

LUMI

A white wolf is the central focus, standing in a snowy, digital landscape. The background is a dark blue/black space filled with vertical light streaks and a grid pattern, suggesting a high-tech or data environment. The wolf is looking towards the viewer.

Process and Thread Distribution and Binding

Jorik van Kemenade
LUMI User Support Team (LUST), SURF

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Slides updated from previous version,
authored by Kurt Lust (LUST, UAntwerp)

What are we talking about?

- Distribute processes and threads across the available resources for the job
- and bind them to the resources to ensure they stay there and only use the assigned resources
 - Across nodes: Only distribution
 - Within a node: Binding necessary
- System software level (Linux/ROCm/Slurm):
 - Control groups used at the job and job step level, sometimes at the task level
 - Affinity mask to control where a thread can get scheduled
 - ROCm runtime also has a mechanism to control access to GPUs
- Tools for verification in the lumi-CPEtools modules

When/where is it done?

- Slurm level
 - Creation of allocation: Slurm reserves resources at the node level using control groups
 - Creation of job step:
 - Distributes tasks across nodes and cores/hardware threads on nodes
 - Default in most cases: Binds tasks to CPUs (affinity mask) and GPUs (control groups unfortunately)
- Application runtime library level
 - Cray MPICH can renumber the ranks and bind to NICs
 - OpenMP runtime: select number of CPU threads and bind threads within the resources of a task using affinity masks
 - ROCm runtime: Select GPUs using [ROCR_VISIBLE_DEVICES](#)
- Does not always make sense on nodes that are not job-exclusive!

Why do I need this?

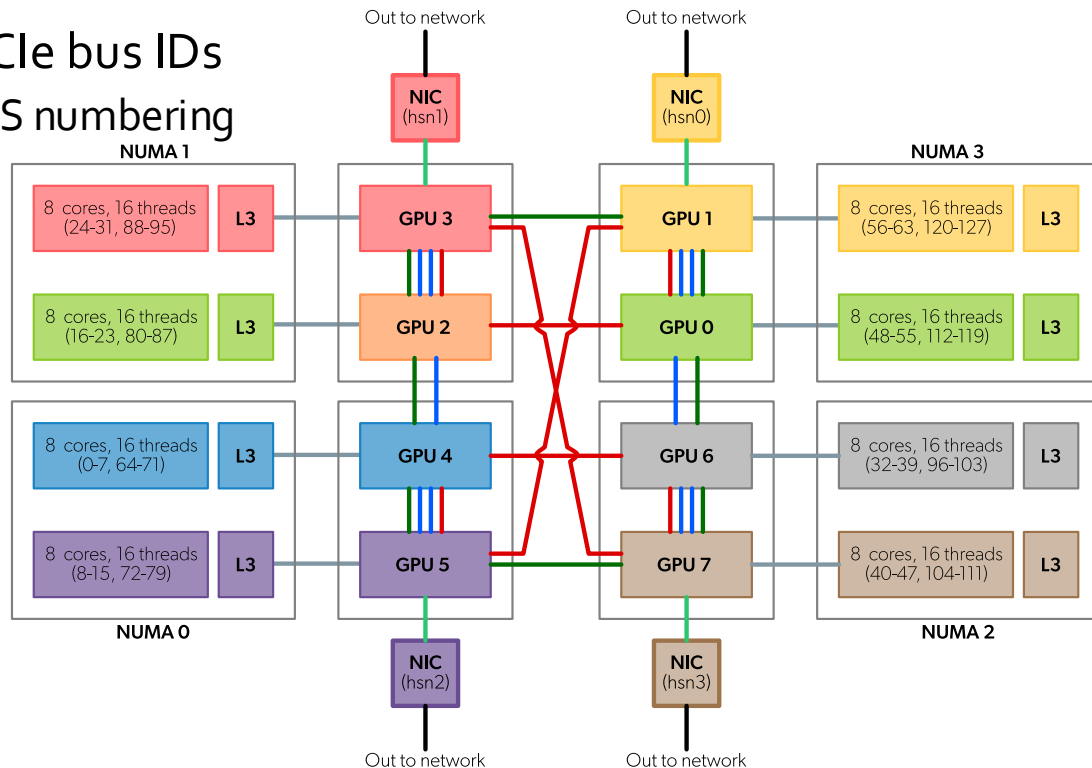
- Importance of memory locality at all levels (cache and main memory)
 - E.g.: MPI application with 14 GB/rank so 16 ranks on node: Spread out across CCDs...
 - Shared memory with lack of memory locality: Maybe need to bundle threads if the application fits in a socket
 - No solution that's always optimal!
- Short connection between CPU and GPU sometimes essential for fast communication between both
 - Cache-coherent accesses to GPU memory by the CPU
- Mapping of MPI ranks to reduce inter-node traffic and maximise intra-node traffic which is much faster
 - Also on the GPU: Map communication pattern on the topology of a node

Core numbering

- Linux core (actually hardware thread/virtual core) numbering does not reflect the hierarchy
 - Numbers 0-127 on LUMI-C are the first hardware thread on each physical core, 128-255 then the second one, so i and $i+128$ map onto the same physical core
 - On LUMI-G: Core 0-63 first hardware thread, core 64-127 second, so i and $i+64$ map onto the same physical core
- Hardware threading on LUMI is turned on when booting a node
 - Slurm does not turn hardware threading off, but doesn't include the second hardware thread in the affinity mask when multithreading is off
 - Slurm only does so at the regular job step level
 - The Slurm batch step will always see both hardware threads for each core!
- Technical discussion in the notes if you're interested

GPU Numbering (1)

- Very tricky
- Numbering based on the PCIe bus IDs
 - Global numbering or bare-OS numbering



GPU Numbering (2)

- Very tricky
- Numbering based on the PCIe bus IDs
 - *Global numbering or bare-OS numbering (0-7)*
- Job-level control group
 - New numbering starting from 0: *job-local numbering*
 - Same order though
- Task-level control group
 - Yet another numbering starting from 0: *task-local numbering*
 - And a headache for MPI and RCCL applications
- Further restricting access via `ROCR_VISIBLE_DEVICES` will start yet another numbering in, e.g., the HIP runtime

GPU Numbering - Remarks

- Very technical demonstrations in the notes
- Slurm works differently with CPUs and GPUs on LUMI
 - CPUs: Control groups at the job level, after that affinity masks
 - GPUs: Control groups at the job and task level, even though `ROCR_VISIBLE_DEVICES` plays a bit the role of an affinity mask
- Affinity masks work differently from `ROCR_VISIBLE_DEVICES`
 - Affinity masks always refer to the global / bare OS numbering of the hardware threads
 - `ROCR_VISIBLE_DEVICES` numbering is based on the local numbering in the context where the variable is used
 - Affinity masks can only shrink as you go deeper in a hierarchy
 - `ROCR_VISIBLE_DEVICES`, being just an environment variable, can be abused to gain access to extra resources (within the confines of the control group)

Task distribution with Slurm (1)

- `srun --distribution={block|cyclic|plane=<s>}[:{block|cyclic|fcyclic}[, {Pack|NoPack}]`
- Level 1: Distribution of tasks across nodes
 - `block`: Fill first node in allocation, then fill second, etc.
 - `Pack`: Fill completely before moving to the next node
 - `NoPack`: More ballanced, trying to fill all nodes as equally as possible
 - `cyclic`: First assign one task to each node, then from the first node again assign a second task, ...
 - `plane=<s>`: As cyclic, but assigning `s` tasks at a time before moving on
 - More options that we do not discuss

Task distribution with Slurm (2)

Example: 10 task of 32 cores each (quarter node) spread across 3 nodes:

- `--distribution=block,pack`

node 1				node 2				node 3			
0	1	2	3	4	5	6	7	8	9		

- `--distribution=block,nopack`

node 1				node 2				node 3			
0	1	2	3	4	5	6		7	8	9	

- `--distribution=cyclic`

node 1				node 2				node 3			
0	3	6	9	1	4	7		2	5	8	

- `--distribution=plane=2`

node 1				node 2				node 3			
0	1	6	7	2	3	8	9	4	5		

Task distribution with Slurm (3)

- `srun --distribution={block|cyclic|plane=<s>}[:{block|cyclic|fcyclic}[, {Pack|NoPack}]`
- Level 2: Distribution of tasks across cores
 - L2 already binds tasks to sets of cores and will conflict with other binding mechanisms
 - **block**: Consecutive sets of cores for each task
 - **cyclic**: First assign one task to each socket on the first set of consecutive cores/virtual cores of each socket, then assign a second task on each socket on the next set of cores, ...
 - **fcyclic**: Will spread tasks out across sockets
 - Not clear where this is useful on an AMD system except for cases with one task per node and a lot of memory for that task
- Level 3 not shown in this simplified version
- Default: **block:block:nopack** but **block:*** results in **block:cyclic**
- L2 and L3 distribution conflicts with the CPU binding mechanism that we will discuss
 - But usefull with `--cpus-per-task`

Task-to-CPU binding with Slurm: Why?

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- For memory access performance reasons, you may want to bundle all threads of a task in a single L3 cache domain, a single NUMA domain or a single socket.
 - And for very memory bandwidth intensive applications, underpopulating cores can be an option
- Or in some cases, if a shared memory code is very NUMA-friendly but cannot use all cores efficiently, you may want to spread out the threads to have maximal memory bandwidth.
- On LUMI-G, proper mapping of CCDs, GCDs and network interfaces can be very important for good performance
 - And the easiest way is often to reorder the tasks in a non-trivial way across the CCDs.

Task-to-CPU binding with Slurm: How?

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- Works with affinity masks
- `srun --cpu-bind=[{quiet|verbose},]<type>`
- Some `<type>` options are for automatic binding
 - `--cpu-bind=threads` is the default behaviour on LUMI
 - Other options: See the manual
- Other `<type>` options define a list of task slots to be used
 - Combination with `--distribution` L2/L3 options does not make sense
 - `--cpu-bind=map_cpu:<cpu_id_for_task_0>,<cpu_id_for_task_1>,...` : Specify a single hardware thread for each task on the node
 - For MPI programs
 - `--cpu-bind=mask_cpu:<mask_for_task_0>,<mask_for_task_1>,...` : Specify afinity mask for each task on the node.
 - For OpenMP or hybrid programs

Task-to-CPU binding with Slurm: Masks

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- Slurm uses hexadecimal masks to select which CPU cores tasks should bind to
 - Bits ordered right to left
 - First bit masks core #0
 - Each task need its mask
- Single mask for 7 cores out of 8 (disabling core #0)
 - Core numbers: 76543210
 - Binary mask: 11111110
 - Hexadecimal value: 0xfe
 - Leading zeros can be omitted, but each element can still be very long
- See the notes for more information

Task-to-CPU binding with Slurm: Examples

- `salloc --nodes=1 --partition=standard-g`
`module load LUMI/24.03 partition/G lumi-CPEtools/1.1-cpeGNU-24.03`
`srun --ntasks=8 --cpu-bind=map_cpu:49,57,17,25,1,9,33,41 mpi_check -r`
 - Example will be relevant for LUMI-G
- `srun --ntasks=8 --cpu-bind=mask_cpu:\`
`7e000000000000,7e00000000000000,7e0000,7e000000,7e,7e00,7e00000000,7e0000000000 \`
`hybrid_check -r`
 - Like the above but now enabling 6 cores per CCD (1-6).
 - Masks with use of both hardware threads can become extremely long, certainly on LUMI-C...
 - Playing with `--cpus-per-task` and then further restricting with OpenMP environment variables may be the easier way on LUMI-C
- Do not combine with `-c/--cpus-per-task`!

Task-to-GPU binding with Slurm

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- **Currently not recommended on LUMI**

- The control groups mechanism that Slurm uses breaks Peer2Peer IPC for GPU-aware MPI
- `srun --gpu-bind=[{quiet|verbose},]<type>`
- Some `<type>` options are for automatic binding
 - `--gpu-bind=none` is the **most useful variant on LUMI**: Turns off Slurm binding
 - Useful when combined with `--gpus-per-task`: unbind and then rebind, see later
 - `--gpu-bind=closest` is broken on LUMI
 - Other options: See the manual
- Other `<type>` options for fully manual distribution
 - `--gpu-bind=map_cpu:<gpu_id_for_task_0>,<gpu_id_for_task_1>,...` : Specify a single GPU for each task on the node
 - `--gpu-bind=mask_cpu:<mask_for_task_0>,<mask_for_task_1>,...` : Specify multiple GPUs via a mask (but only 2 hexadecimal digits as there are only 8 GPUs per node)

MPI rank redistribution with Cray MPICH (1)

- Default behaviour: MPI rank i on task i
- Cray MPICH has its own mechanism to reorder MPI ranks on Slurm tasks that is more powerful than Slurm's
 - Best to use block distribution in Slurm for this.
 - `export MPICH_RANK_REORDER_METHOD=0` : Round-robin (like Slurm cyclic ordering)
 - `export MPICH_RANK_REORDER_METHOD=1` : Default, preserve the ordering from Slurm
 - `export MPICH_RANK_REORDER_METHOD=2` : Folded rank placement: First assign ranks on first task slot of each node from 0 till ..., then assign a rank on the second task slot but now from ... till 0, and so on.
 - `export MPICH_RANK_REORDER_METHOD=3` : Custom ordering set by the file `MPICH_RANK_ORDER` (or `$MPICH_RANK_REORDER_FILE`)
- The CPE has profiling tools that help you determine the optimal rank ordering
- See the 4/5-day Advanced LUMI course for more details

MPI rank redistribution with Cray MPICH (2)

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- Assume 12 quarter node tasks and 3 nodes, starting from a Slurm block ordering
- `export MPICH_RANK_REORDER_METHOD=0` (Cyclic)

node 1				node 2				node 3			
0	3	6	9	1	4	7	10	2	5	8	11

- `export MPICH_RANK_REORDER_METHOD=1` (Preserve Slurm)

node 1				node 2				node 3			
0	1	2	3	4	5	6	7	8	9	10	11

- `export MPICH_RANK_REORDER_METHOD=2` (Folded)

node 1				node 2				node 3			
0	5	6	11	1	4	7	10	2	3	8	9

MPI network adapter binding with Cray MPICH LUMI

- The environment variable `MPICH_OFI_NIC_POLICY` can be used to map processes on Network Interface Controllers (NICs).
 - Useful on LUMI-G as each node has 4 NICs
 - Some values, first 2 are most relevant on LUMI:
 - `MPICH_OFI_NIC_POLICY=GPU`: Use the NIC closest to the GPU.
 - Should be used if MPI operations mostly access GPU-attached memory regions
 - `MPICH_OFI_NIC_POLICY=NUMA`: Use the NIC closest to the CPU cores of the MPI rank
 - Should be used if MPI communications are done from CPU buffers
 - `MPICH_OFI_NIC_POLICY=BLOCK`: Consecutive local ranks equally distributed among NICs.
- ➡ **Default value**
- `MPICH_OFI_NIC_POLICY=ROUND-ROBIN`: With 4 NICs: rank 0, 4, 8, ... to NIC 0, rank 1, 5, 9, ... to NIC 1, etc.
 - User mapping possible in combination with `MPICH_OFI_NIC_MAPPING`.

Refining core binding in OpenMP

- Slurm will assign cores up to the task/process level
 - Special case: Batch job step: All hardware threads of all cores of the first node of the job
- Thread-level control in OpenMP through library functions or environment variables
 - Debug: `export OMP_DISPLAY_AFFINITY=true`
 - `export OMP_NUM_THREADS=<num>` : Set number of threads
 - Multiple comma-separated numbers possible for multi-level parallelism
 - `OMP_PLACES` to define the places to use for binding: hardware thread level, core level or socket level, or an explicit list
 - `OMP_PROC_BIND` to set distribution and binding strategy over places
- Single level parallelism: Experiment with `omp_check` and `hybrid_check` in `lumi-CPEtools`

Refining core binding in OpenMP: OMP_PLACES

- Defines the places to use for binding
 - `OMP_PLACES=threads` : OpenMP threads restricted to a single hardware thread (default)
 - `OMP_PLACES=cores` : OpenMP threads restricted to both hardware threads of a core
 - `OMP_PLACES=socket` : OpenMP threads restricted to all hardware threads of a single socket
 - Or define a set of locations (very technical)
`export OMP_PLACES="{0,1,2,3},{8,9,10,11},{16,17,18,19}"`
`export OMP_PLACES="{0:4}:3:8"`
 - Core numbers here are relative to those available to the process and not physical numbers

Refining core binding in OpenMP: OMP_PROC_BIND

- Distribution over the places and binding selection:
 - `OMP_PROC_BIND=false` : Turn off OpenMP thread binding, use the task affinity mask
 - `OMP_PROC_BIND=close` : Try to keep the OpenMP threads as close as possible with one in each place (unless oversubscribed)
 - `OMP_PROC_BIND=spread` : Try to spread the OpenMP threads out as much as possible
 - `OMP_PROC_BIND=master` : Keep threads in the same place as the master thread.
 - Mostly useful if the place is a socket
- Multiple comma-separated options possible for nested parallelism
- Non-standard option in CCE: `auto` which is the default (other compilers: `false`)
 - CCE does a very reasonable job in many cases
- Many implementations have additional environment variables to tune the distribution

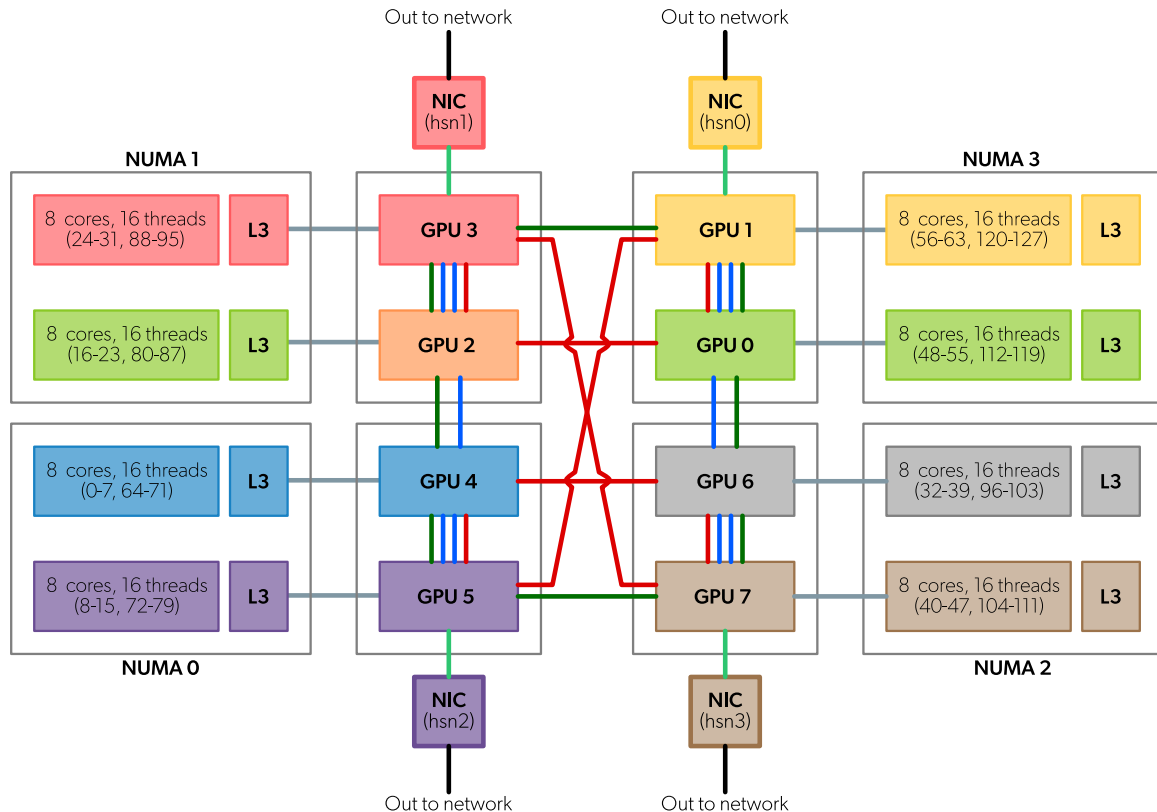
GPU binding with `ROCR_VISIBLE_DEVICES`

- Works at a very low level of the ROCm software stack
- Limits visibility to certain GPUs for all applications using the ROCm runtime
 - So also covers HIP and OpenCL
- Value: Comma-separated list of all device indices exposed to the application
 - Uses the local numbering in the control group
- Differences with affinity masks for CPUs
 - Affinity masks are OS-controlled
 - Therefore the OS can ensure you can only make masks more restrictive than the parent
 - Affinity masks always use the global numbering of hardware threads while `ROCR_VISIBLE_DEVICES` uses the local numbering in the control group

GPU binding: Optimal mapping (1)

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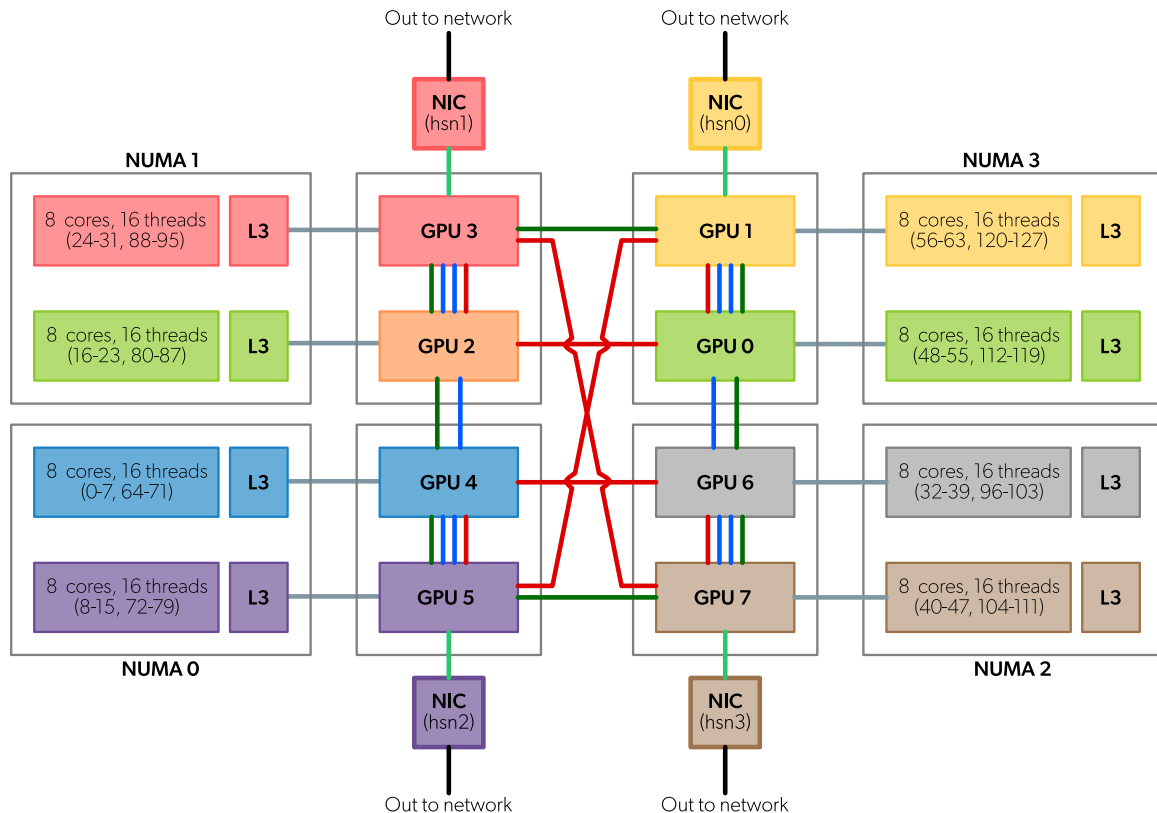
CCD	Available HWTs	GCD
0	1-7, 65-71	4
1	9-15, 73-79	5
2	17-23, 81-87	2
3	25-32, 89-95	3
4	33-39, 97-103	6
5	41-47, 105-111	7
6	49-55, 113-119	0
7	57-63, 121-127	1



GPU binding: Optimal mapping (2)

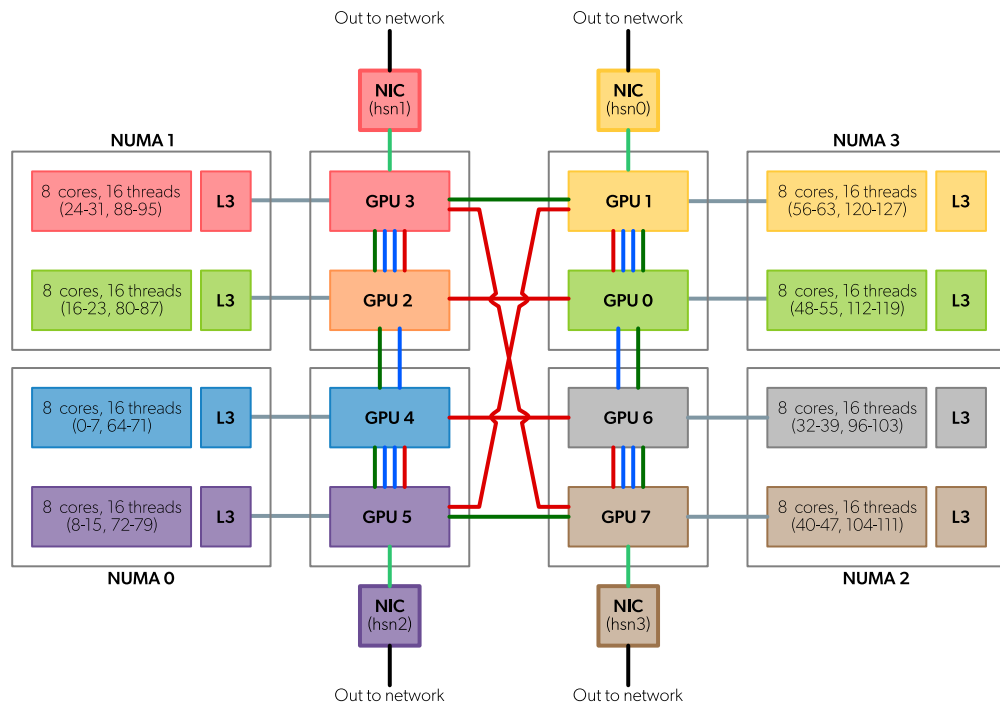
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GCD	CCD	Available HWTs
0	6	49-55, 113-119
1	7	57-63, 121-127
2	2	17-23, 81-87
3	3	25-32, 89-95
4	0	1-7, 65-71
5	1	9-15, 73-79
6	4	33-39, 97-103
7	5	41-47, 105-111



GPU binding: Embedded rings

- Green ring: 0 – 1 – 3 – 2 – 4 – 5 – 7 – 6 – 0
- Red ring: 0 – 1 – 5 – 4 – 6 – 7 – 3 – 2 – 0



GPU binding: Implementation

- Combination of three mechanisms:
 - CPU side: Use `--cpu-bind`, or in some cases simply `--cpus-per-task`
 - GPU side: Manual binding required by setting `ROCR_VISIBLE_DEVICES` because Slurm uses a mechanism with unwanted side effects.
 - Use a wrapper script that computes the proper GPU(s) from the Slurm local task id, sets `ROCR_VISIBLE_DEVICES` and then starts the application
 - NIC side: Ensure the use of the closest NIC for each task/rank by setting `MPICH_OFI_NIC_POLICY`

GPU binding: Linear GCD, match cores (1)

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```
...
#SBATCH --partition=standard-g
#SBATCH --gpus-per-node=8
...
cat << EOF > select_gpu_$SLURM_JOB_ID
#!/bin/bash
export ROCR_VISIBLE_DEVICES=\$SLURM_LOCALID
exec \$*
EOF
chmod +x select_gpu_$SLURM_JOB_ID
...
CPU_BIND1="map_cpu:49,57,17,25,1,9,33,41"
srun --ntasks=$((SLURM_NNODES*8)) --cpu-bind=$CPU_BIND1 \
    ./select_gpu_$SLURM_JOB_ID gpu_check -l
```



GPU binding: Linear GCD, match cores (2)

L U M I

```
...
#SBATCH --partition=standard-g
#SBATCH --gpus-per-node=8
...
cat << EOF > select_gpu_$SLURM_JOB_ID
#!/bin/bash
export ROCR_VISIBLE_DEVICES=\$SLURM_LOCALID
exec \$*
EOF
chmod +x select_gpu_$SLURM_JOB_ID
...
CPU_BIND2="mask_cpu:0xfe000000000000,0xfe00000000000000"
CPU_BIND2="$CPU_BIND2,0xfe0000,0xfe000000"
CPU_BIND2="$CPU_BIND2,0xfe,0xfe00"
CPU_BIND2="$CPU_BIND2,0xfe00000000,0xfe0000000000"
srun --ntasks=$((SLURM_NNODES*8)) --cpu-bind=$CPU_BIND2 \
    ./select_gpu_$SLURM_JOB_ID gpu_check -l
```



GPU binding: Linear CCD, match GCD (1)

L U M I

```
...
#SBATCH --partition=standard-g
#SBATCH --gpus-per-node=8
...
cat << EOF > select_gpu_$SLURM_JOB_ID
#!/bin/bash
GPU_ORDER=(4 5 2 3 6 7 0 1)
export ROCR_VISIBLE_DEVICES=${GPU_ORDER[${SLURM_LOCALID}]}
exec \*$*
EOF
chmod +x select_gpu_$SLURM_JOB_ID
...
CPU_BIND1="map_cpu:1,9,17,25,33,41,49,57"
srun --ntasks=$((SLURM_NNODES*8)) --cpu-bind=$CPU_BIND1 \
    ./select_gpu_$SLURM_JOB_ID gpu_check -l
```



GPU binding: Linear CCD, match GCD (2)

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```
...
#SBATCH --partition=standard-g
#SBATCH --gpus-per-node=8
...
cat << EOF > select_gpu_$SLURM_JOB_ID
#!/bin/bash
GPU_ORDER=(4 5 2 3 6 7 0 1)
export ROCR_VISIBLE_DEVICES=${GPU_ORDER[`${SLURM_LOCALID}`]}
exec \${*}
EOF
chmod +x select_gpu_$SLURM_JOB_ID
...
CPU_BIND2="mask_cpu"
CPU_BIND2="$CPU_BIND2:0x00000000000000fe,0x000000000000fe00"
CPU_BIND2="$CPU_BIND2,0x0000000000fe0000,0x00000000fe000000"
CPU_BIND2="$CPU_BIND2,0x000000fe00000000,0x0000fe0000000000"
CPU_BIND2="$CPU_BIND2,0x00fe000000000000,0xfe00000000000000"
srun --ntasks=$((SLURM_NNODES*8)) --cpu-bind=$CPU_BIND2 \
    ./select_gpu_$SLURM_JOB_ID gpu_check -l
```



GPU binding: Linear CCD, match GCD (3)

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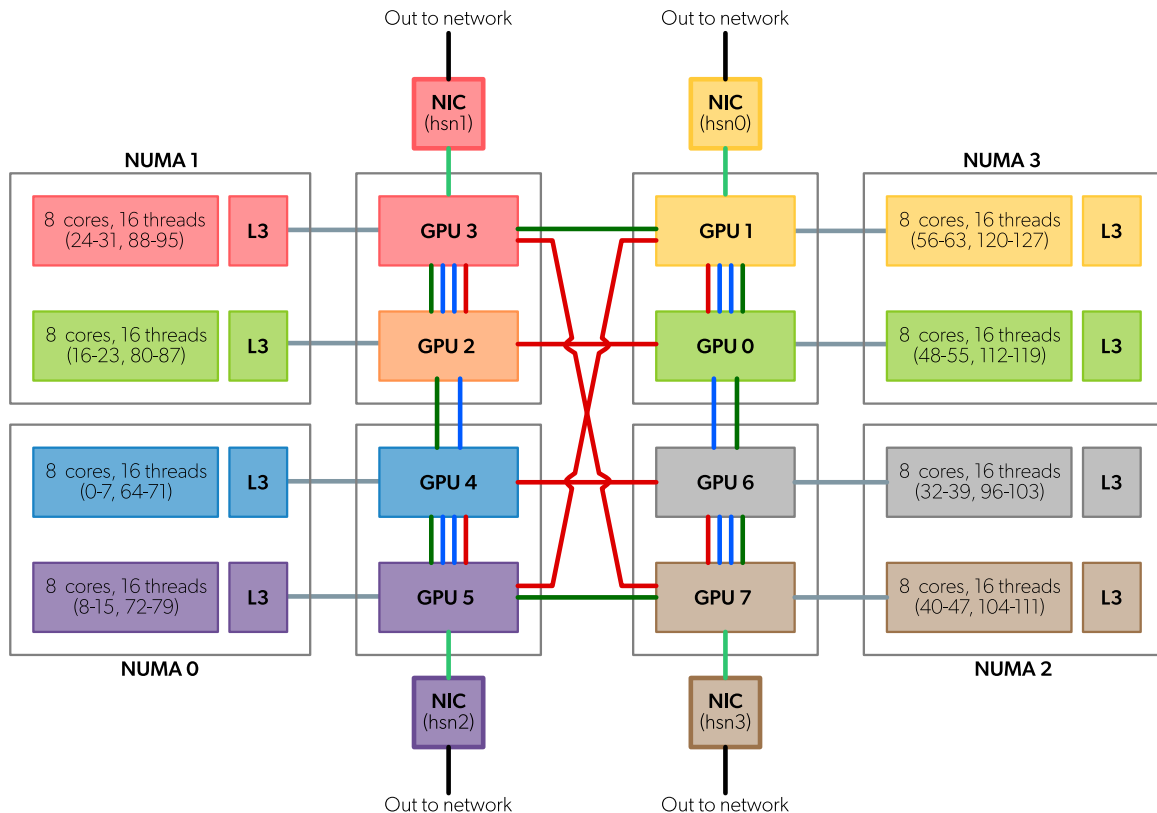
```
...
#SBATCH --partition=standard-g
#SBATCH --gpus-per-node=8
...
cat << EOF > select_gpu_$SLURM_JOB_ID
#!/bin/bash
GPU_ORDER=(4 5 2 3 6 7 0 1)
export ROCR_VISIBLE_DEVICES=${GPU_ORDER[ \ $SLURM_LOCALID ]}
exec \ $*
EOF
chmod +x select_gpu_$SLURM_JOB_ID
...
srun --ntasks=$((SLURM_NNODES*8)) --cpus-per-task=7 \
    ./select_gpu_$SLURM_JOB_ID gpu_check -l
...
export OMP_NUM_THREADS=6
srun --ntasks=$((SLURM_NNODES*8)) --cpus-per-task=7 \
    ./select_gpu_$SLURM_JOB_ID gpu_check -l
```



GPU binding: Green ring (1)

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Task	GCD	CCD	HWTs
0	0	6	49-55, 113-119
1	1	7	57-63, 121-127
2	3	3	25-32, 89-95
3	2	2	17-23, 81-87
4	4	0	1-7, 65-71
5	5	1	9-15, 73-79
6	7	5	41-47, 105-111
7	6	4	33-39, 97-103



GPU binding: Green ring (2)

L U M I

```
...
#SBATCH --partition=standard-g
#SBATCH --gpus-per-node=8
...
cat << EOF > select_gpu_$SLURM_JOB_ID
#!/bin/bash
GPU_ORDER=(0 1 3 2 4 5 7 6)
export ROCR_VISIBLE_DEVICES=${GPU_ORDER[${SLURM_LOCALID}]}
exec \*$*
EOF
chmod +x select_gpu_$SLURM_JOB_ID
...
CPU_BIND1="map_cpu:49,57,25,17,1,9,41,33"
srun --ntasks=$((SLURM_NNODES*8)) --cpu-bind=$CPU_BIND1 \
    ./select_gpu_$SLURM_JOB_ID gpu_check -l
```



GPU binding: Green ring (3)

L U M I

```
cat << EOF > select_gpu_$SLURM_JOB_ID
#!/bin/bash
GPU_ORDER=(0 1 3 2 4 5 7 6)
export ROCR_VISIBLE_DEVICES=\${GPU_ORDER[\$SLURM_LOCALID]}
exec \$*
EOF
chmod +x select_gpu_$SLURM_JOB_ID
...
CCD_MASK=( 0x00000000000000fe \
           0x000000000000fe00 \
           0x0000000000fe0000 \
           0x00000000fe000000 \
           0x000000fe00000000 \
           0x0000fe0000000000 \
           0x00fe000000000000 \
           0xfe00000000000000 )

CPU_BIND2="mask_cpu"
CPU_BIND2="$CPU_BIND2:${CCD_MASK[6]},${CCD_MASK[7]}"
CPU_BIND2="$CPU_BIND2:${CCD_MASK[3]},${CCD_MASK[2]}"
CPU_BIND2="$CPU_BIND2:${CCD_MASK[0]},${CCD_MASK[1]}"
CPU_BIND2="$CPU_BIND2:${CCD_MASK[5]},${CCD_MASK[4]}"
srun --ntasks=$((SLURM_NNODES*8)) --cpu-bind=$CPU_BIND2 \
    ./select_gpu_$SLURM_JOB_ID gpu_check -l
```



“Allocate by resources” partitions

- Proper binding not possible unless exclusively allocating entire nodes only
- Slurm will use a control group per task for the GPUs
 - You almost have to use `--gpu-per-task` to ensure that GPUs and tasks are on the same nodes (unless you use just a single node)
 - Problems with Peer2Peer IPC
 - Solution:
 - Turn off with `--gpu-bind=none`
 - This will number visible GPUs for the job on each node from 0,
 - and we can then again use the local task ID to assign a GPU to each task via `ROCR_VISIBLE_DEVICES` via the `select_gpu` script trick.
- Optimal mapping is not possible, but a proper setting of `MPICH_OFI_NIC_POLICY` may still make sense.

Questions?