



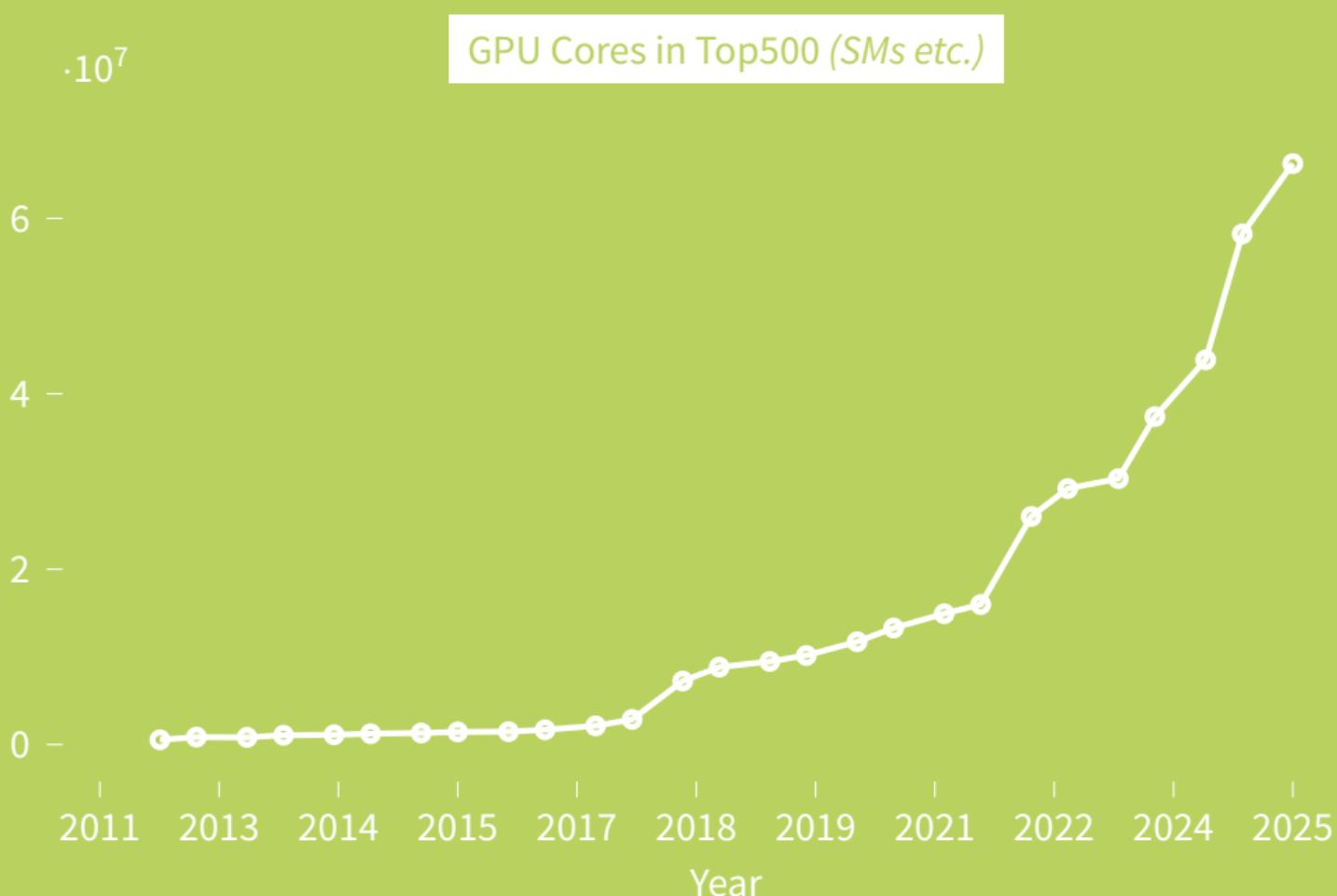
DISTRIBUTED GPU PROGRAMMING FOR EXASCALE SC25 TUTORIAL SESSION 1

16 November 2025 | Andreas Herten | Jülich Supercomputing Centre, Forschungszentrum Jülich

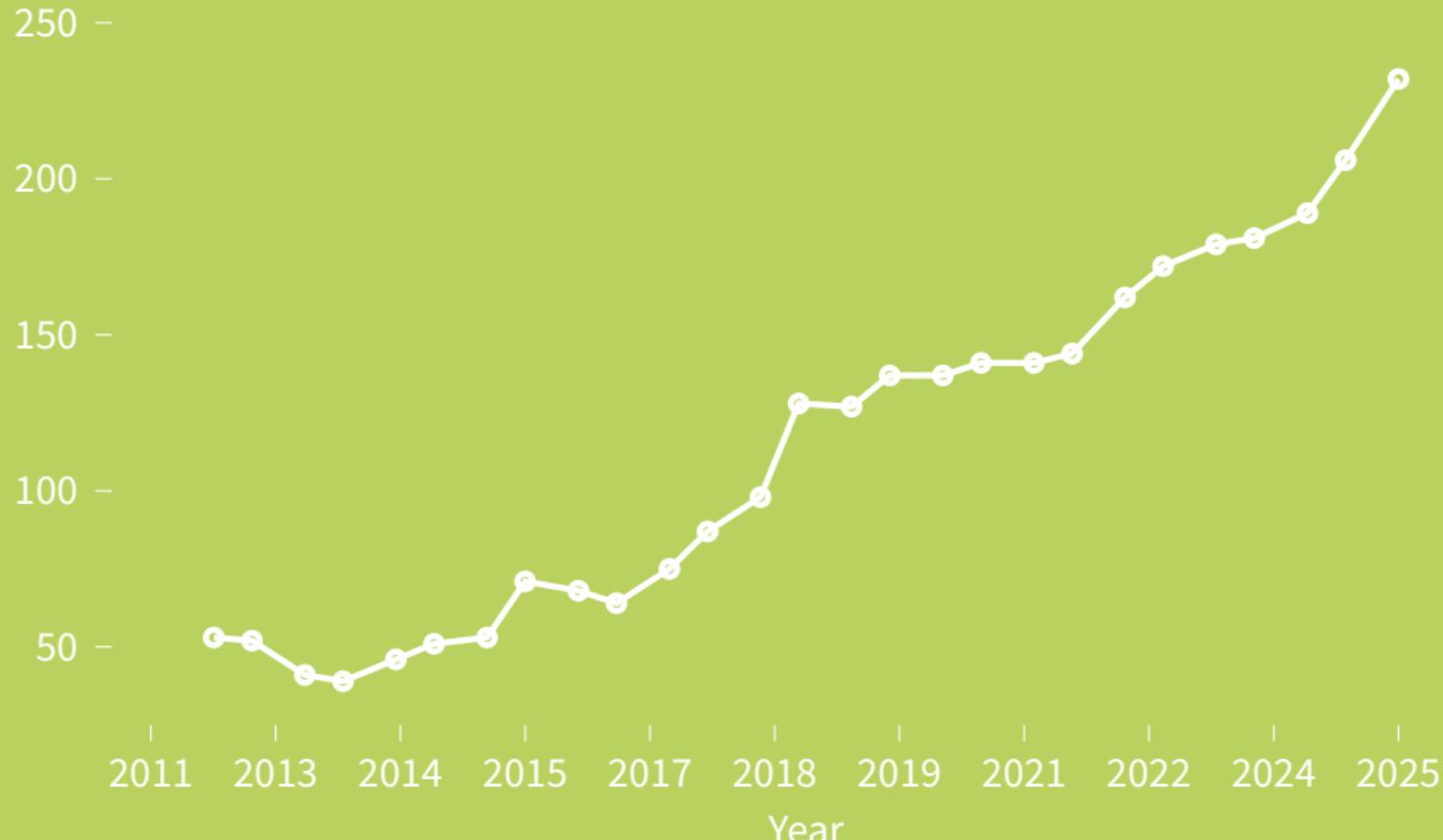
Welcome to

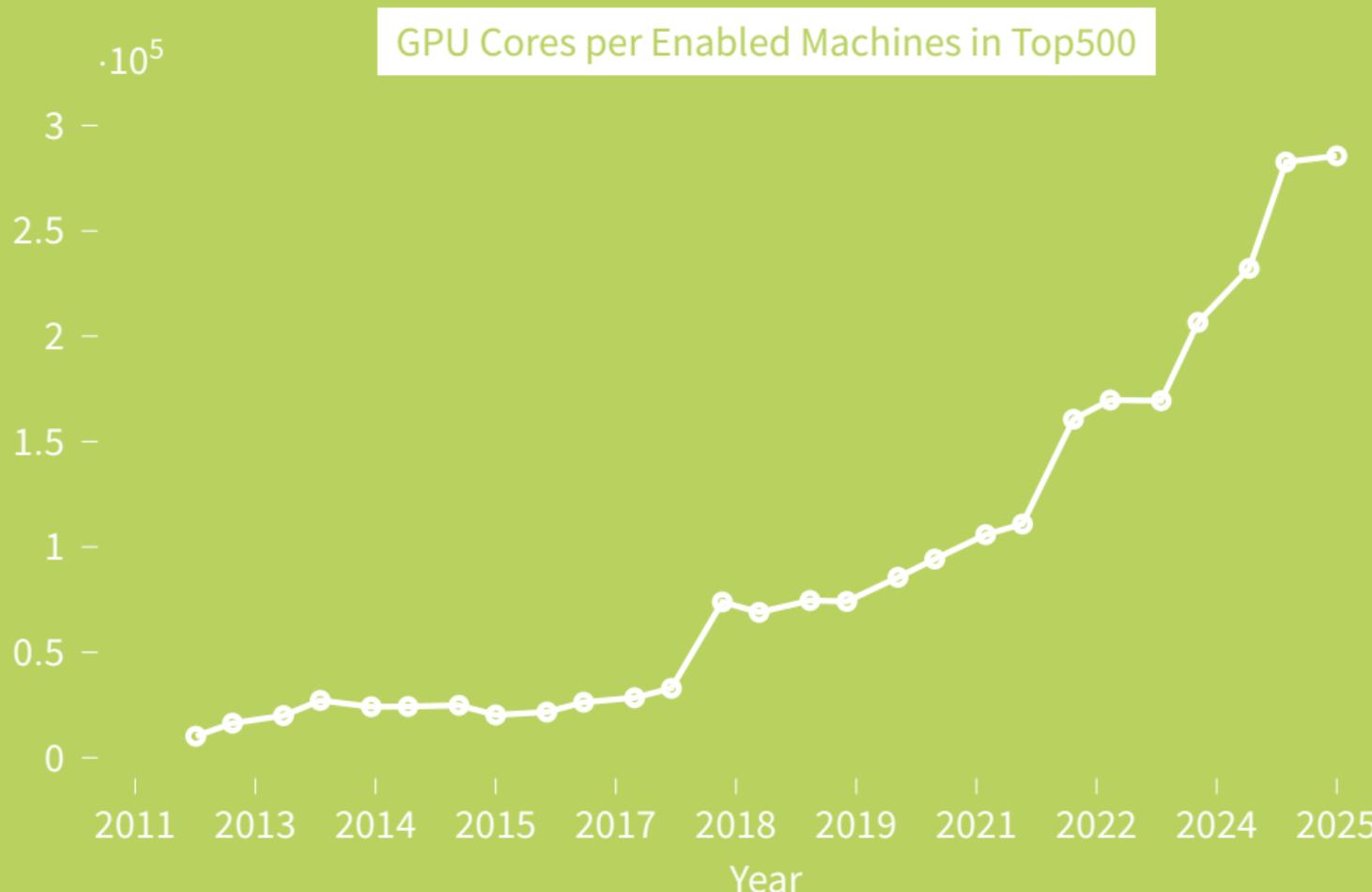
Efficient Distributed GPU Programming for Exascale,

an SC25 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

● : AMD, ● : Intel, ● : NVIDIA

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- Future
 - GPUs selected as technology for enabling Exascale
→ Even larger GPU machines with larger GPUs
 - Pre-Exascale systems: LUMI^A, Leonardo^N; Perlmutter^N
 - Exascale systems: Frontier^A, El Capitan^A, Aurora^I; JUPITER^N



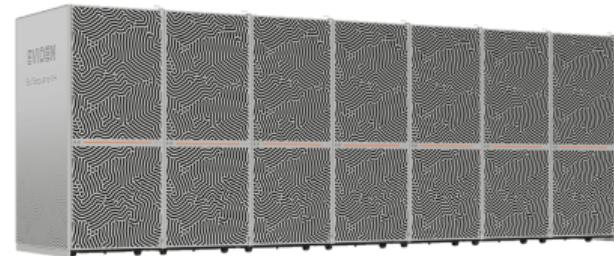
LLNL's El Capitan: ≈ 44 544 GPUs (APUs),
1.74 EFLOP/s, 2024
Rendering by LLNL

● : AMD, ● : Intel, ● : NVIDIA

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JSC's JUPITER: ≈ 24 000 GPUs, 0.8 EFLOP/s,
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: AMD, : Intel, : NVIDIA

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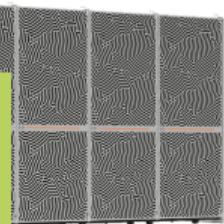
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- GPUs
 - Even

We help to Tame the Beasts!



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About Tutorial

Goals

- Prepare for large-scale GPU systems
- Learn GPU+MPI basics
- Show CPU-less GPU+MPI
- Outline advanced libraries to improve scaling efficiency
- Learn interactively!

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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>10:00 - 10:30: 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>12:00 - 13:30: Lunch Break</i>
7L	Lecture	Overview of NCCL and NVSHMEM in MPI Programs
8H	Hands-On	Using NCCL and NVSHMEM <i>15:00 - 15:30: Coffee Break</i>
9L	Lecture	Device-initiated Communication with NVSHMEM
10H	Hands-On	Device-initiated Communication with NVSHMEM
11L	Lecture	Outline of Advanced Topics and Conclusion

Tutorial Team



Simon Garcia

Scalable Computer Architectures
Sandia National Laboratories



Andreas Herten

Accelerating Devices Lab
Jülich Supercomputing Centre



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Prof. for Computer Engineering
University Hagen



David Appelhans

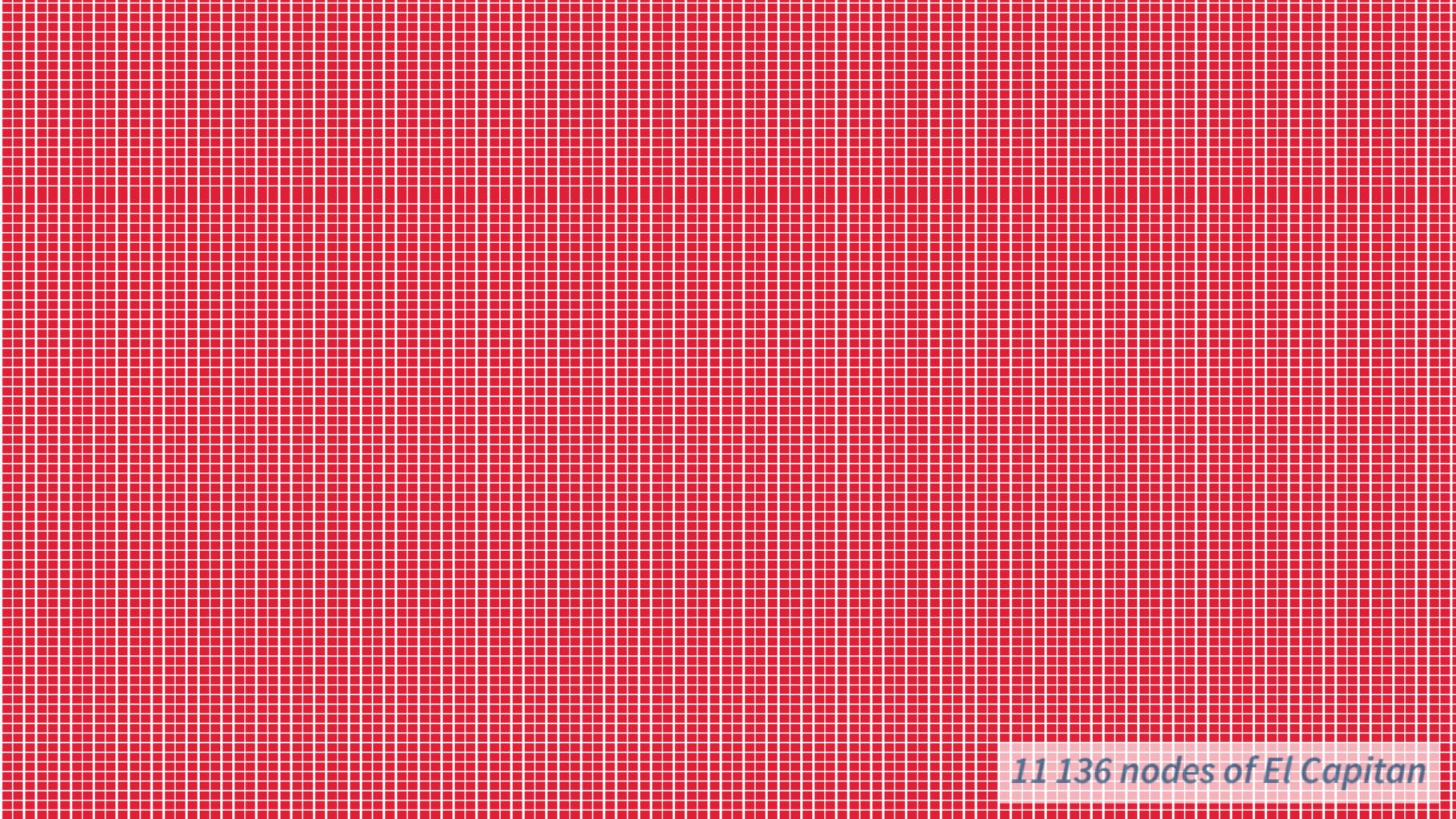
DevTech
NVIDIA

Support by

Jiri Kraus, NVIDIA

Markus Hrywniak, NVIDIA

Exascale GPU Systems

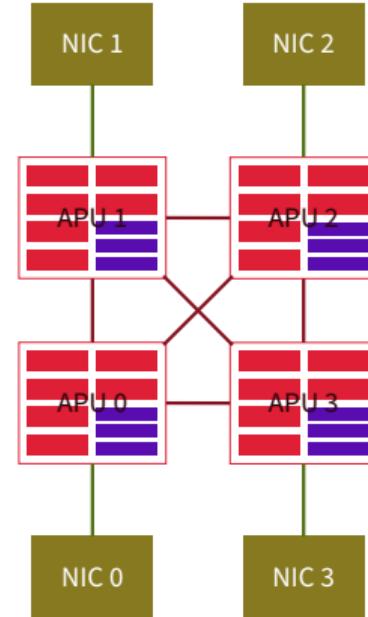


11 136 nodes of El Capitan

El Capitan

■

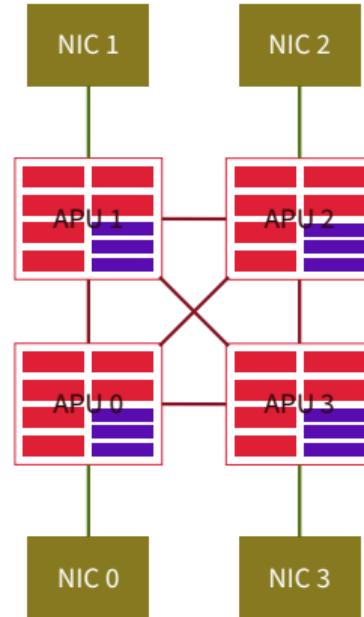
El Capitan

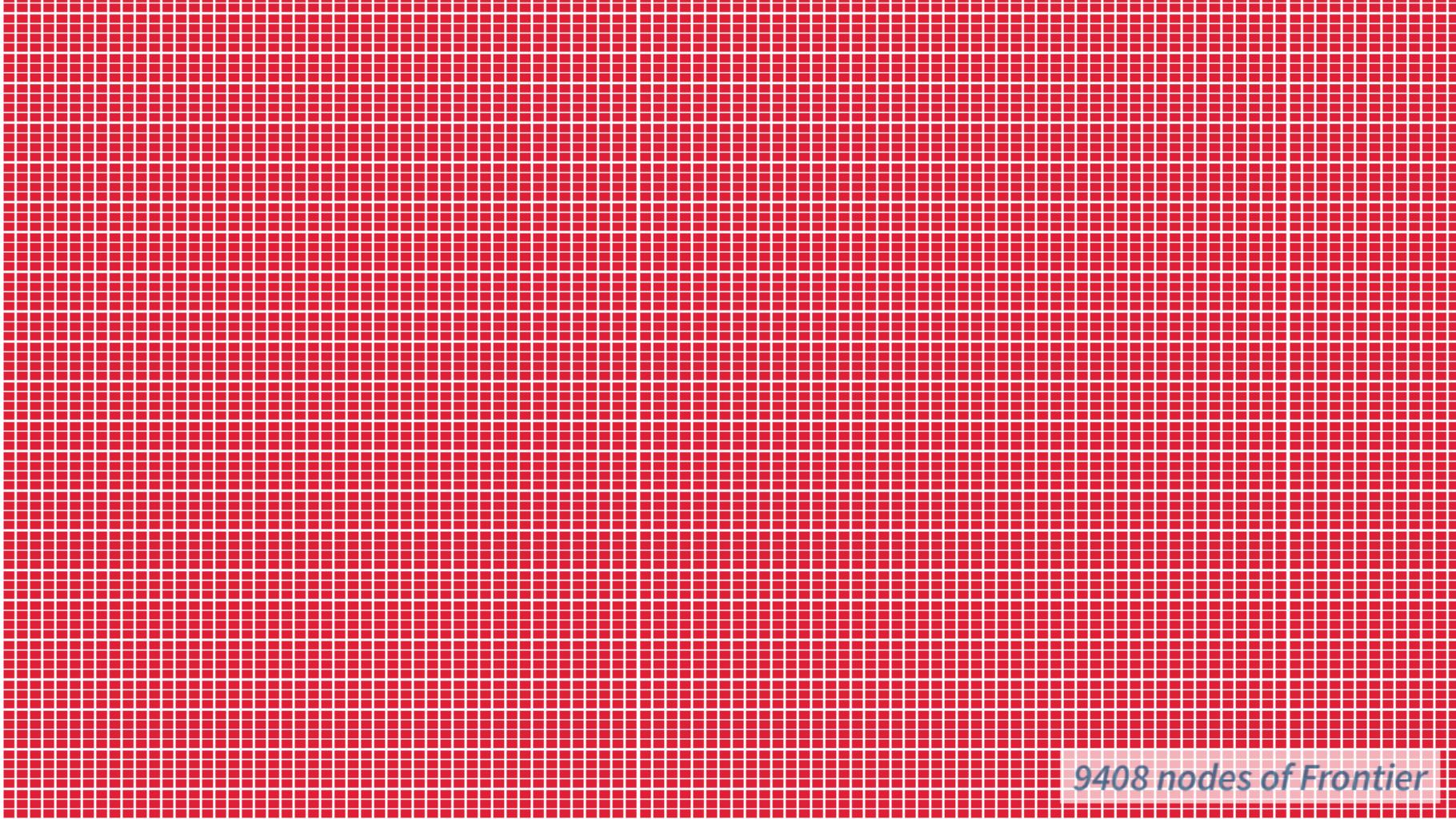


El Capitan



- At Lawrence Livermore National Lab, US
 - Largest Exascale system
 - HPL: 1.7 EFLOP/s
 - APU : 4× AMD Instinct MI300A
CPU+GPU chiplets combined, 128 GB per APU (HBM)
 - Network : 4× HPE Slingshot, 4 × 50 GB/s
- 11 136 nodes, 44 544 GPUs, 44 544 network devices



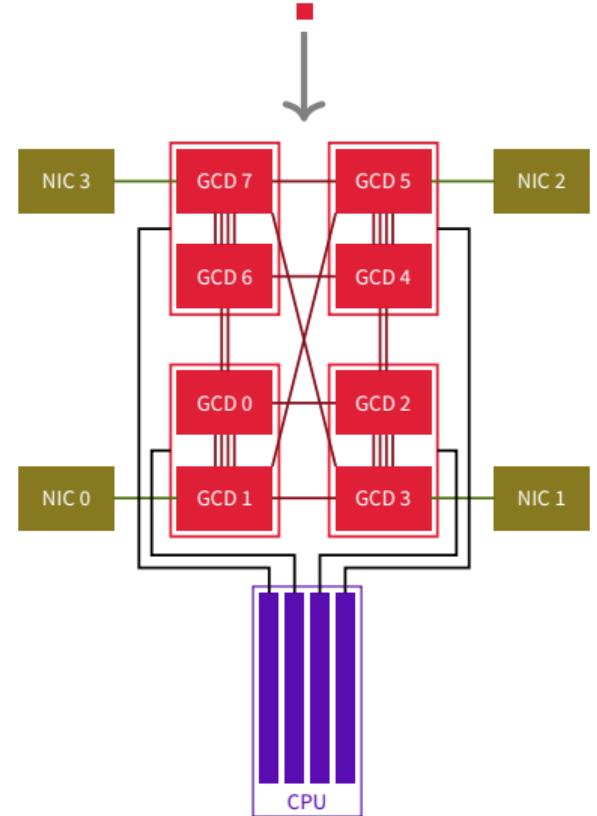


9408 nodes of Frontier

Frontier

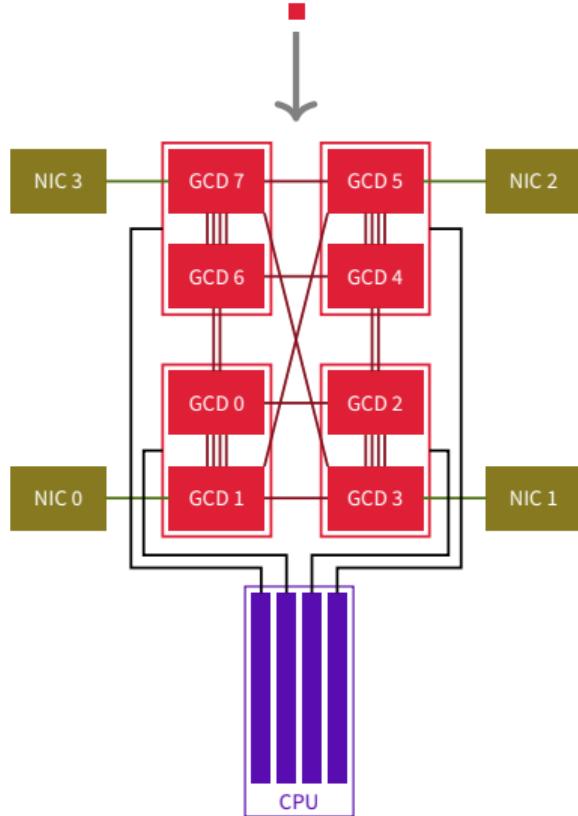


Frontier



Frontier

- At Oak Ridge Nation Lab, US
 - First Exascale system
 - HPL: 1.4 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

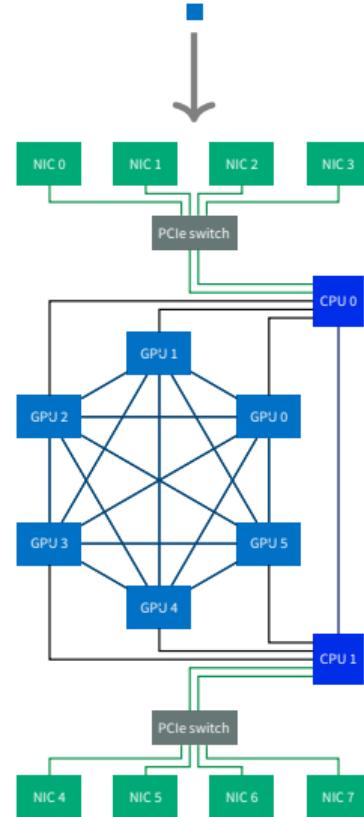


10 624 nodes of Aurora

Aurora

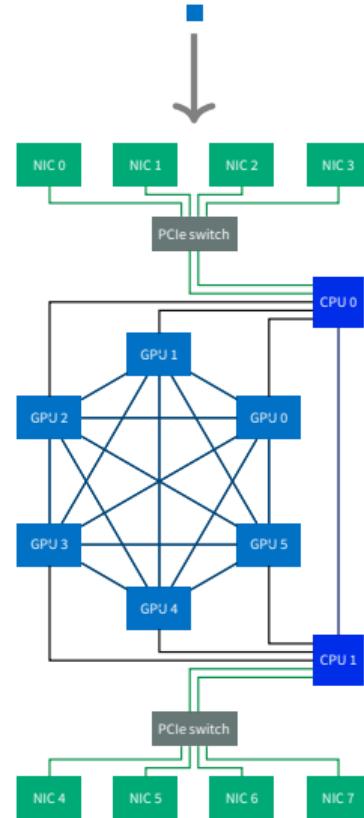


Aurora



Aurora

- At Argonne National Lab, US
 - Highest theoretical peak
 - HPL: 1 EFLOP/s
 - 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

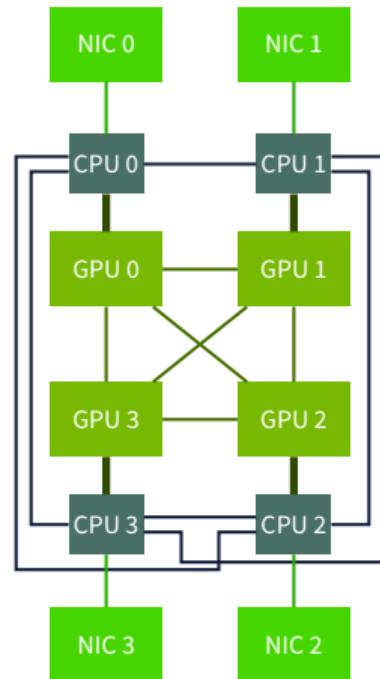


\approx 6000 nodes of JUPITER

JUPITER

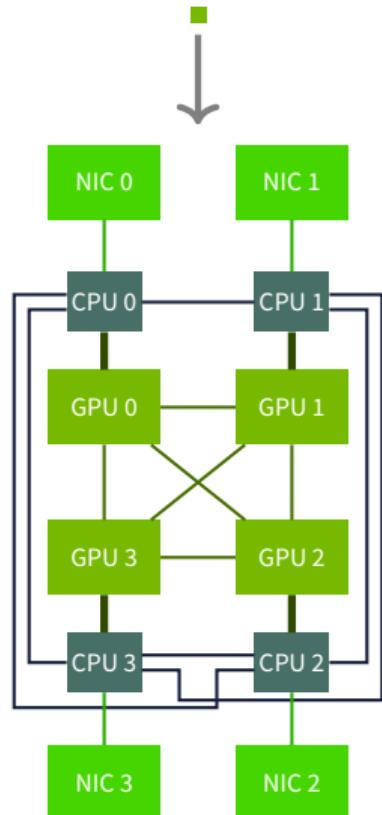


JUPITER



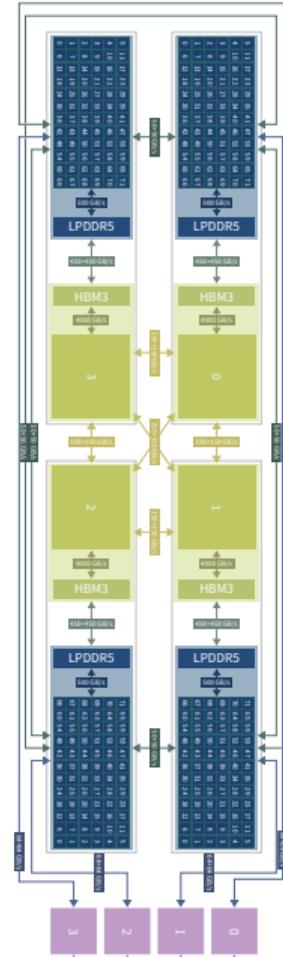
JUPITER

- At Jülich Supercomputing Center, Germany; procured by EuroHPC JU
 - First European Exascale system
 - **Booster**, Cluster
 - HPL June 2025: 0.8 EFLOP/s
 - 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 InfiniBand NDR200, 4 × 25 GB/s
- ≈6000 nodes, ≈24 000 GPUs, ≈24 000 network devices



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Today: JUWELS Booster!



JUPITER vs JUWELS

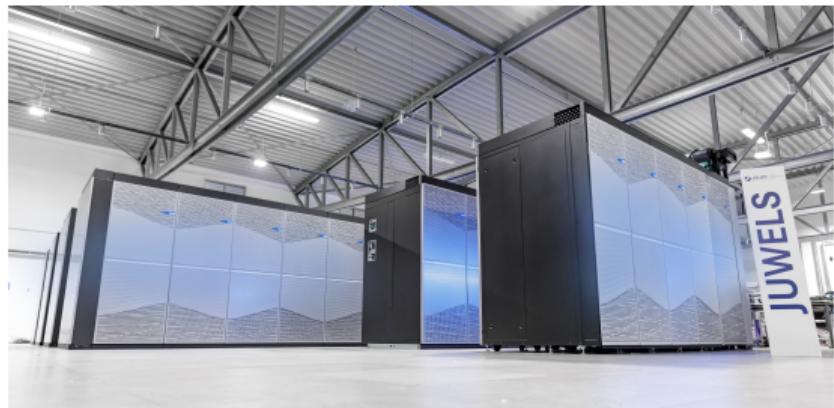
JUPITER vs JUWELS

JUPITER Booster



- Exascale system
- 5884 nodes, 23 536 GPUs
- NVIDIA GH200 superchip (Hopper GPU)
- Per node: 4× GPU, 4× IB, 4× CPU
- DragonFly+ network

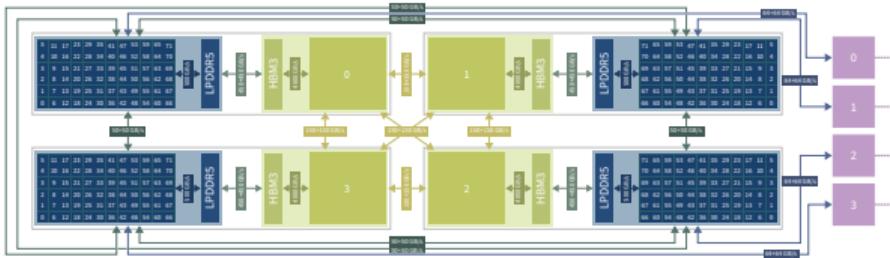
JUWELS Booster



- Petascale system, exascale explorer
- 936 nodes, 3744 GPUs
- NVIDIA A100 GPU
- Per node: 4× GPU, 4× IB, 2× CPU
- DragonFly+ network

Topology

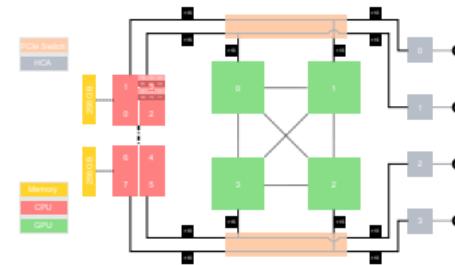
JUPITER Booster



- 4 GH200 superchips → 4 NUMA domains
- 1:1:1 affinity of CPU, GPU, HCA; coherent access between GPU-GPU, CPU-GPU, CPU-CPU

No fear: Slurm – and we – take care about affinity!

JUWELS Booster

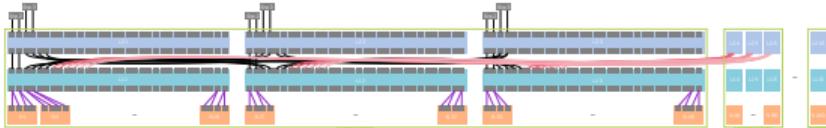


- 2 AMD EPYC CPUs, each 4 chiplets → 8 NUMA domains
- Affinity between GPUs and some CPU chiplets, HCA

Some fear: But Slurm still takes care

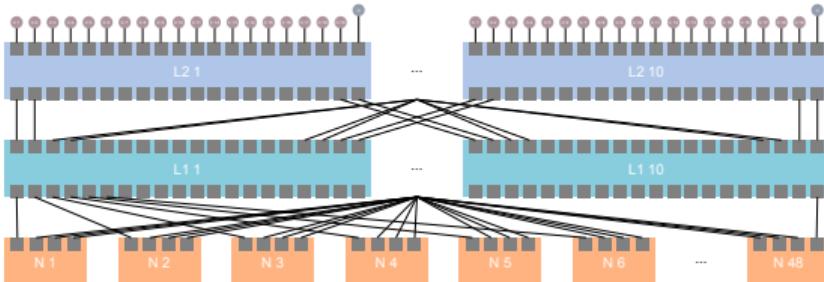
Network

JUPITER Booster



- NVIDIA Mellanox Quantum InfiniBand NDR200 network
- Dragonfly+ topology: 25 sparsely interconnected groups of 240 well-connected nodes (5 racks, each 48 nodes)
- Per group: 15 L1 switches, 16 L2 switches (*rack 3 has one more*)
- 400 Gbit/s links between switches, 200 Gbit/s links from nodes

JUWELS Booster



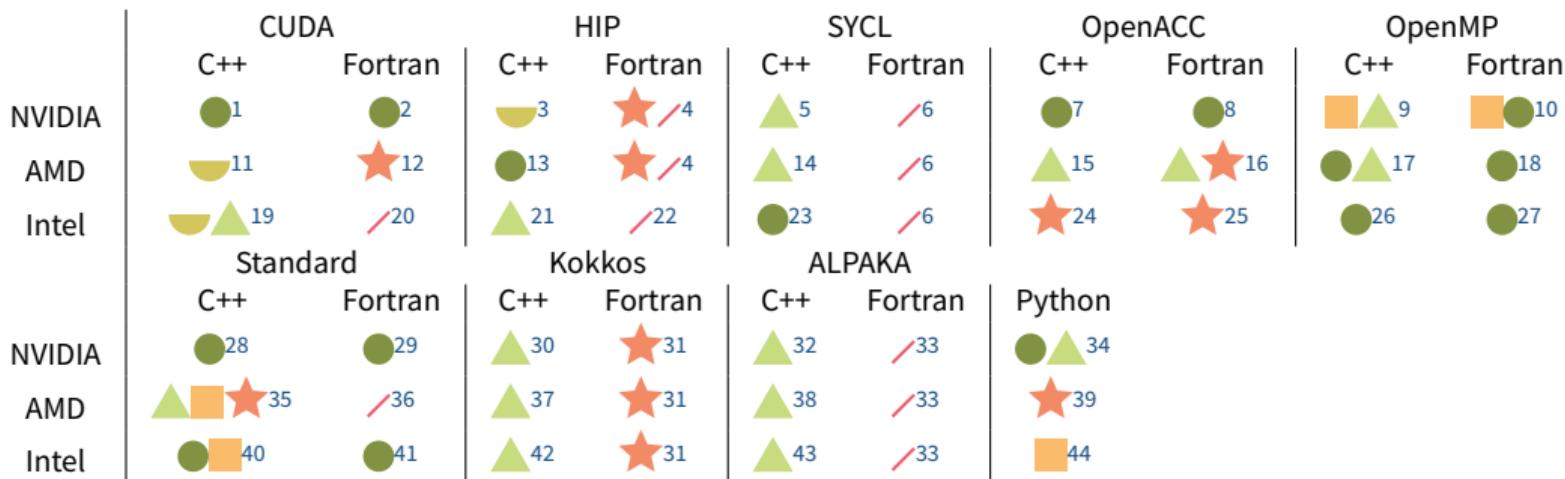
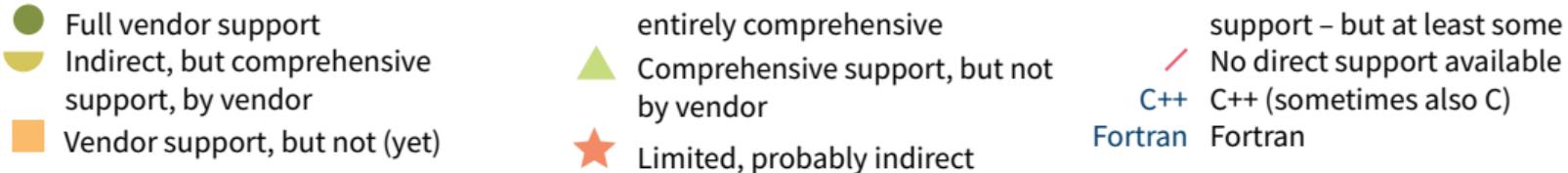
- NVIDIA Mellanox Quantum InfiniBand HDR200 network
- Dragonfly+ topology: 20 groups of 48 nodes (2 racks, each 24 nodes)
- Per group: 10 L1 switches, 10 L2 switches
- 200 Gbit/s links

Vendors, Models

GPU Vendors in Tutorial

- First Exascale machine: Frontier, with **AMD** GPUs!
- This tutorial: **NVIDIA** examples
 - We have most experience with NVIDIA
 -  JUPITER: NVIDIA GPUs
 - JUWELS as well
- **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

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- 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: JUPITER JUWELS Booster
- Most important tools for performance analysis: Nsight Systems, Nsight Compute, Score-P stack; great overview at in [B. Mohr's and M. Knobloch's recent article](#)

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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++.