-mpi:2020
gromacs/cmake-3.15.7-llvm-7-tsan:2020
gromacs/cmake-3.11.4-llvm-3:2020
gromacs/cmake-3.11.4-llvm-8:2020
gromacs/cmake-3.9.6-gcc-9-cuda-10.0-mpi:2020
```

#3 - 03/20/2020 11:22 AM - Paul Bauer

Full set of configs that should cover both pre- and post-submit for 2020

```
gromacs/cmake-3.9.6-gcc-5-cuda-9-mpi:2020
gromacs/cmake-3.15.7-gcc-8-cuda-10.1:2020
gromacs/cmake-3.9.6-gcc-6-cuda-10.1-opencl-clfft-mpi:2020
gromacs/cmake-3.15.7-llvm-7-tsan:2020
gromacs/cmake-3.11.4-llvm-3:2020
gromacs/cmake-3.11.4-llvm-8:2020
gromacs/cmake-3.9.6-gcc-9-cuda-10.0-mpi:2020
gromacs/cmake-3.15.7-llvm-8-cuda-10.1-mpi:2020
gromacs/cmake-3.15.7-llvm-8-intel-opencl:2020
```

#4 - 03/20/2020 02:41 PM - Paul Bauer

Images for master

```
gromacs/cmake-3.13.0-gcc-7-cuda-9.0-mpi:master
gromacs/cmake-3.15.7-gcc-8-cuda-10.1-opencl-clfft-mpi:master
gromacs/cmake-3.13.0-llvm-8-tsan:master
gromacs/cmake-3.15.7-llvm-9:master
gromacs/cmake-3.15.7-llvm-9-cuda-10.2-mpi:master
gromacs/cmake-3.13.0-llvm-9-intel-opencl:master
```

#5 - 03/21/2020 10:19 PM - Eric Irrgang

Does "intel" mean Intel's MPI implementation? If so, I suggest "impi," and consistent ordering of "opencl" and MPI flavor.

I suggest "openmpi," "mpich," or "impi" instead of "mpi".

I don't see these images on Docker Hub. Are they only going to exist on the GitLab Runner hosts or have they just not been pushed yet?

#6 - 03/22/2020 12:51 PM - Paul Bauer

Eric Irrgang wrote:

> Does "intel" mean Intel's MPI implementation? If so, I suggest "impi," and consistent ordering of "opencl" and MPI flavor.
>
> I suggest "openmpi," "mpich," or "impi" instead of "mpi".
>
> I don't see these images on Docker Hub. Are they only going to exist on the GitLab Runner hosts or have they just not been pushed yet?

I didn't upload them yet because they weren't ready before the latest fixes, will be up later today.
The intel refers to intel opencl

#7 - 03/22/2020 02:46 PM - Paul Bauer

for 2020,

```
gromacs/cmake-3.15.7-llvm-7-tsan:2020
```

needs to be changed to

```
gromacs/cmake-3.15.7-llvm-8-tsan:2020
```

to be able to run static analyser version 8 :)

#8 - 03/23/2020 09:19 AM - Paul Bauer

we also need to change

```
gromacs/cmake-3.15.7-llvm-9-cuda-10.2-mpi:master
```

to

```
gromacs/cmake-3.15.7-llvm-8-cuda-10.2-mpi:master
```

or the CUDA toolkit complains

#9 - 03/23/2020 10:09 AM - Paul Bauer

Paul Bauer wrote:

> we also need to change
> [...]
> to
> [...]
> or the CUDA toolkit complains

actually needs to be

```
gromacs/cmake-3.15.7-llvm-8-cuda-10.0-mpi:master
```

for clang-cuda compilation to work, and

```
gromacs/cmake-3.15.7-llvm-8-cuda-10.1-mpi:master
```

for general CUDA compilation

```
gromacs/cmake-3.15.7-llvm-8-cuda-10.1-mpi:master
```

for general CUDA compilation