



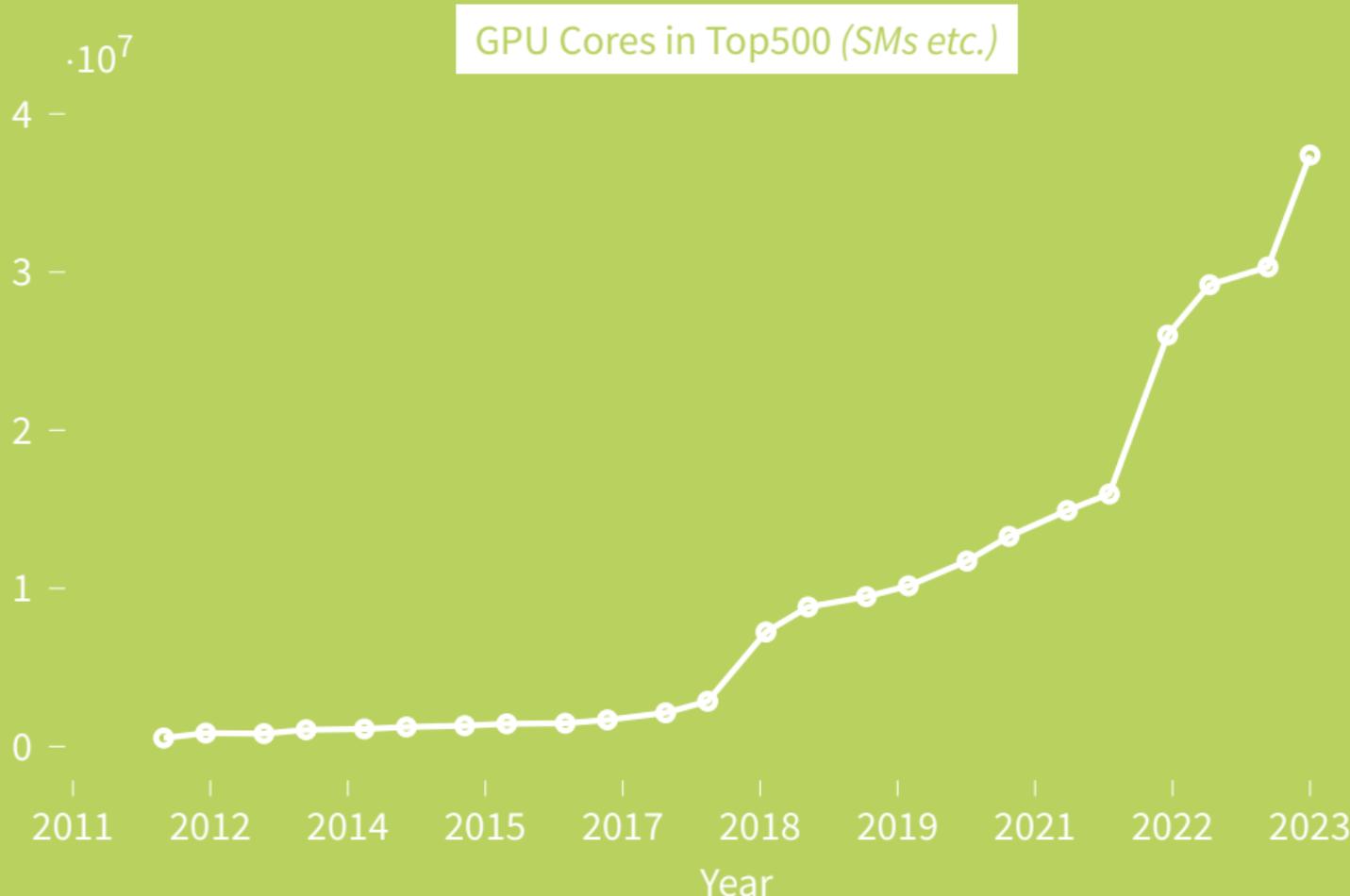
DISTRIBUTED GPU PROGRAMMING FOR EXASCALE ISC24 TUTORIAL SESSION 1

12 May 2024 | Andreas Herten | Jülich Supercomputing Centre, Forschungszentrum Jülich

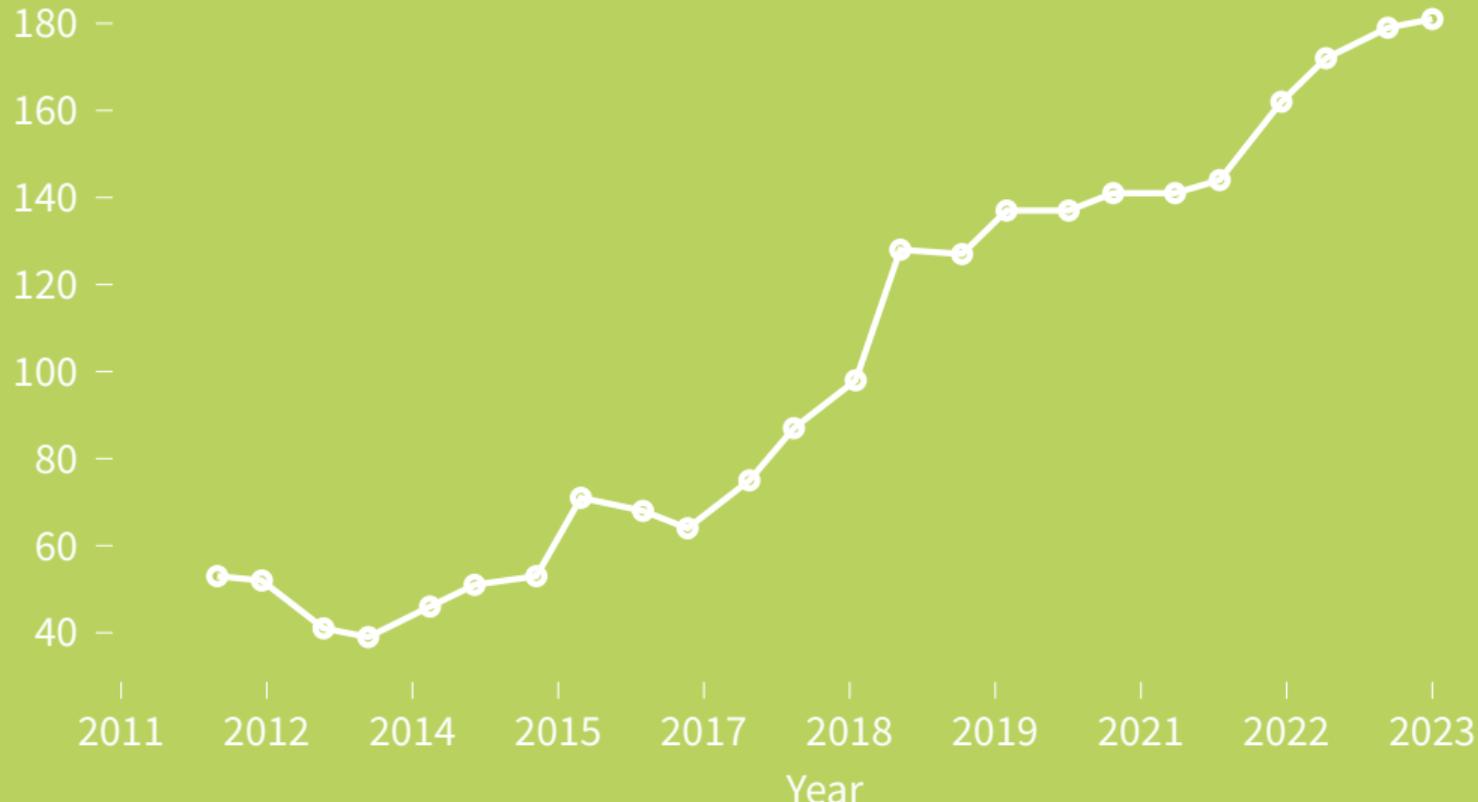
Welcome to

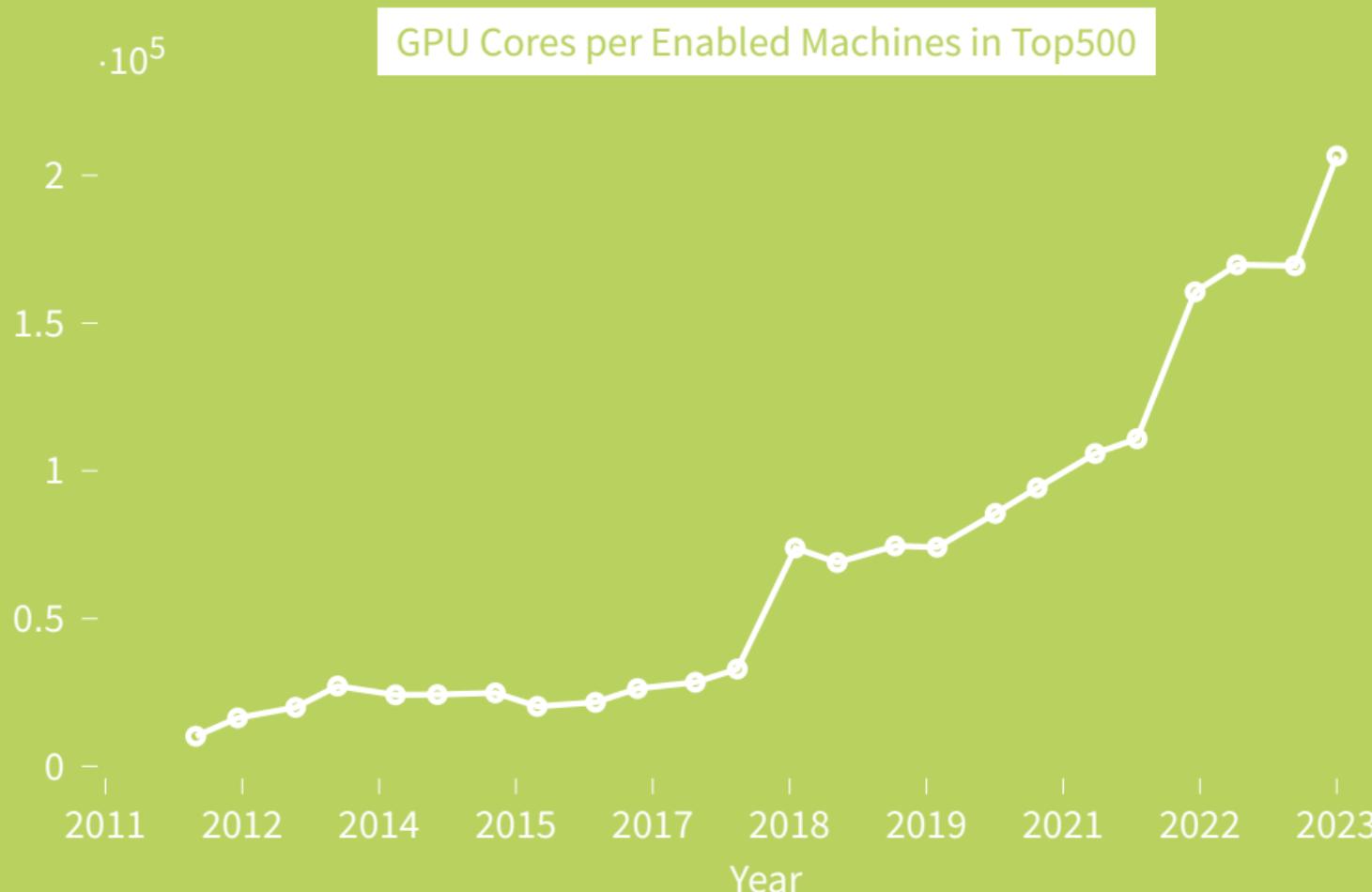
Efficient Distributed GPU Programming for Exascale,

an *ISC24 Tutorial*



GPU-enabled Machines in Top500





State of the GPUUnion

Landscape Overview

- Last decade
 - More and more GPUs installed in HPC machines
 - More and more HPC machines with GPUs
 - More and more GPUs in each machine

State of the GPUunion

Landscape Overview

- Last decade
 - More and more GPUs installed in HPC machines
 - More and more HPC machines with GPUs
 - More and more GPUs in each machine
- Future
 - GPUs selected as technology for enabling Exascale
→ Even larger GPU machines with larger GPUs
 - Pre-Exascale systems: LUMI^A, Leonardo^N; JUWELS Booster^N, Perlmutter^N
 - Exascale systems: Frontier^A, El Capitan^A, Aurora^I; JUPITER^N



ORNL's Frontier: > 35 000 GPUs, 1.5 EFLOPs/s, 2022

32 % of all installed GPU cores in Frontier!
Rendering by ORNL

State of the GPUUnion

Landscape Overview

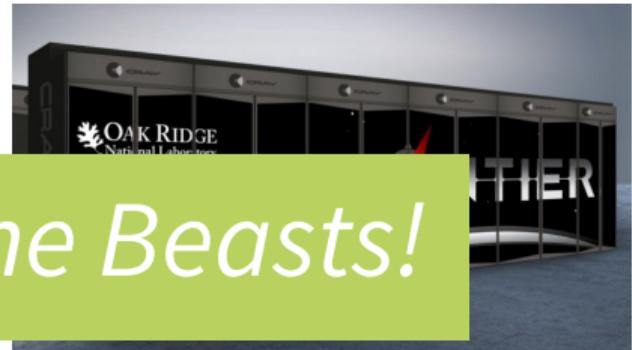
- Last decade
 - More and more GPUs installed in HPC machines
 - More and more HPC machines with GPUs
 - More and more GPUs in each machine

- Future

- GPU
 - Evolution

We help to Tame the Beasts!

- Pre-Exascale systems: LUMI^A, Leonardo^N; JUWELS Booster^N, Perlmutter^N
- Exascale systems: Frontier^A, El Capitan^A, Aurora^I; JUPITER^N



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About Tutorial

Goals

- Prepare for large-scale GPU systems
- Learn GPU+MPI basics
- Apply optimization, analysis techniques
- Study CPU-less GPU+MPI
- Use advanced libraries to improve scaling efficiency

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Non-Goals

- Optimize your GPU application; we teach tools and techniques, you need to apply!
- Learn MPI; we expect base-level knowledge of MPI, you don't need more.
- Discuss general scalability; GPU-independent features (like load balancing) are too broad a topic
- Learn CUDA; we expect principle knowledge of GPU programming
- Showcase all GPU platforms; we use an NVIDIA system and teach NVIDIA libraries and tools, other platforms (AMD) follow along (see last lecture)

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Curriculum

1L	Lecture <i>Onboarding</i>	Tutorial Overview, Introduction to System <i>Accessing JUWELS Booster</i>
2L	Lecture	Introduction to MPI-Distributed Computing with GPUs
3H	Hands-On	Multi-GPU Parallelization <i>11:00 - 11:30: Coffee Break</i>
4L	Lecture	Performance and Debugging Tools
5L	Lecture	Optimization Techniques for Multi-GPU Applications
6H	Hands-On	Overlap Communication and Computation with MPI <i>13:00 - 14:00: Lunch Break</i>
7L	Lecture	NCCL and Host-Initiated NVSHMEM
8H	Hands-On	Using NCCL and NVSHMEM <i>16:00 - 16:30: Coffee Break</i>
9L	Lecture	CUDA Graphs and Device-Initiated NVSHMEM
10H	Hands-On	CUDA Graphs and Device-Initiated NVSHMEM
11L	Lecture	Outline of Advanced Topics and Conclusion

Tutorial Team

Hello from Europe



Simon Garcia

Scalable Computer Architectures
Sandia National Laboratories



Jiri Kraus

DevTech Compute
NVIDIA



Andreas Herten

Accelerating Devices Lab
Jülich Supercomputing Centre



Lena Oden

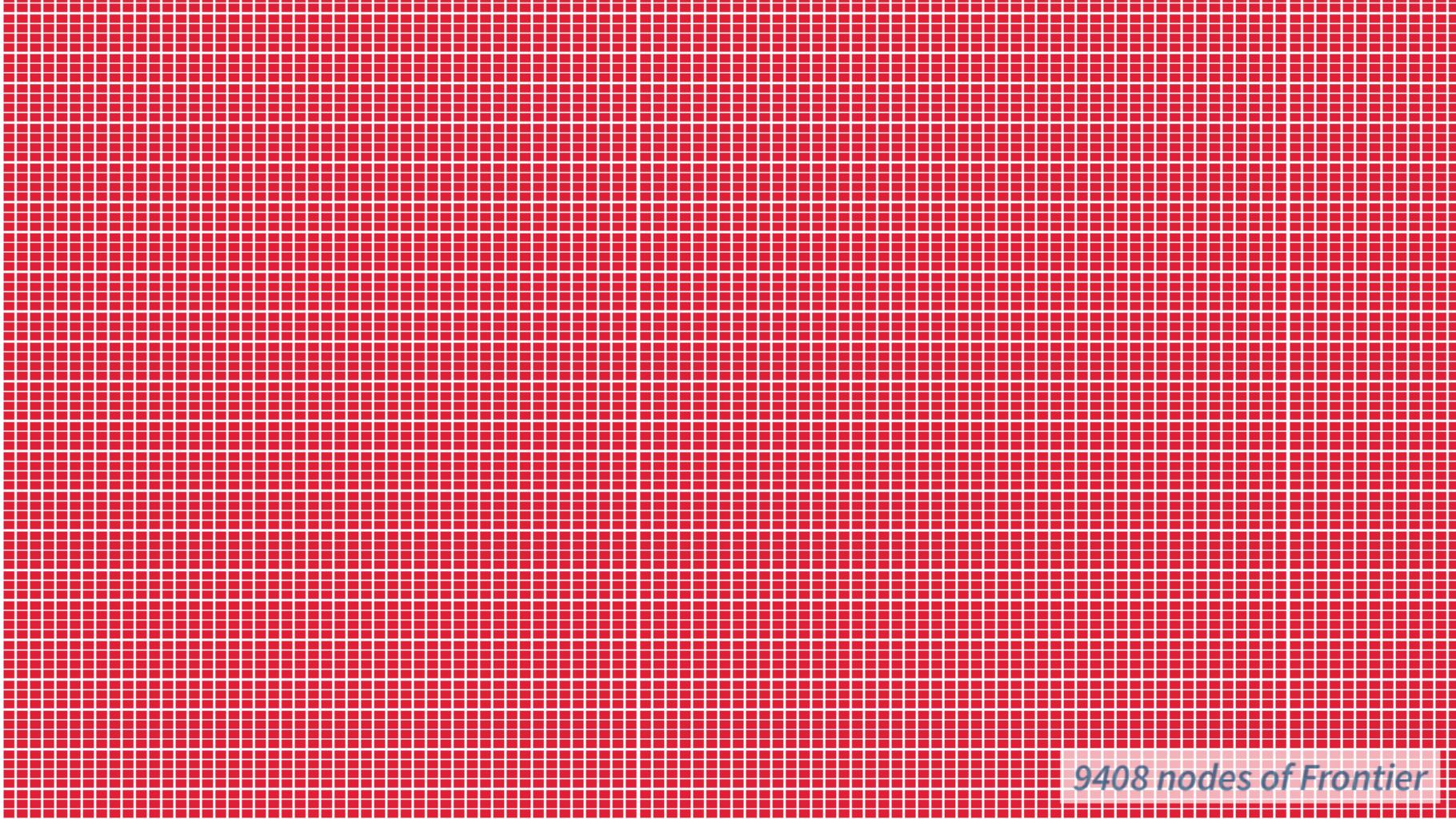
Prof. for Computer Engineering
University Hagen



Markus Hrywniak

DevTech Compute
NVIDIA

Exascale GPU Systems

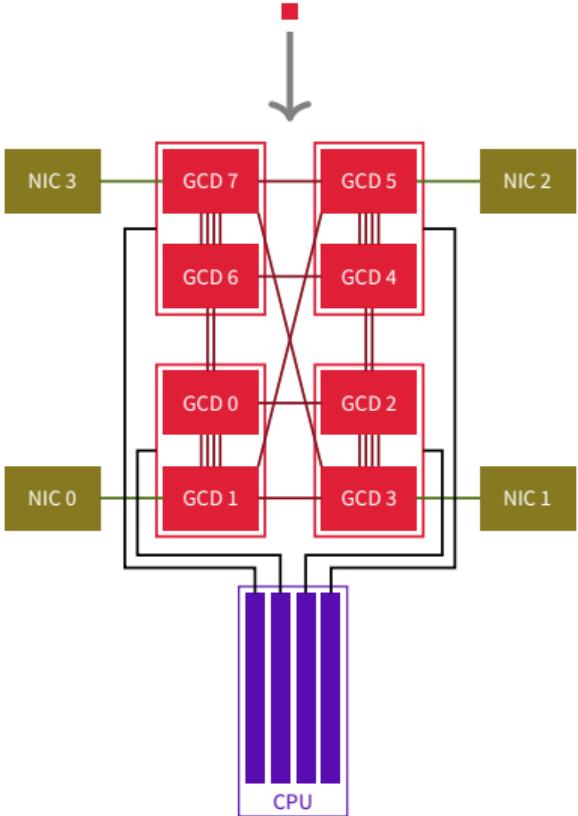


9408 nodes of Frontier

Frontier

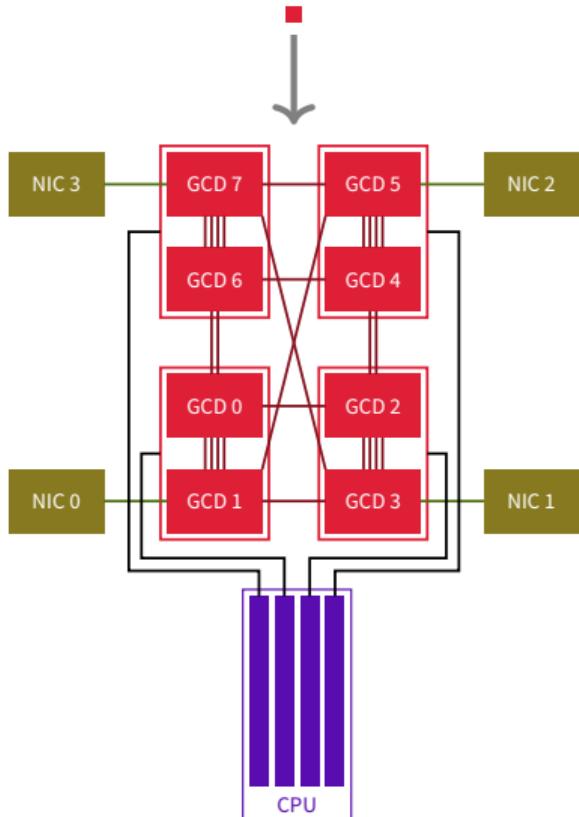


Frontier



Frontier

- At Oak Ridge Nation Lab, US
 - First Exascale system
 - HPL: 1.194 EFLOP/S
 - GPU : 4× AMD Radeon Instinct MI250X
2 GCDs per GPU, 64 GB memory per GCD
 - CPU : 1× AMD Epyc Trento, 64 cores; 4 NUMA domains, one per GCD; 512 GB DDR memory
 - Network : 4× HPE Slingshot, 4 × 50 GB/s
- 9408 nodes, 37 632 GPUs, 75 264 GCDs, 37 632 network devices

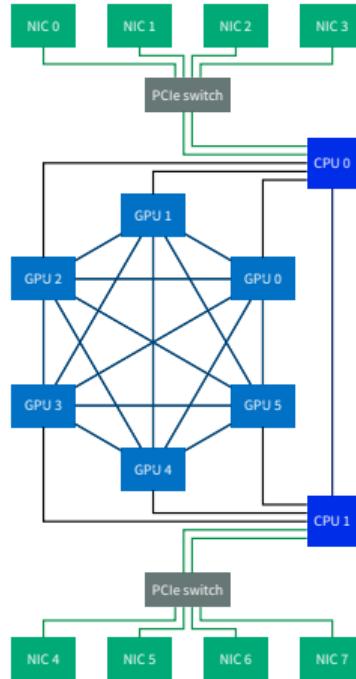


10 624 nodes of Aurora

Aurora

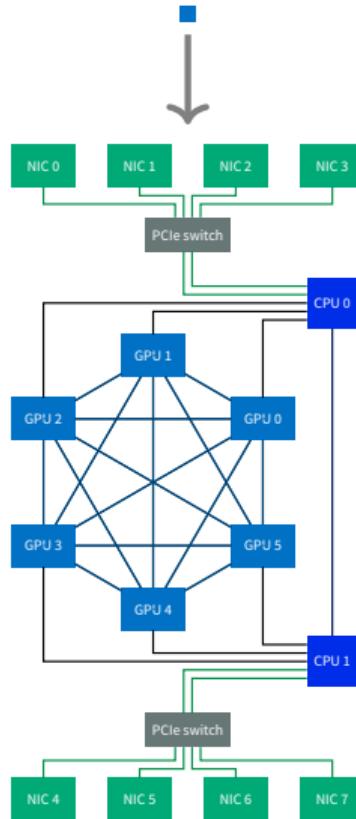


Aurora



Aurora

- At Argonne National Lab, US
 - First 2 EFOp/s system?
 - HPL: ???
 - GPU : 6× Intel Ponte Vecchio (*Data Center GPU Max*)
128 GB memory per GPU
 - CPU : 2× Intel Sapphire Rapids, 2× 56 cores; 2×
56 GB HBM memory; 1 TB DDR memory
 - Network : 4× HPE Slingshot, 8 × 50 GB/s
- 10 624 nodes, 63 744 GPUs, 84 992 network devices



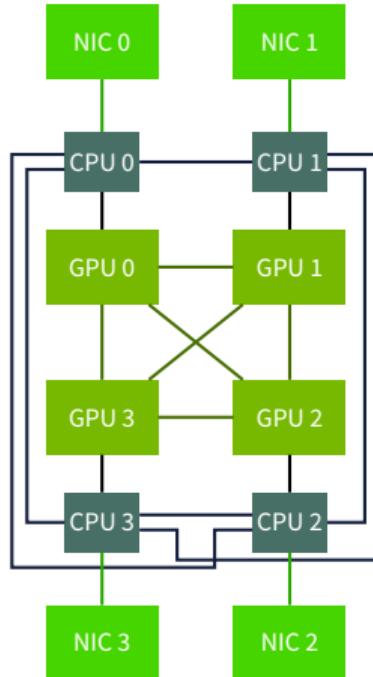
\approx 6000 nodes of JUPITER

JUPITER



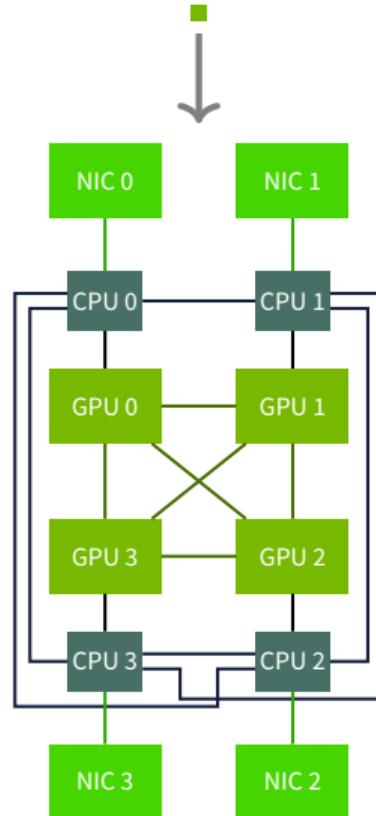
JUPITER

↓



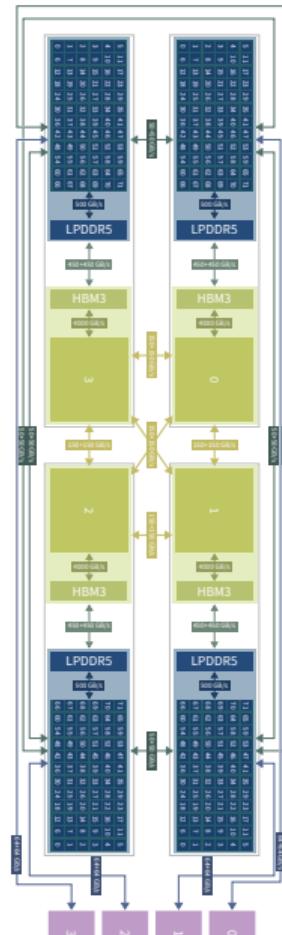
JUPITER

- At Jülich Supercomputing Center, Germany; procured by EuroHPC JU
 - First European Exascale system
 - HPL: ???
 - GPU : 4× NVIDIA H100 *Grace-Hopper flavor*
96 GB memory per GPU
 - CPU : 4× NVIDIA Grace, 4× 72 cores; 4× 120 GB LPDDR5X memory
 - Network : 4× NVIDIA Mellanox InfiniBand NDR200,
4 × 25 GB/s
- ≈6000 nodes, ≈24 000 GPUs, ≈24 000 network devices



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 - CPU : 4× Intel Xeon Gold 6242R, 4× 120 GB LPDDR5X memory
 - Network : 4× NVIDIA Mellanox InfiniBand NDR200,
4 × 25 GB/s
- ≈6000 nodes, ≈24 000 GPUs, ≈24 000 network devices

Today: JUWELS Booster!



System: JUWELS Booster



JUWELS Booster – Scaling Higher!

- 936 nodes with AMD EPYC Rome CPUs (2×24 cores)
- Each with 4 NVIDIA A100 Ampere GPUs (each: FP64TC : 19.5 TFLOP/S, FP64 : 9.7 GB memory)
- InfiniBand DragonFly+ HDR-200 network; 4×200 Gbit/s per node



Top500 List Nov 2020:

- #1 Europe
- #7 World
- #4* Top/Green500

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 FP64 : 9.7
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JUWELS Booster Overview

Node Configuration

Arch Atos Bull Sequana XH2000

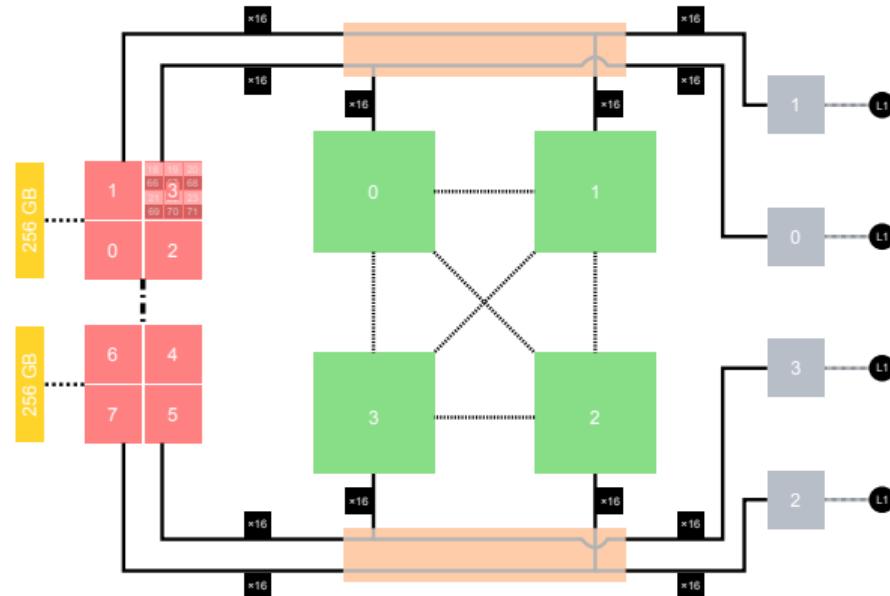
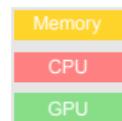
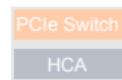
CPU 2 × AMD EPYC 7402:

2Socket × 24Core × 2SMT,
2 × 256 GB DDR4-3200 RAM;
NPS-4

GPU 4 × NVIDIA A100 40 GB, NVLink3

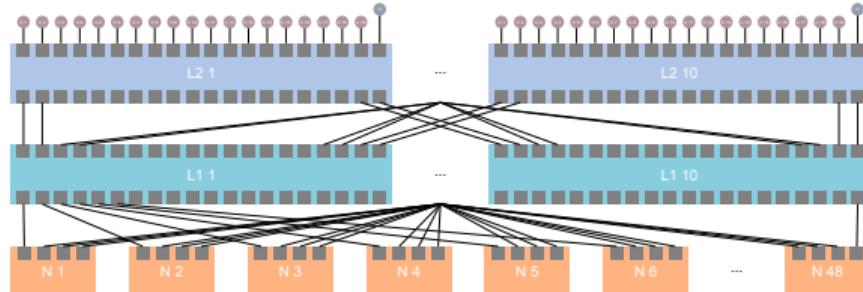
HCA 4 × Mellanox HDR200
(200 Gbit/s) InfiniBand ConnectX
6

etc 2 × PCIe Gen 4 switch

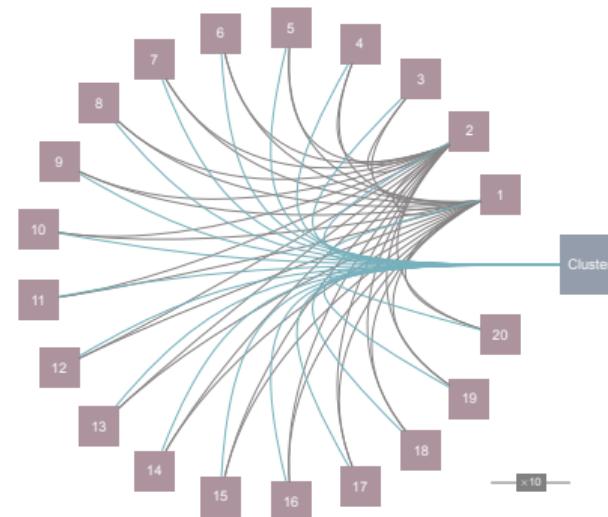


JUWELS Booster Overview

Network Configuration: DragonFly+ Network



In-Cell (48 nodes): Full fat-tree in 2 levels



Inter-Cell (20 cells): 10 links between each pair of cells

AMD EPYC Rome

Some Processor Basics

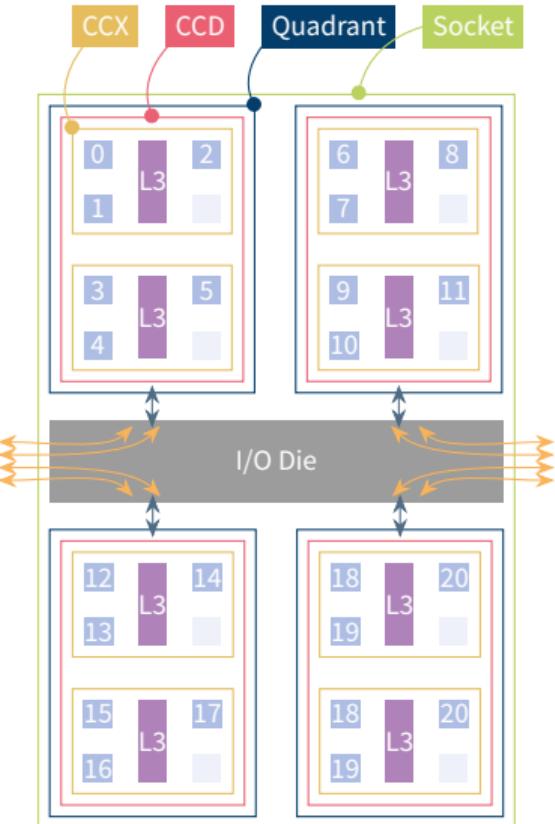
- JUWELS Booster: AMD EPYC Rome 7402 (24 core (SMT-2) × 2 sockets)
- EPYC processor: Built as Multi-Chip Module
→ Many building blocks, hierarchies

AMD EPYC Rome

Some Processor Basics

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- EPYC processor: Built as Multi-Chip Module
→ Many building blocks, hierarchies

3 cores	Core-Complex (CCX), shared L3 (<i>max 4 cores</i>)
2 CCXs	Core Complex Die (CCD)
1 CCD	1 quadrant (<i>max 2 CCDs per quadrant</i>)
4 quadrants	1 socket; NPS-4: 4 NUMA domains per socket
2 sockets	1 node (<i>only 1 shown</i>)
I/O Die	Connections between quadrants and outside
RAM	8 memory channels, 2 per quadrant



AMD EPYC Rome

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2 CCXs Core Complex Die (CCD)

1 CCD 1 quadrant (*max 2 CCDs per quadrant*)

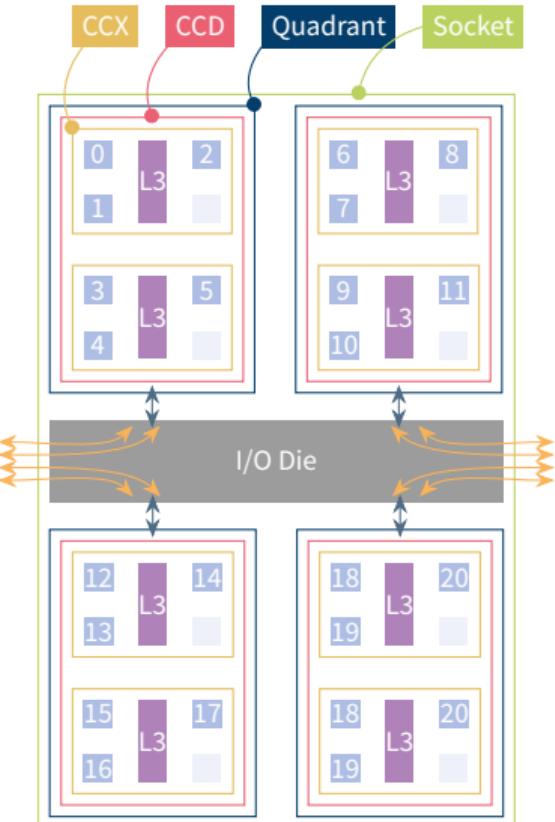
4 quadrants 1 socket; NPS-4: 4 NUMA domains per socket

2 sockets 1 node (*only 1 shown*)

I/O Die Connections between quadrants and outside

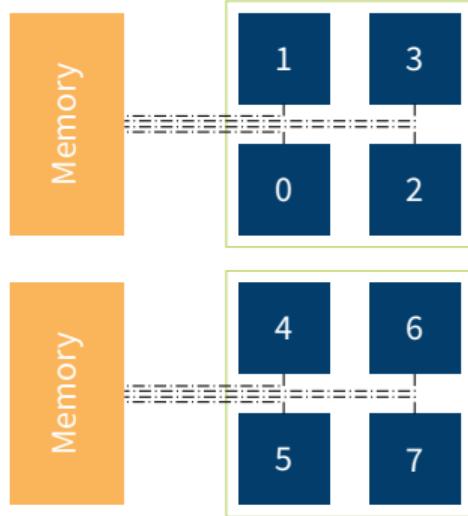
RAM 8 memory channels, 2 per quadrant

⇒ Complex topology!



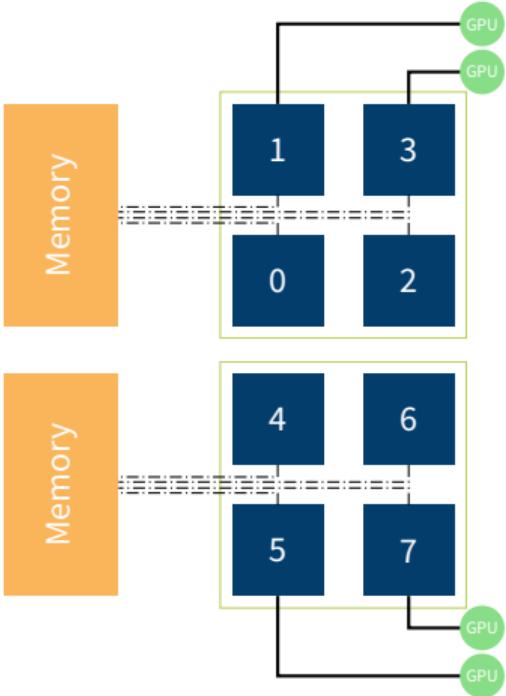
NUMA Overview

- GPUs, HCAs associated to one CPU quadrant (NUMA)
- NUMA domains are numbered



NUMA Overview

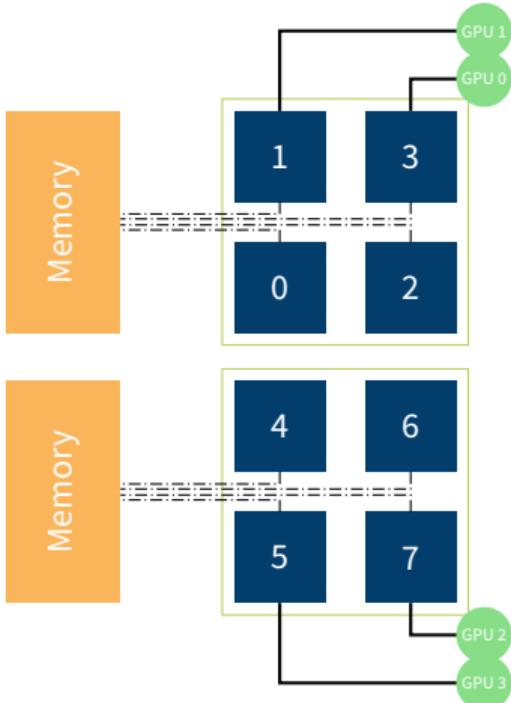
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- Complete affinity table

Rank	NUMA Domain	GPU ID	HCA ID
0	3	0	0
1	1	1	1
2	7	2	2
3	5	3	3

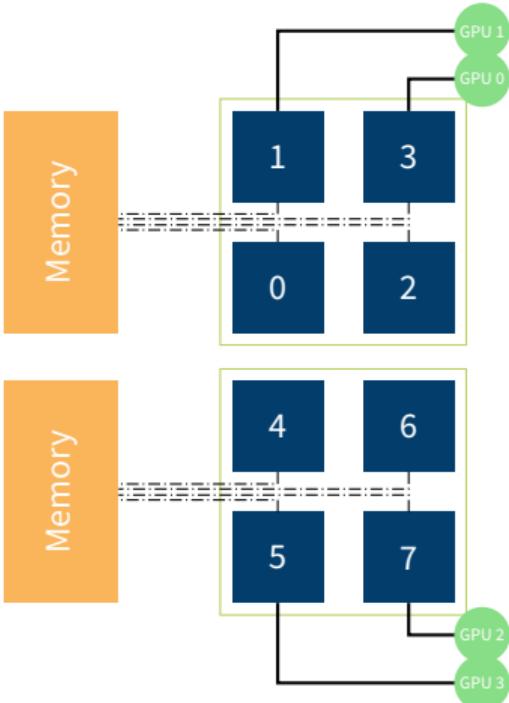


NUMA Overview

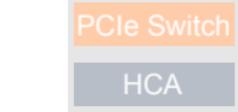
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→ Slurm configured to automatically use best topology



NUMA Overview



- GPUs, HCAs associated with the CPU queue (NUMA)

- NUMA domains are assigned to each HCA

- But no 1:1 relationship between HCA IDs

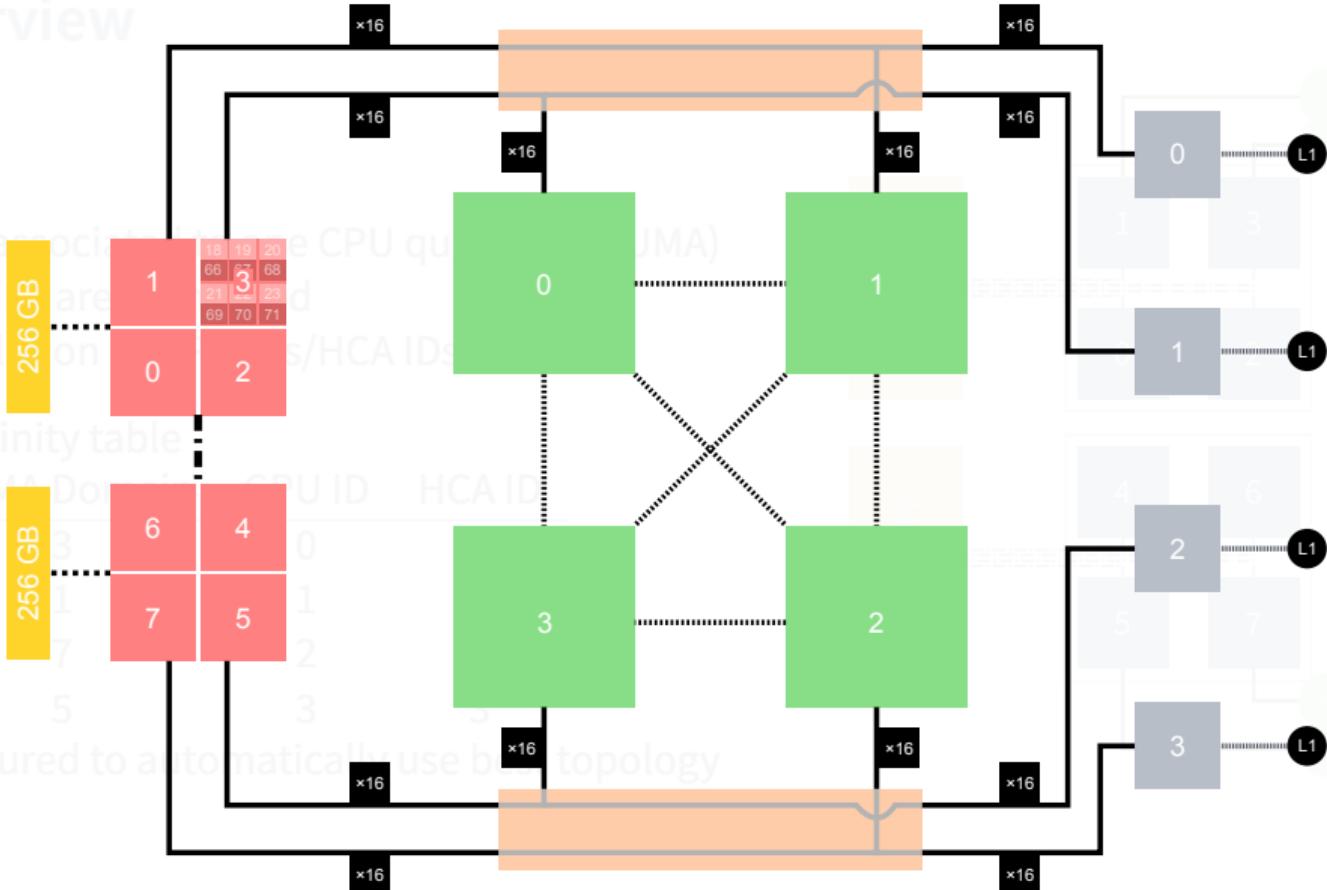
- Complete affinity table

- Rank NUMA Domains CPU ID HCA ID

Rank	0	0	0
0	256 GB	1	16
1	256 GB	0	16
2	256 GB	2	16

Rank	0	1	2	3	4	5	6	7
0	Memory	CPU						
1	GPU	GPU	GPU	GPU	GPU	GPU	GPU	GPU
2	GPU	GPU	GPU	GPU	GPU	GPU	GPU	GPU
3	GPU	GPU	GPU	GPU	GPU	GPU	GPU	GPU

→ Suggested to automatically use best topology



DragonFly+ Topology

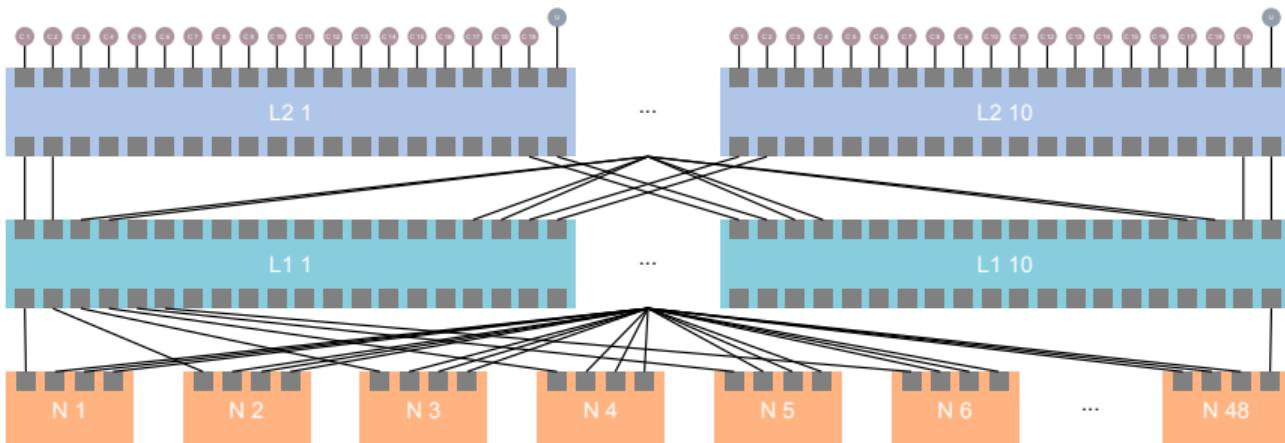
Overview

- 3744 end points; adaptive routing
- HDR200: 200 Gbit/s per link per direction
- Dragonfly+ Topology selected as good way to balance factors (space, investment, performance)
- Two-level topology: local (in-cell), non-local (inter-cell)
- Still learning practical implications of topology

DragonFly+ Topology

In-Cell Topology

- In-cell: full fat-tree in 2 levels
 - 48 nodes, each 4 links (*strided to 4 L1 switches*)
 - 10 L1 switches, 40 port (*each L1 switch: 2 links to L2, strided to 10 L2 switches*)
 - 10 L2 switches, 40 port (*each L2 switch: 1 link to L2 switch of all other cells, 1 link to cluster*)



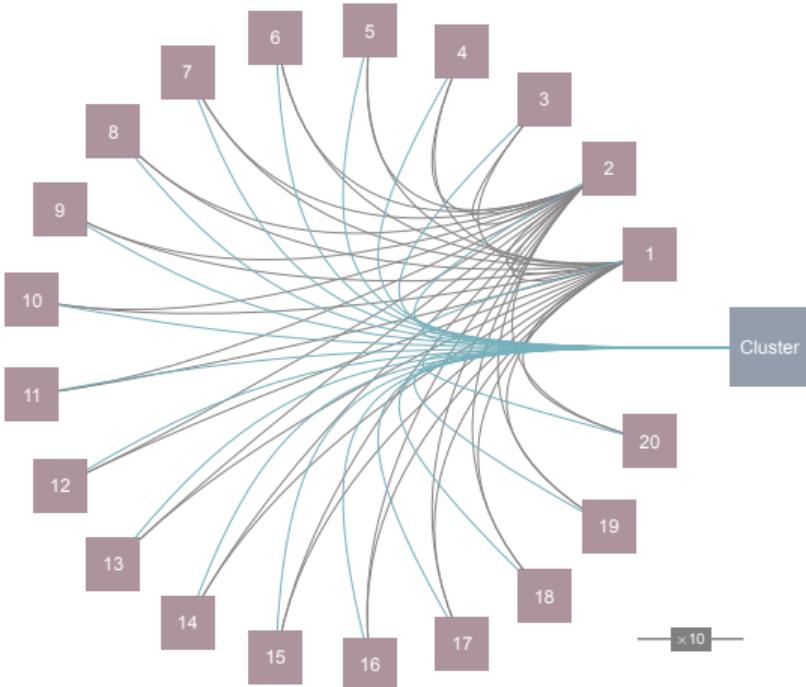
DragonFly+ Topology

Intra-Cell Topology

- Inter-cell: 20 cells

- 10 links between each pair of cells
- 10 links per cell to JUWELS Cluster
- Filesystem access via cell 20
- Bi-section bandwidth between N cells:

$$\mathcal{B}(N) = \lfloor (N/2)^2 \rfloor \times (10 \times bw_1)$$



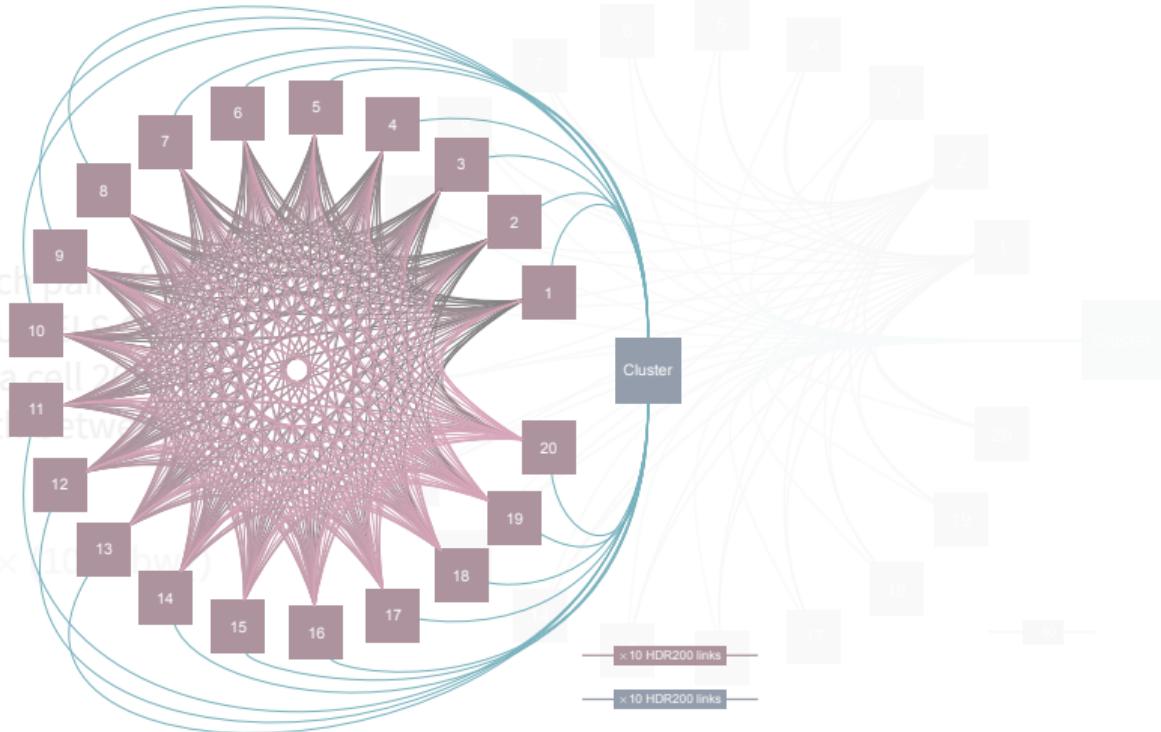
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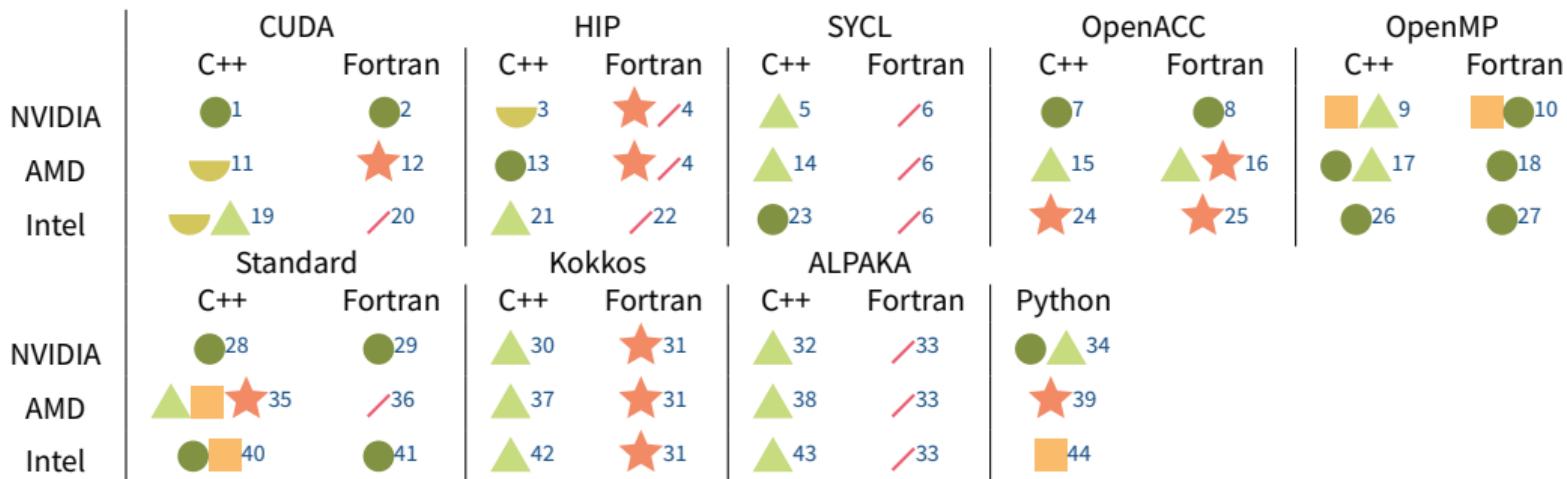
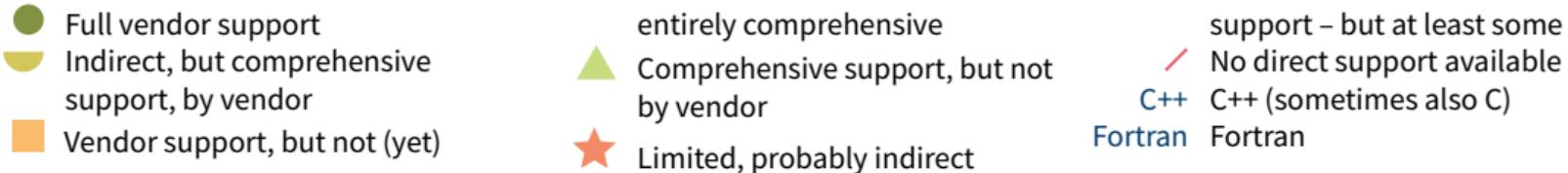


Vendors, Models

GPU Vendors in Tutorial

- First Exascale machine: Frontier, with **AMD** GPUs!
- This tutorial: **NVIDIA** examples
 - JUWELS Booster: machine for tutorial
 - We have most experience with NVIDIA
 -  JUPITER: NVIDIA GPUs
- **But:** Everything similar for other vendors (especially AMD)
- More on other vendors in last session

GPU Programming Models



See appendix for explanations, or doi:10.34732/xdvblg-r1bvif/doi:10.48550/arXiv.2309.05445

Programming Model in Tutorial

- Tutorial: **CUDA** for GPU programming
 - Many other possibilities, especially for NVIDIA GPUs
 - Some: higher-level abstractions, mapping back to CUDA
 - Conceptionally all similar
 - No significant changes needed to use MPI
- Transfer CUDA knowledge to other models

Summary and Conclusions

Summary and Conclusions

- Exascale and Pre-Exascale systems mainly based on GPUs, with thousands of devices
- Many advanced technologies in place to enable large-scale GPU applications
- Tutorial with team experienced in distributed GPU workloads
- Supercomputer of tutorial: JUWELS Booster, European flagship system based on A100 GPUs and HDR200 InfiniBand network

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Thank you
for your attention!
a.herten@fz-juelich.de

Appendix

Appendix

Vendor/Programming Model Table

Appendix

Vendor/Programming Model Table:

GPU Vendor/Programming Model Table I

- 1: CUDA C/C++ is supported on NVIDIA GPUs through the [CUDA Toolkit](#)
- 2: CUDA Fortran, a proprietary Fortran extension, is supported on NVIDIA GPUs via the [NVIDIA HPC SDK](#)
- 3: HIP programs can directly use NVIDIA GPUs via a CUDA backend; HIP is maintained by AMD
- 4: No such thing like HIP for Fortran, but AMD offers Fortran interfaces to HIP and ROCm libraries in [hipfort](#)
- 5: SYCL can be used on NVIDIA GPUs with *experimental* support either in [SYCL](#) directly or in [DPC++](#), or via [hipSYCL](#)
- 6: No such thing like SYCL for Fortran
- 7: OpenACC C/C++ supported on NVIDIA GPUs directly (and best) through NVIDIA HPC SDK; additional, somewhat limited support by [GCC C compiler](#) and in LLVM through [Clacc](#)
- 8: OpenACC Fortran supported on NVIDIA GPUs directly (and best) through NVIDIA HPC SDK; additional, somewhat limited support by GCC Fortran compiler and [Flacc](#)
- 9: OpenMP in C++ supported on NVIDIA GPUs through NVIDIA HPC SDK (albeit [with a few limits](#)), by GCC, and Clang; see [OpenMP ECP BoF on status in 2022](#).
- 10: OpenMP in Fortran supported on NVIDIA GPUs through NVIDIA HPC SDK (but not full OpenMP feature set available), by GCC, and Flang
- 28: pSTL features supported on NVIDIA GPUs through [NVIDIA HPC SDK](#)
- 29: Standard Language parallel features supported on NVIDIA GPUs through NVIDIA HPC SDK
- 30: [Kokkos](#) supports NVIDIA GPUs by calling CUDA as part of the compilation process
- 31: Kokkos is a C++ model, but an official compatibility layer ([Fortran Language Compatibility Layer, FLCL](#)) is available.

GPU Vendor/Programming Model Table II

- 32: [Alpaka](#) supports NVIDIA GPUs by calling CUDA as part of the compilation process; also, an OpenMP backend can be used
- 33: Alpaka is a C++ model
- 34: There is a vast community of offloading Python code to NVIDIA GPUs, like [CuPy](#), [Numba](#), [cuNumeric](#), and many others; NVIDIA actively supports a lot of them, but has no direct product like *CUDA for Python*; so, the status is somewhere in between
- 11: [hipify](#) by AMD can translate CUDA calls to HIP calls which runs natively on AMD GPUs
- 12: AMD offers a Source-to-Source translator to convert some CUDA Fortran functionality to OpenMP for AMD GPUs ([gpufort](#)); in addition, there are ROCm library bindings for Fortran in [hipfort](#) OpenACC/CUDA Fortran Source-to-Source translator
- 13: [HIP](#) is the preferred native programming model for AMD GPUs
- 14: SYCL can use AMD GPUs, for example with [hipSYCL](#) or [DPC++](#) for HIP AMD
- 15: OpenACC C/C++ can be used on AMD GPUs via GCC or Clacc; also, Intel's OpenACC to OpenMP Source-to-Source translator can be used to generate OpenMP directives from OpenACC directives
- 16: OpenACC Fortran can be used on AMD GPUs via GCC; also, AMD's [gpufort](#) Source-to-Source translator can move OpenACC Fortran code to OpenMP Fortran code, and also Intel's translator can work
- ???: AMD offers a dedicated, Clang-based compiler for using OpenMP on AMD GPUs: [AOMP](#); it supports both C/C++ (Clang) and Fortran (Flang, [example](#))
- ???: Currently, no (known) way to launch Standard-based parallel algorithms on AMD GPUs
- 37: Kokkos supports AMD GPUs through HIP
- 38: Alpaka supports AMD GPUs through HIP or through an OpenMP backend

GPU Vendor/Programming Model Table III

- 39: AMD does not officially support GPU programming with Python (also not semi-officially like NVIDIA), but third-party support is available, for example through [Numba](#) (currently inactive) or a [HIP version of CuPy](#)
- 19: [SYCLomatic](#) translates CUDA code to SYCL code, allowing it to run on Intel GPUs; also, Intel's [DPC++ Compatibility Tool](#) can transform CUDA to SYCL
- 20: No direct support, only via ISO C bindings, but at least an example can be [found on GitHub](#); it's pretty scarce and not by Intel itself, though
- 21: [CHIP-SPV](#) supports mapping CUDA and HIP to OpenCL and Intel's Level Zero, making it run on Intel GPUs
- 22: No such thing like HIP for Fortran
- 23: SYCL is the prime programming model for Intel GPUs; actually, SYCL is only a standard, while Intel's implementation of it is called [DPC++ \(Data Parallel C++\)](#), which extends the SYCL standard in various places; actually actually, Intel namespaces everything *oneAPI* these days, so the *full* proper name is Intel oneAPI DPC++ (which incorporates a C++ compiler and also a library)
- ???: OpenACC can be used on Intel GPUs by translating the code to OpenMP with [Intel's Source-to-Source translator](#)
- ???: Intel has [extensive support for OpenMP](#) through their latest compilers
- ???: Intel supports pSTL algorithms through their [DPC++ Library](#) (oneDPL; [GitHub](#)). It's heavily namespaced and not yet on the same level as NVIDIA
- 41: With [Intel oneAPI 2022.3](#), Intel supports DO CONCURRENT with GPU offloading
- 42: Kokkos supports Intel GPUs through SYCL

GPU Vendor/Programming Model Table IV

- 43: Alpaka v0.9.0 introduces experimental SYCL support; also, Alpaka can use OpenMP backends
- 44: Not a lot of support available at the moment, but notably DPNP, a SYCL-based drop-in replacement for Numpy, and numba-dpex, an extension of Numba for DPC++.