LUMI

Scaling up GPU computing on LUMI

Case Study with GROMACS

Goals

GROMACS is a widely used molecular dynamics package, open-source and community-driven with mature support for GPU computing

This case study presents:

- How to work with the LUMI software stack
- Running a job on GPU partition (LUMI-G)
- Distributing work across available CPU cores and GPUs
- Correct binding to a GPU and CPU
- Difference between multi-process and multithreaded execution

Remarks on code's version

For this purpose unofficial branch of Gromacs is used

- HIP port from AMD
- The containerized version from the AMD Infinity Hub
  - https://www.amd.com/en/technologies/infinity-hub/gromacs
  - https://hub.docker.com/r/amdih/gromacs
- Source code from ROCm GitHub repository
  - https://github.com/ROCmSoftwarePlatform/Gromacs

The Benchmark Systems

- HECBioSim Benchmarks

  https://www.hecbiosim.ac.uk/access-hpc/benchmarks
- A free GROMACS benchmark set
  https://www.mpinat.mpg.de/grubmueller/bench

Using LUMI software stack

- I will start with the containerized version
- There are guidelines on execution on the AMD's page
  - https://www.amd.com/en/technologies/infinity-hub/gromacs
  - Including singularity which is supported container runtime on LUMI

- The container supports only single-node execution
- I would need to use custom version of the application to enable MPI (multi-node) execution
- There is a recipe for self-building in the "software library"
  - https://lumi-supercomputer.github.io/LUMI-EasyBuild-docs/g/GROMACS
  - GPU enabled version is marked with `-MPI-GPU` name prefix

Running a job on GPU partition

There are generic allocation options required to use GPU resources

- Either allocate resource access or define batch job with SLURM
  - Use `salloc` command to get on-demand access
  - Submit job defined with job script using `sbatch` command

- Define required resources (LUMI specific):
  - GPU partition with `--partition=small-g  standard-g dev-g`
  - Learn about allocation policy https://docs.lumi-supercomputer.eu/runjobs/scheduled-jobs/partitions/
  - Define number of nodes with `--nodes=NN`
  - Define per-node resources: GPUs (`--gpus-per-node=NG`), tasks (`--ntasks-per-node=NT`), CPUs (`--cpus-per-task=NCPUS`)

Managing program execution

Resource and task distribution with SLURM

- Number of nodes
- Number of tasks
- Number of GPUs and CPUs
- Distribution of tasks
- Multithreading of taks
- CPUs and GPUs binding/mapping

Additional control with environmental variables

- Thread placement (multi-threading)
- GPU exposure (multi-gpu)
- GPU awareness in MPI (multi-node)
- NIC binding (multi-gpu, multi-node)
- Diagnostics on resource distribution

Features and runtime mode

- Use of GPU kernel offloading (application specific)
- Data decomposition (application specific)
- Multi-gpu management

Distributing work

- Remark: LUMI GPU nodes are running in the "low-noise" mode with first core reserved for OS and there 63 core available for user to allocate
- Starting set of SLURM directives (job script preamble)

```
#!/bin/bash                          shebang line
#SBATCH --exclusive                  required for task binding
#SBATCH --ntasks=1                   for single-node run
#SBATCH --ntasks-per-node=1          for the container multi-theaded run
#SBATCH --cpus-per-task=48           avoid using core 0
#SBATCH --gpus-per-node=8            for multi-gpu run
#SBATCH --partition small-g          select one of the GPU partitions
#SBATCH --account=project_XXXXXXXX   project account number
#SBATCH --hint=nomultithread         avoid hardware threads to be enabled
```

- Learn more on SLURM distribution modes using docs
  https://docs.lumi-supercomputer.eu/runjobs/scheduled-jobs/slurm-quickstart/

Running the container

- Singularity is (HPC) container runtime on LUMI
- You can run docker containers directly from DockerHub
- Command line:

```
singularity exec \
docker://amdih/gromacs:2022.3.amd1_174 \
gmx mdrun \
-notunepme -noconfout \
-ntomp 6 -ntmpi 8 \
-pin on -pinoffset 1 \
-npme 1 -bonded cpu \
-nb gpu -pme gpu \
-gpu_id 0,1,2,3,4,5,6,7 \
-s benchmark.tpr
```

Tuning the environment

- Some of the GROMACS features need to be enabled with runtime environment variables (for GPU execution)

```
export GMX_GPU_DD_COMMS=true \
export GMX_GPU_PME_PP_COMMS=true \
export GMX_FORCE_UPDATE_DEFAULT_GPU=true
```

- Thread placement also can be managed with environment variables

```
export OMP_NUM_THREADS=6 \
export OMP_PROC_BIND=close \
export OMP_PLACES=cores
```

- Variable names need `SINGULARITYENV_` prefix to be exported to the container
- Thread placement is managed by GROMACS internally

Complete jobscript for a container

```
#!/bin/bash

#SBATCH --ntasks=1
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=48
#SBATCH --time=0:15:0
#SBATCH --exclusive
#SBATCH --partition small-g
#SBATCH --account=project_465000XXX
#SBATCH --hint=nomultithread
#SBATCH --gpus-per-node=8

module load LUMI/22.08                                  # Use LUMI software stack

module load partition/G                                 # Use software components for GPU execution (ROCm)

export SINGULARITYENV_GMX_GPU_DD_COMMS=true

export SINGULARITYENV_GMX_GPU_PME_PP_COMMS=true

export SINGULARITYENV_GMX_FORCE_UPDATE_DEFAULT_GPU=true

export SINGULARITYENV_OMP_NUM_THREADS=6

export SINGULARITYENV_OMP_PROC_BIND=close

export SINGULARITYENV_OMP_PLACES=cores

srun singularity exec docker://amdih/gromacs:2022.3.amd1_174 \
gmx mdrun -notunepme -noconfout -resethway -ntomp 6 -ntmpi 8 -pin on -pinoffset 1 -npme 1 -bonded cpu -nb gpu -pme gpu -gpu_id 0,1,2,3,4,5,6,7  -s benchmark.tpr
```

- Launch program on allocated nodes with `srun` (the only launcher for LUMI)
- Submit with `sbatch job_script.sh`

Building native application

- I would need to use custom version of the application to enable MPI multi-node, multi-gpu execution
- There is ready to use recipe to build (self-install) version
- Code-base similar to the containerized version but with MPI enabled
  - Precisely commit `7bbbb2de208ac1a42c7144ac28ecc5fb0dc0dd4e` of the `develop_2022_amd` branch
  - Recipe name `GROMACS-2023-dev-cpeGNU-22.08-MPI-GPU`

Building native application cont.

- Simple steps for installation (on the system)
  - Select the Software stack version with: `` `module load LUMI/22.08` ``
  - Select target HW partition with: `` `module load partition/G` ``
  - Enable user based EasyBuild installation with: `` `module load EasyBuild-user` ``
  - Run installation with: `` `eb --robot --trace GROMACS-2023-dev-cpeGNU-22.08-MPI-GPU.eb` ``
- After completing these steps, software is available with `` `module load GROMACS/2023-dev-cpeGNU-22.08-MPI-GPU` ``

Running the MPI version

- Need to add tasks (multi-process) distribution
- Targeting one MPI rank per GPU and six threads per MPI task
- Add SLURM directives:

```
#SBATCH --ntasks-per-node=8
#SBATCH --cpus-per-task=6
```

- Refine job script, adding software modules

```
module load LUMI/22.08
module load partition/G
module load GROMACS/2023-dev-cpeGNU-22.08-MPI-GPU
```

- Remove singularity executor, `tmpi` option and change executable name

```
srun gmx_mpi mdrun -nsteps 4000 -notunepme -noconfout -npme 1 -bonded cpu
-nb gpu -pme gpu -update gpu -ntomp 6 -gpu_id 0,1,2,3,4,5,6,7
```

Complete jobscript

```
#!/bin/bash

#SBATCH --ntasks=1
#SBATCH --ntasks-per-node=8
#SBATCH --cpus-per-task=6
#SBATCH --time=0:15:0
#SBATCH --exclusive
#SBATCH --partition small-g
#SBATCH --account=project_465000XXX
#SBATCH --hint=nomultithread
#SBATCH --gpus-per-node=8

module load LUMI/22.08
module load partition/G
module load GROMACS/2023-dev-cpeGNU-22.08-MPI-GPU

export GMX_GPU_DD_COMMS=true
export GMX_GPU_PME_PP_COMMS=true
export GMX_FORCE_UPDATE_DEFAULT_GPU=true

export SRUN_CPUS_PER_TASK=6
export OMP_NUM_THREADS=6
export OMP_PLACES=cores
export OMP_PROC_BIND=close

srun gmx_mpi mdrun -nsteps 4000 -notunepme -noconfout -npme 1 -bonded cpu -nb gpu -pme gpu -update gpu -ntomp 6 -gpu_id 0,1,2,3,4,5,6,7 \
-s benchmark.tpr
```

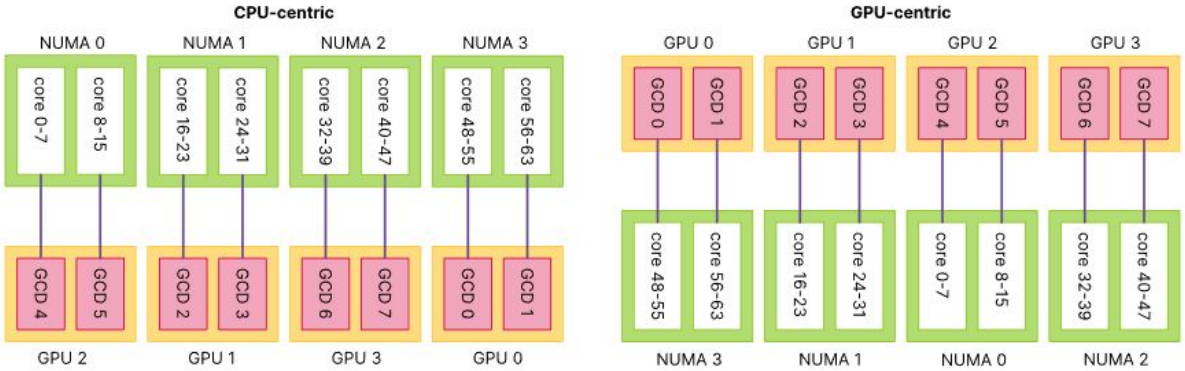
- Submit with `sbatch job_script.sh`

Failure

- Expected performance with this run mode is very low (comparing with the multi-threaded container)
- GROMACS is doing good job with thread placement (binding to CPUs) in the multi-threaded mode (tMPI plus OpenMP)
- How to improve?

Binding to GPU to CPUs

- Proper binding the NUMA node to the GPU is crucial for achieving optimal performance
- It may be beneficial to avoid each first core of the NUMA region while they are used for GPU management



Source https://docs.lumi-supercomputer.eu/hardware/lumig/

Binding to GPU to CPUs cont.

- To allocate specific CPU cores to job tasks (processes) there are SLURM's options:
  - `--cpu-bind=map_cpu:MAPPING`
  - `--cpu-bind=mask_cpu:MASK`
- I need to bind CPUs using "GPU-centric" policy with custom NUMA region order

Understanding bitmasks

- In this case I decided to mask every first (and last) core of the NUMA region
- Mask first and last core of the CCD (8 cores) to accommodate 6 threads
  - binary mask: `0111110`
  - hexadecimal mask: `0x7e`
- Combining masks for NUMA regions (CCDs)
  - `mask_cpu:7e,7e00,7e0000,7e000000,7e00000000,7e0000000000,7e000000000000,7e000000000000`
- Correct order:
  - `48-55 , 56-63 , 16-23 , 24-31 , 0-7 , 8-15, 32-39 , 40-47`
  - `mask_cpu:7e000000000000,7e000000000000,7e0000,7e000000,7e,7e00,7e00000000,7e0000000000`

Complete jobscript

```
#!/bin/bash

#SBATCH --ntasks=1
#SBATCH --ntasks-per-node=8
#SBATCH --cpus-per-task=6
#SBATCH --time=0:15:0
#SBATCH --exclusive
#SBATCH --partition small-g
#SBATCH --account=project_465000XXX
#SBATCH --hint=nomultithread
#SBATCH --gpus-per-node=8

module load LUMI/22.08
module load partition/G
module load GROMACS/2023-dev-cpeGNU-22.08-MPI-GPU

export GMX_GPU_DD_COMMS=true
export GMX_GPU_PME_PP_COMMS=true
export GMX_FORCE_UPDATE_DEFAULT_GPU=true

export SRUN_CPUS_PER_TASK=6
export OMP_NUM_THREADS=6
export OMP_PLACES=cores
export OMP_PROC_BIND=close

export SLURM_CPU_BIND="mask_cpu:7e000000000000,7e00000000000000,7e0000,7e000000,7e,7e00,7e00000000,7e0000000000"

srun gmx_mpi mdrun -nsteps 4000 -notunepme -noconfout -npme 1 -bonded cpu -nb gpu -pme gpu -update gpu -ntomp 6 -gpu_id 0,1,2,3,4,5,6,7 \
-s benchmark.tpr
```

- Submit with `sbatch job_script.sh`

Problems with a performance

- Again performance with this run mode is not comparable to the multi-threaded container
- You can observe large overheads associated with GPU communication
- How to improve?

Enabling GPU-aware MPI

- To improve performance you need to enable direct communication between GPUs binded to the different MPI tasks
- GROMACS is not able to detect if MPI on LUMI is GPU aware
- This is controlled with environmental variables:

```
export GMX_ENABLE_DIRECT_GPU_COMM=true
export GMX_FORCE_CUDA_AWARE_MPI=true (GROMACS 2022)
```

- MPI also needs to be enabled with GPU awareness:

```
export MPICH_GPU_SUPPORT_ENABLED=1
export MPICH_GPU_IPC_ENABLED=1
```

Complete jobscript

```
#!/bin/bash

#SBATCH --ntasks=1
#SBATCH --ntasks-per-node=8
#SBATCH --time=0:15:0
#SBATCH --exclusive
#SBATCH --partition small-g
#SBATCH --account=project_465000XXX
#SBATCH --hint=nomultithread
#SBATCH --gpus-per-node=8

module load LUMI/22.08
module load partition/G
module load GROMACS/2023-dev-cpeGNU-22.08-MPI-GPU

export GMX_GPU_DD_COMMS=true
export GMX_GPU_PME_PP_COMMS=true
export GMX_FORCE_UPDATE_DEFAULT_GPU=true
export GMX_ENABLE_DIRECT_GPU_COMM=true
export GMX_FORCE_CUDA_AWARE_MPI=true

export MPICH_GPU_SUPPORT_ENABLED=1
export MPICH_GPU_IPC_ENABLED=1

export OMP_NUM_THREADS=6
export OMP_PLACES=cores
export OMP_PROC_BIND=close

export SLURM_CPU_BIND="mask_cpu:7e000000000000,7e00000000000000,7e0000,7e000000,7e,7e00,7e00000000,7e0000000000"

srun gmx_mpi mdrun -nsteps 4000 -notunepme -noconfout -npme 1 -bonded cpu -nb gpu -pme gpu -update gpu -ntomp 6 -gpu_id 0,1,2,3,4,5,6,7 \
-s benchmark.tpr
```

Still Problems with a performance

- Some of the features allowing efficient GPU usage are not implemented in this code version
- How to update code version?

Upgrading code version

- Upgrade your build to more recent version of GROMACS
- Create custom EasyBuild recipe by adding specific commit from the `develop_2023_amd` branch (change commit hash)
- Reinstall GROMACS with the new recipe
  - Use `--force` and `--force-download=all` options for EasyBuild
- Update `GMX_FORCE_CUDA_AWARE_MPI` variable with `GMX_FORCE_GPU_AWARE_MPI`

Conclusion

- Containerized version provide easy to start, performance friendly approach
- Building custom version with a multi-node support requires care
- Correct, non-default CPU and GPU binding make huge difference in performance
- GPU-awareness of MPI is not enabled by default
- You still need to update to the latest GROMACS release (2023) to get best performance on multiple nodes!

LUMI

Maciej Szpindler

m.szpindler@cyfronet.pl

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www.lumi-supercomputer.eu

contact@lumi-supercomputer.eu

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