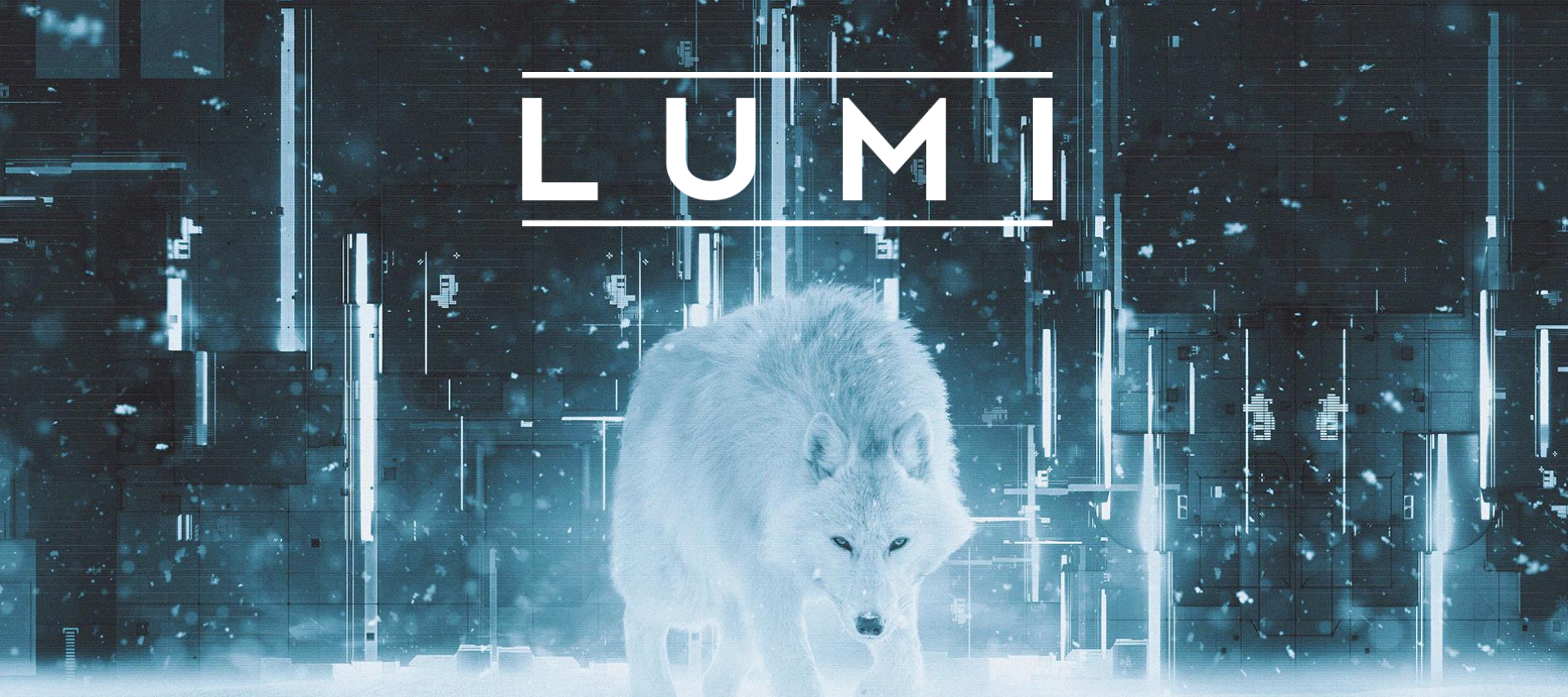

LUMI update January 2026

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Main LUMI stack: 25.03

LUMI

- Motivation:
  - CPE 25.03 is the only one fully validated on the current system configuration (current libfabric build + ROCm 6.3 + SUSE 15 SP6)
  - Could move from almost the start as the stack was sufficiently ready since we had containers available for development and a test system for the last tests
- Secondary stack: 25.09
  - Newest compilers available for LUMI.
  - Way to gain experience with Cray MPICH 9
  - Will likely work with our own ROCm 6.4.4 module instead
  - But still in the early stages as we could not prepare for this one
  - Need to load lumi-CrayPath after loading all modules, or use the LD_LIBRARY_PATH trick
- New developments happen exclusively on 25.03 or newer unless an older version could solve a burning problem with little effort

Main LUMI stack: 25.03

LUMI

- Already a fairly complete set of EasyBuild recipes for software, but focus on recent versions of packages
  - We don't support versions older than 2 years unless it only requires little effort
  - Old software and new compilers don't always go together well if the author was not careful following standards, and packages have disappeared temporarily from the LUMI stacks due to compatibility problems with new compilers
  - Software with commercial licenses (anyone say VASP?) slower to appear as we may need help from partners with access to a valid license
  - Offer ROCm downgrade to 6.2 also
- Default answer in case of problems will often be: "move to 25.03 (or even 25.09) as then we can exclude a number of causes".

Other stacks

LUMI

- All older LUMI stacks now use ROCm 6.3 instead of the version they were built for
  - Driver support issue
- LUMI/24.03:
  - Cray PE 24.03 was built for ROCm 6.0, but we run it with ROCm 6.3
  - Most software still compiles, but we did not really test-run all of these binaries
  - Offered as-is with little extra development from LUST
- LUMI/23.09: Offered as-is and known broken
  - Cray PE 23.09 was built for ROCm 5.2 and 5.5, but we run it now with ROCm 6.3
  - Only there for a project that really wanted to keep trying to use it, but we expect issues not only with GPU but also with MPI.
  - MPI for GNU definitely broken
- Older LUMI stacks have been removed
- No ROCm 7.0-based stack yet as there are too many issues

Other stacks (2)

LUMI

- CrayEnv: Some version updates of packages (mostly build tools)
- Will offer Spack configuration when ready
  - Changes in the LUST team have slowed down spack developement
  - As usual, spack will be offered "as is" but we cannot do any development in Spack packages
  - We will encourage the use of spack environments more over the use of a more classic stack as we have now as that seems to solve problems we've run into
- Cannot tell much about stacks in /appl/local
  - Change in development for the AI containers: They will now come from the AI factory.
  - CSC has been working hard on checking and updating software in /appl/local/csc. Much is already there

Minor changes and issues

LUMI

- Move to EasyBuild 5
  - Overview of all dependencies now with `-Dr` instead of `-D`
  - Prints a lot more information about the build which may be a bit overwhelming
- Hugepages support is broken; not clear yet if it will be fixed
  - Disabled in EasyBuild recipes where we used it (basically GROMACS and PLUMED)

Bindings in Slurm

LUMI

- The srun `--gpu-bind` flag now kind of works (at least with explicit mapping of the GPU)
  - Has to be used in combination with `--gres-flags=allow-task-sharing` or communication will fail
  - Documentation and training materials will follow
- Example 1:

```
ml LUMI/25.03 partition/G lumi-CPEtools/1.2-cpeAMD-25.03-hpcat-0.9
srun -N2 -G16 -pstandard-g -n16 -c7 \
     --gpu-bind=map:4,5,2,3,6,7,0,1 --gres-flags=allow-task-sharing \
     hpcat
```

HPC Affinity Tracker (v0.9)

LUMI

FABRIC GROUP ID	HOST (NODE)	MPI RANK	CPU			ACCELERATORS			NETWORK	
			LOGICAL PROC	PHYSICAL CORE	NUMA	ID	PCIE ADDR.	NUMA	INTERFACE	NUMA
16	nid005391									
	>>> d)e)	0	1-7	1-7	0	4	[0:d1]	0	cxi0	3
	>>> d)e)	1	9-15	9-15	0	5	[0:d6]	0	cxi0	3
		2	17-23	17-23	1	2	[0:c9]	1	cxi1	1
		3	25-31	25-31	1	3	[0:ce]	1	cxi1	1
	>>> d)e)	4	33-39	33-39	2	6	[0:d9]	2	cxi2	0
	>>> d)e)	5	41-47	41-47	2	7	[0:de]	2	cxi2	0
	>>> d)e)	6	49-55	49-55	3	0	[0:c1]	3	cxi3	2
	>>> d)e)	7	57-63	57-63	3	1	[0:c6]	3	cxi3	2
16	nid005392									
	>>> d)e)	8	1-7	1-7	0	4	[0:d1]	0	cxi0	3
	>>> d)e)	9	9-15	9-15	0	5	[0:d6]	0	cxi0	3
		10	17-23	17-23	1	2	[0:c9]	1	cxi1	1
		11	25-31	25-31	1	3	[0:ce]	1	cxi1	1
	>>> d)e)	12	33-39	33-39	2	6	[0:d9]	2	cxi2	0
	>>> d)e)	13	41-47	41-47	2	7	[0:de]	2	cxi2	0
	>>> d)e)	14	49-55	49-55	3	0	[0:c1]	3	cxi3	2
	>>> d)e)	15	57-63	57-63	3	1	[0:c6]	3	cxi3	2

FABRIC GROUP ID	HOST (NODE)	MPI RANK	CPU			ACCELERATORS			NETWORK	
			LOGICAL PROC	PHYSICAL CORE	NUMA	ID	PCIE ADDR.	NUMA	INTERFACE	NUMA

TOTAL: 1	2	16	WARNING(S): d) Task(s) have different CPU and NIC NUMA affinities e) Task(s) have different GPU and NIC NUMA affinities

Bindings in Slurm

LUMI

- Example 1 corrected:

```
ml LUMI/25.03 partition/G lumi-CPEtools/1.2-cpeAMD-25.03-hpcat-0.9

export MPICH_OFI_NIC_POLICY=GPU
export MPICH_GPU_SUPPORT_ENABLED=1

srun -N2 -G16 -pstandard-g -n16 -c7 \
     --gpu-bind=map:4,5,2,3,6,7,0,1 --gres-flags=allow-task-sharing \
     hpcat
```

HPC Affinity Tracker (v0.9)

LUMI

FABRIC GROUP ID	HOST (NODE)	MPI RANK	CPU			ACCELERATORS			NETWORK	
			LOGICAL PROC	PHYSICAL CORE	NUMA	ID	PCIE ADDR.	NUMA	INTERFACE	NUMA
14	nid005203									
		0	1-7	1-7	0	4	[0:d1]	0	cxi2	0
		1	9-15	9-15	0	5	[0:d6]	0	cxi2	0
		2	17-23	17-23	1	2	[0:c9]	1	cxi1	1
		3	25-31	25-31	1	3	[0:ce]	1	cxi1	1
		4	33-39	33-39	2	6	[0:d9]	2	cxi3	2
		5	41-47	41-47	2	7	[0:de]	2	cxi3	2
		6	49-55	49-55	3	0	[0:c1]	3	cxi0	3
		7	57-63	57-63	3	1	[0:c6]	3	cxi0	3
14	nid005204									
		8	1-7	1-7	0	4	[0:d1]	0	cxi2	0
		9	9-15	9-15	0	5	[0:d6]	0	cxi2	0
		10	17-23	17-23	1	2	[0:c9]	1	cxi1	1
		11	25-31	25-31	1	3	[0:ce]	1	cxi1	1
		12	33-39	33-39	2	6	[0:d9]	2	cxi3	2
		13	41-47	41-47	2	7	[0:de]	2	cxi3	2
		14	49-55	49-55	3	0	[0:c1]	3	cxi0	3
		15	57-63	57-63	3	1	[0:c6]	3	cxi0	3
FABRIC GROUP ID	HOST (NODE)	MPI RANK	CPU			ACCELERATORS			NETWORK	
			LOGICAL PROC	PHYSICAL CORE	NUMA	ID	PCIE ADDR.	NUMA	INTERFACE	NUMA
TOTAL: 1	2	16								

Bindings in Slurm

- Example 2 with restricted cores:

```
ml LUMI/25.03 partition/G lumi-CPEtools/1.2-cpeAMD-25.03-hpcat-0.9

export MPICH_OFI_NIC_POLICY=GPU
export MPICH_GPU_SUPPORT_ENABLED=1

srun -N2 -G16 -pstandard-g -n16 \
     --cpu-bind=mask_cpu:7e,7e00,7e0000,7e000000,7e00000000,7e0000000000,7e000000000000,7e00000000000000 \
     --gpu-bind=map:4,5,2,3,6,7,0,1 --gres-flags=allow-task-sharing \
     hpcat
```

HPC Affinity Tracker (v0.9)

LUMI

FABRIC GROUP ID	HOST (NODE)	MPI RANK	CPU			ACCELERATORS			NETWORK	
			LOGICAL PROC	PHYSICAL CORE	NUMA	ID	PCIE ADDR.	NUMA	INTERFACE	NUMA
17	nid005540									
		0	1-6	1-6	0	4	[0:d1]	0	cxi2	0
		1	9-14	9-14	0	5	[0:d6]	0	cxi2	0
		2	17-22	17-22	1	2	[0:c9]	1	cxi1	1
		3	25-30	25-30	1	3	[0:ce]	1	cxi1	1
		4	33-38	33-38	2	6	[0:d9]	2	cxi3	2
		5	41-46	41-46	2	7	[0:de]	2	cxi3	2
		6	49-54	49-54	3	0	[0:c1]	3	cxi0	3
		7	57-62	57-62	3	1	[0:c6]	3	cxi0	3
17	nid005541									
		8	1-6	1-6	0	4	[0:d1]	0	cxi2	0
		9	9-14	9-14	0	5	[0:d6]	0	cxi2	0
		10	17-22	17-22	1	2	[0:c9]	1	cxi1	1
		11	25-30	25-30	1	3	[0:ce]	1	cxi1	1
		12	33-38	33-38	2	6	[0:d9]	2	cxi3	2
		13	41-46	41-46	2	7	[0:de]	2	cxi3	2
		14	49-54	49-54	3	0	[0:c1]	3	cxi0	3
		15	57-62	57-62	3	1	[0:c6]	3	cxi0	3

FABRIC GROUP ID	HOST (NODE)	MPI RANK	CPU			ACCELERATORS			NETWORK	
			LOGICAL PROC	PHYSICAL CORE	NUMA	ID	PCIE ADDR.	NUMA	INTERFACE	NUMA
TOTAL: 1	2	16								