



DISTRIBUTED GPU PROGRAMMING FOR EXASCALE SC25 TUTORIAL SESSION 1

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

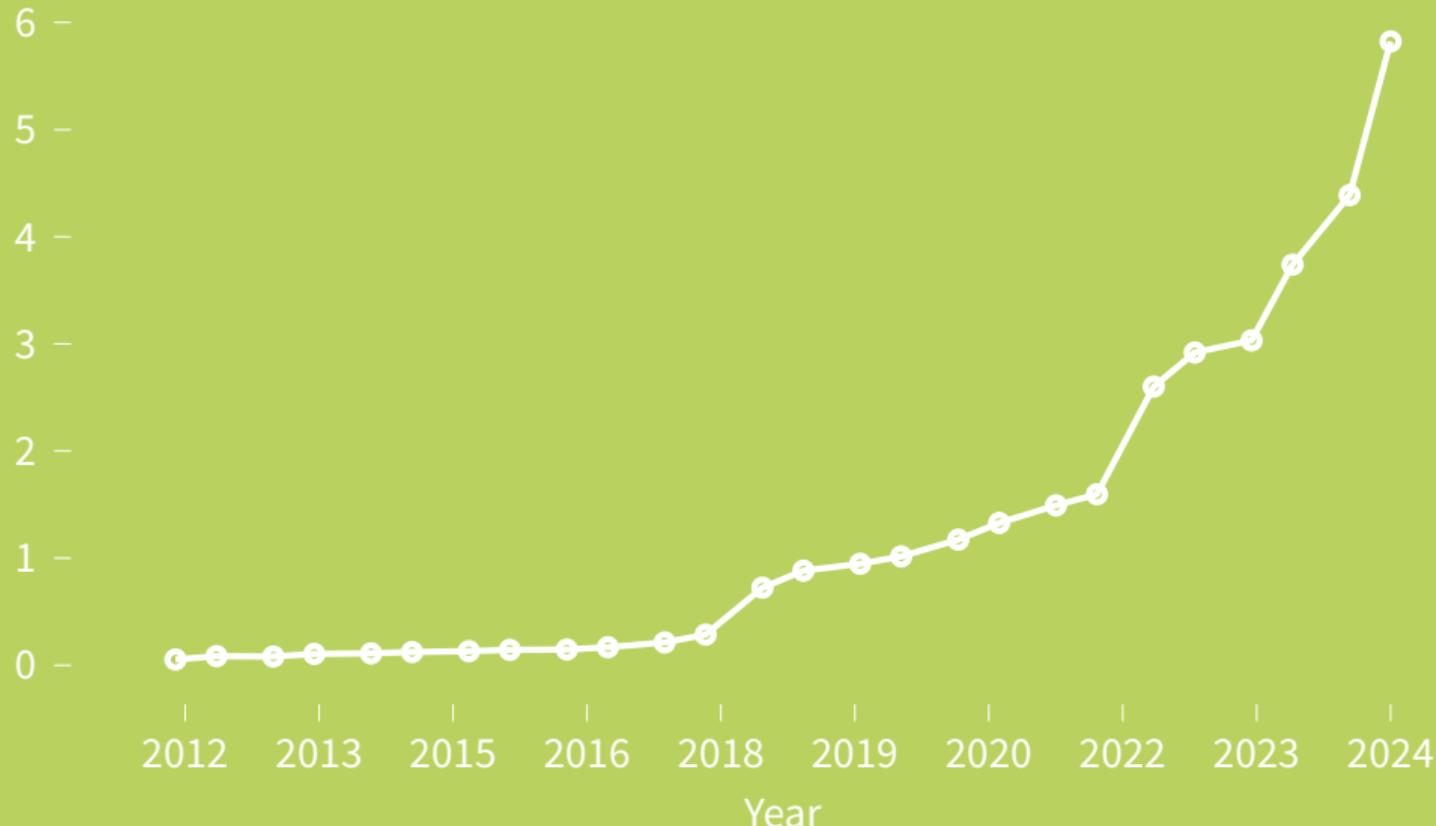
Welcome to

Efficient Distributed GPU Programming for Exascale,

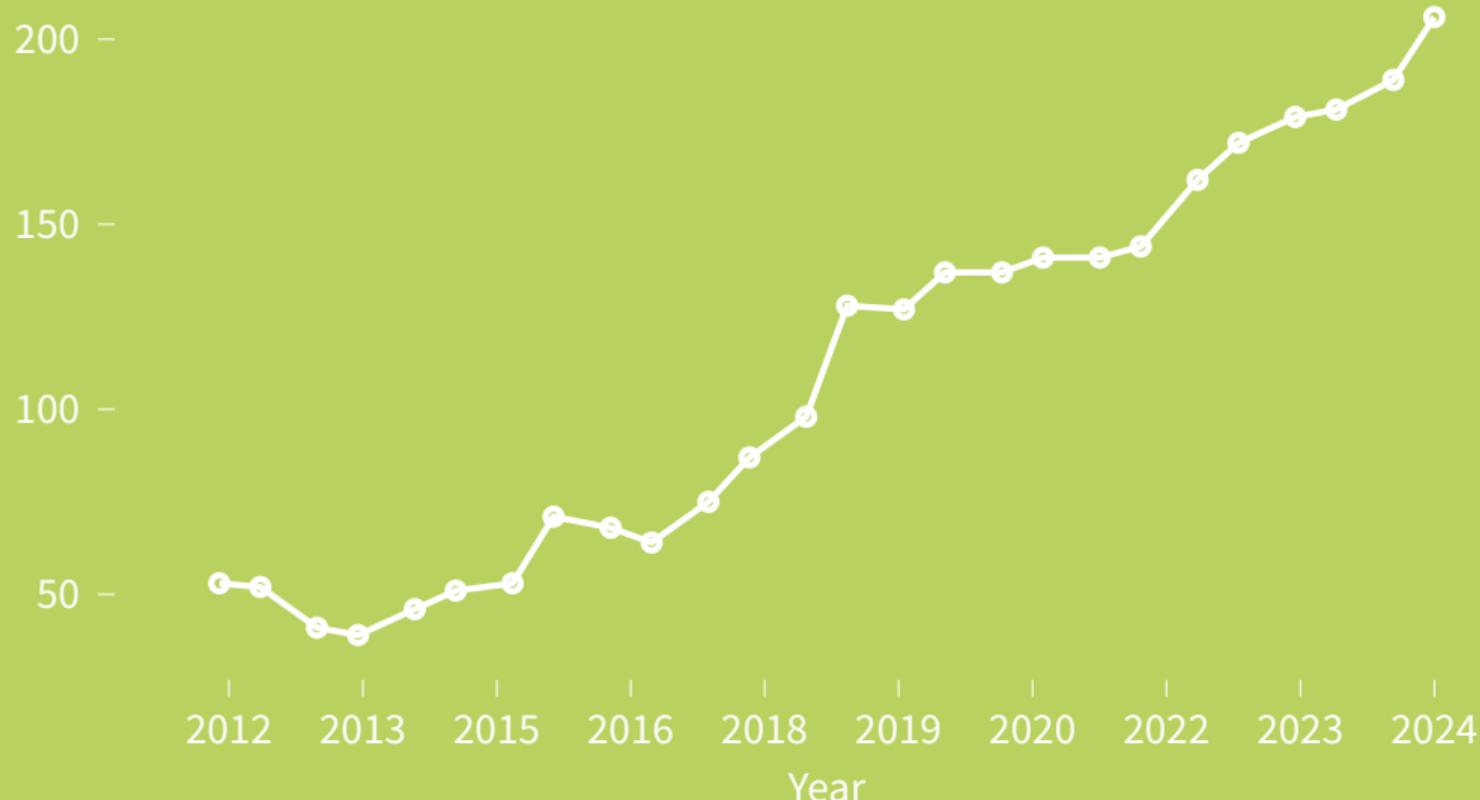
an SC25 Tutorial

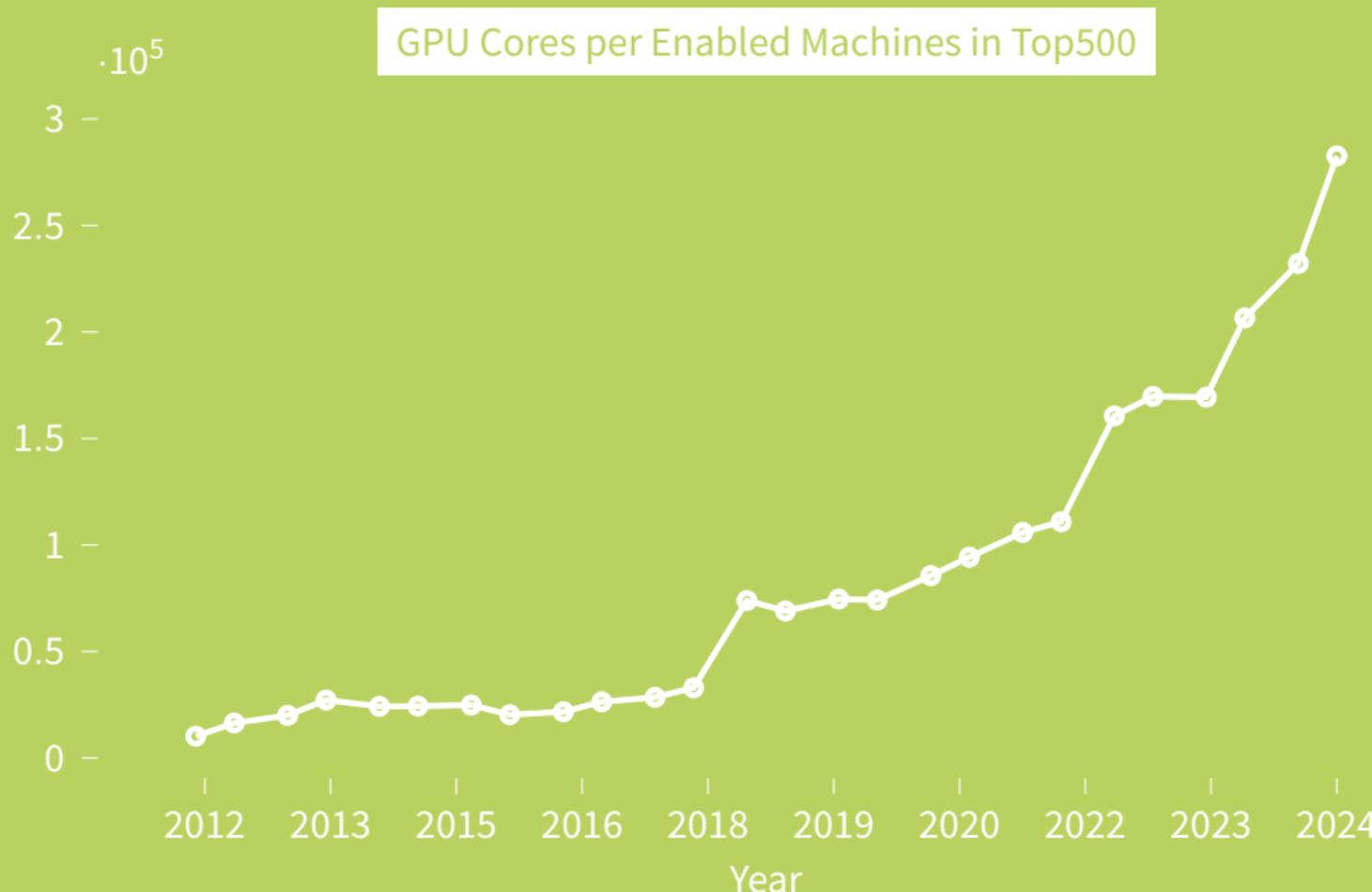
$\cdot 10^7$

GPU Cores in Top500 (*SMs etc.*)



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



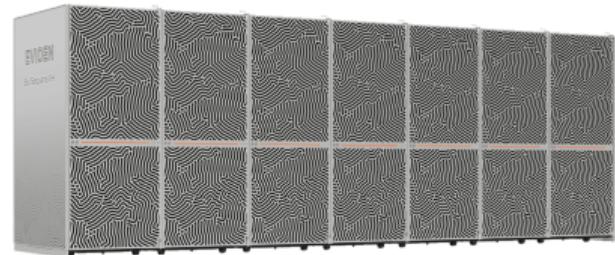
LLNL's El Capitan: ≈ 44 544 GPUs (APUs),
1.74 EFLOP/s, 2024
Rendering by LLNL

● : AMD, ● : Intel, ● : NVIDIA

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JSC's JUPITER: ≈ 24 000 GPUs, 0.8 EFLOP/s,
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Rendering by Atos

State of the GPU Union

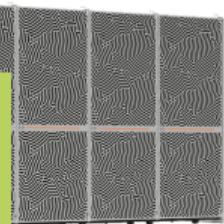
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- GPUs
 - Even

We help to Tame the Beasts!



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: AMD, : Intel, : NVIDIA

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 JEDI</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



Lena Oden

Prof. for Computer Engineering
University Hagen



David Appelhans

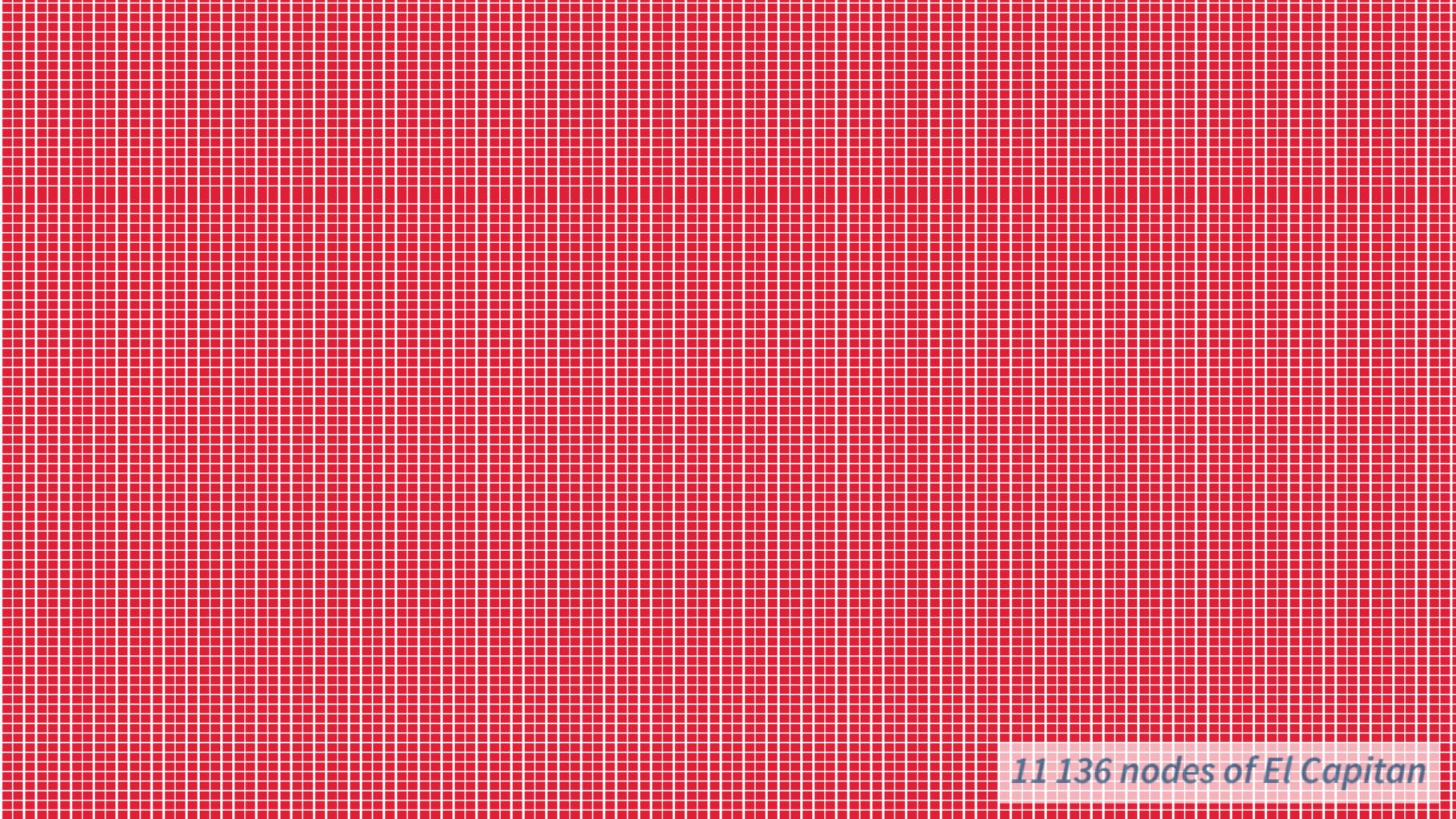
DevTech
NVIDIA

Support by

Jiri Kraus, NVIDIA

Markus Hrywniak, NVIDIA

Exascale GPU Systems

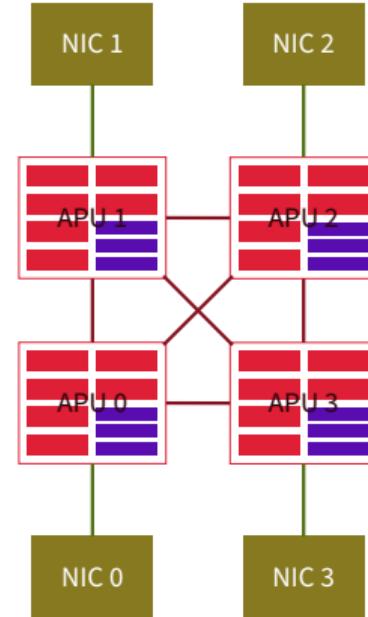


11 136 nodes of El Capitan

El Capitan

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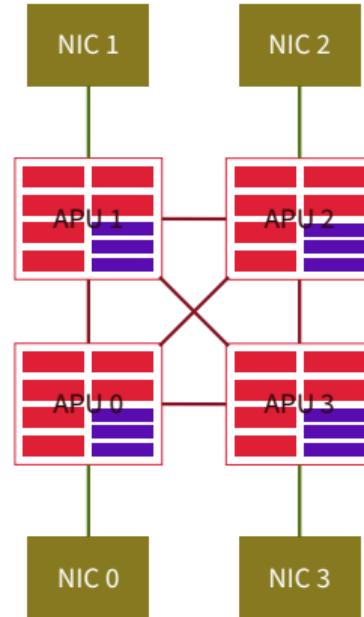
El Capitan

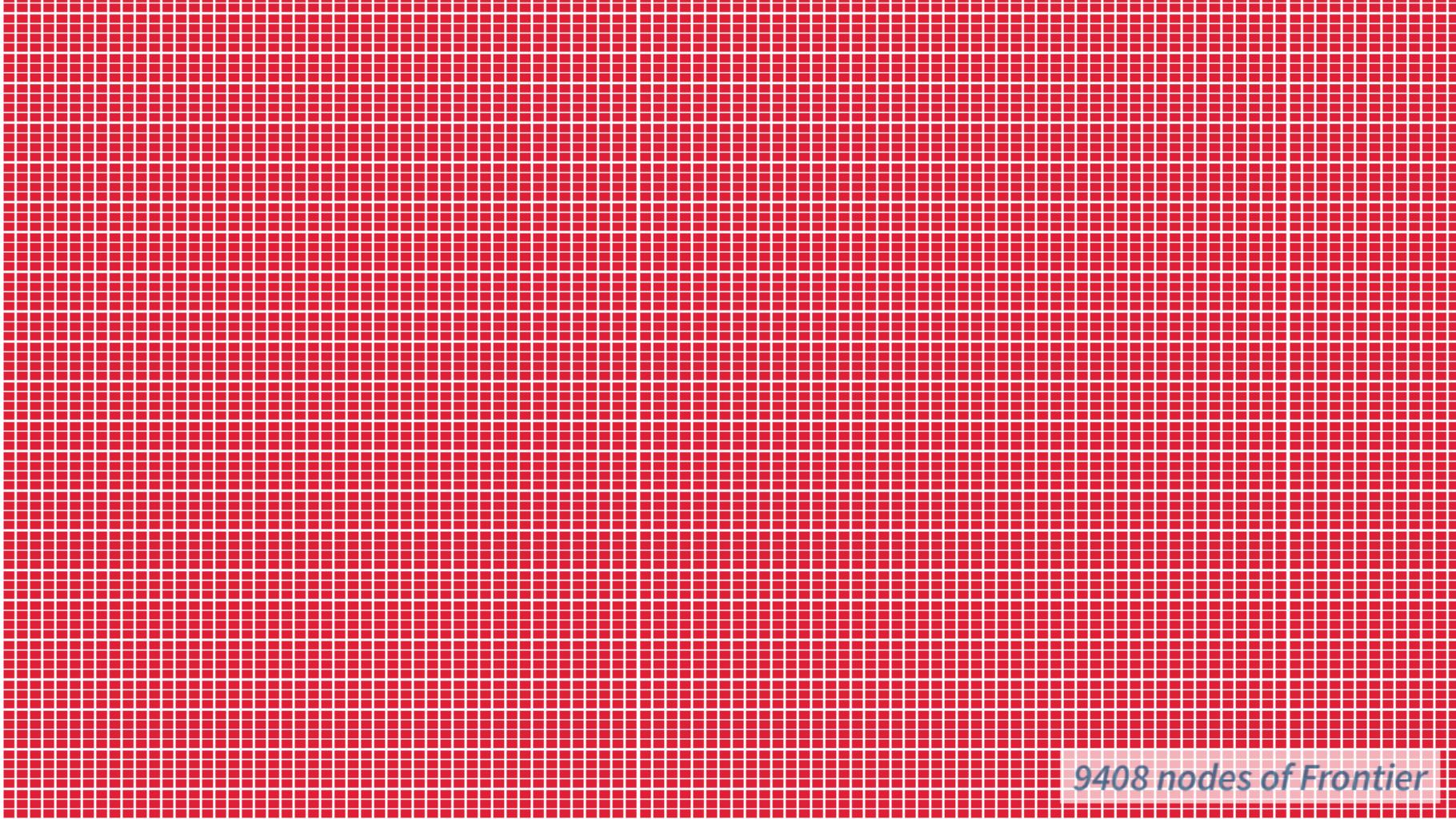


El Capitan



- 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



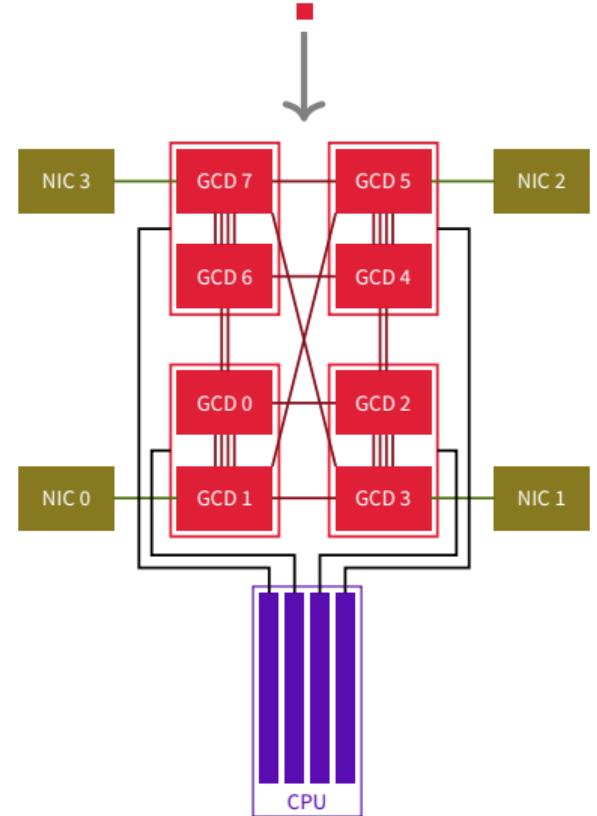


9408 nodes of Frontier

Frontier

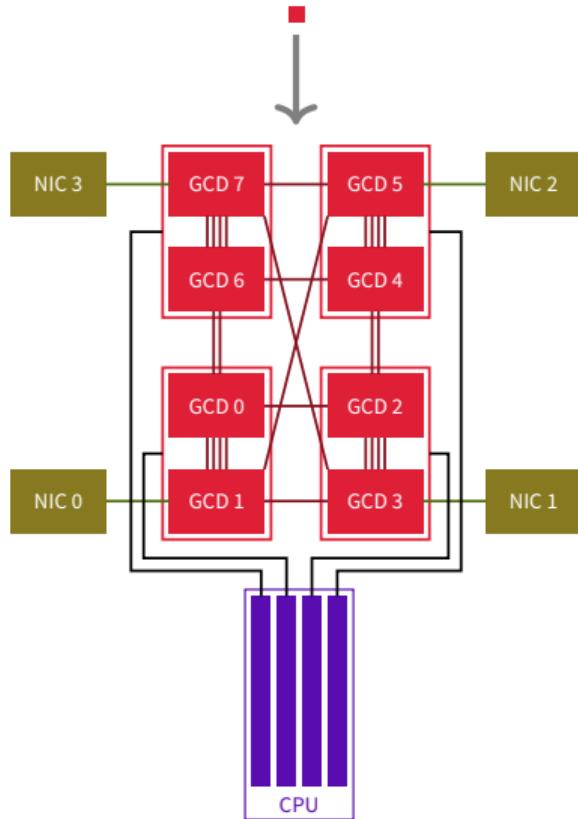


Frontier



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

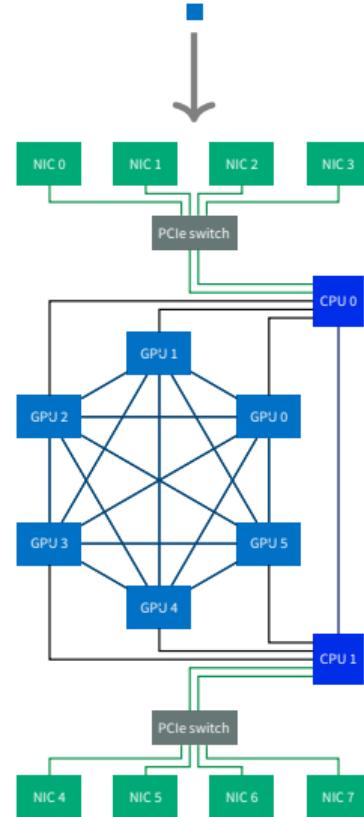


10 624 nodes of Aurora

Aurora

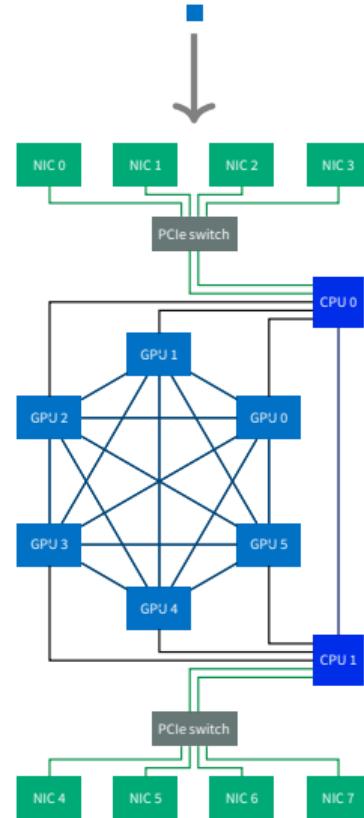


Aurora



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

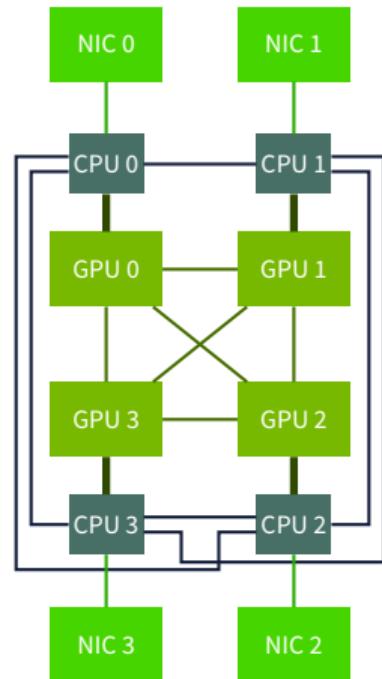


\approx 6000 nodes of JUPITER

JUPITER

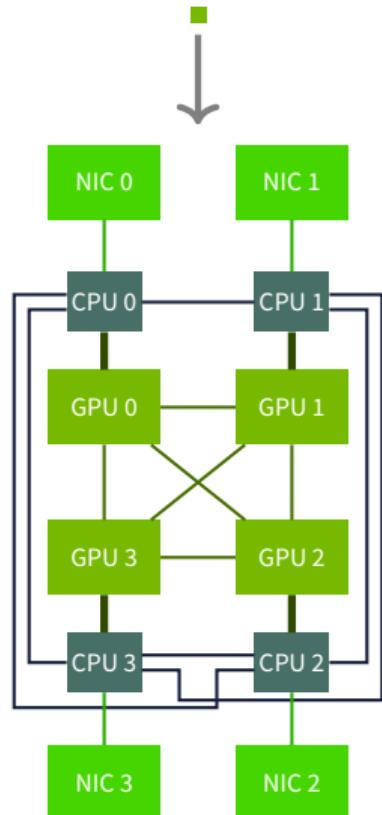


JUPITER



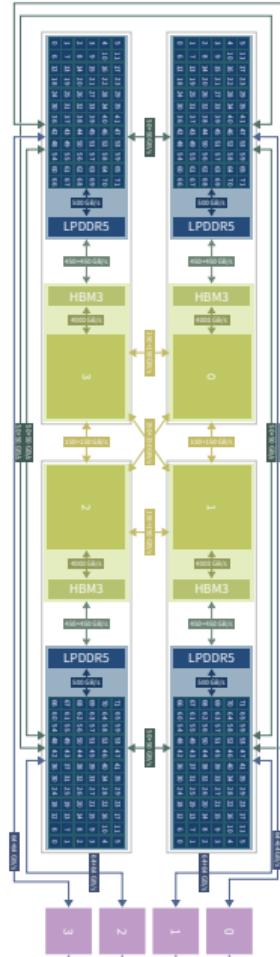
JUPITER

- At Jülich Supercomputing Center, Germany; procured by EuroHPC JU
 - First European Exascale system *soon!*
 - **Booster**, Cluster
 - HPL: 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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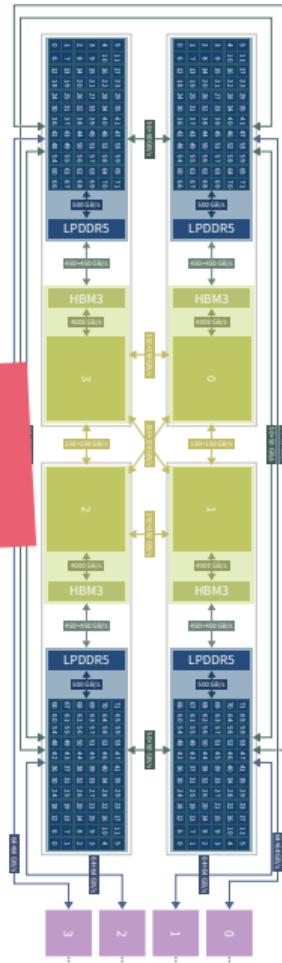


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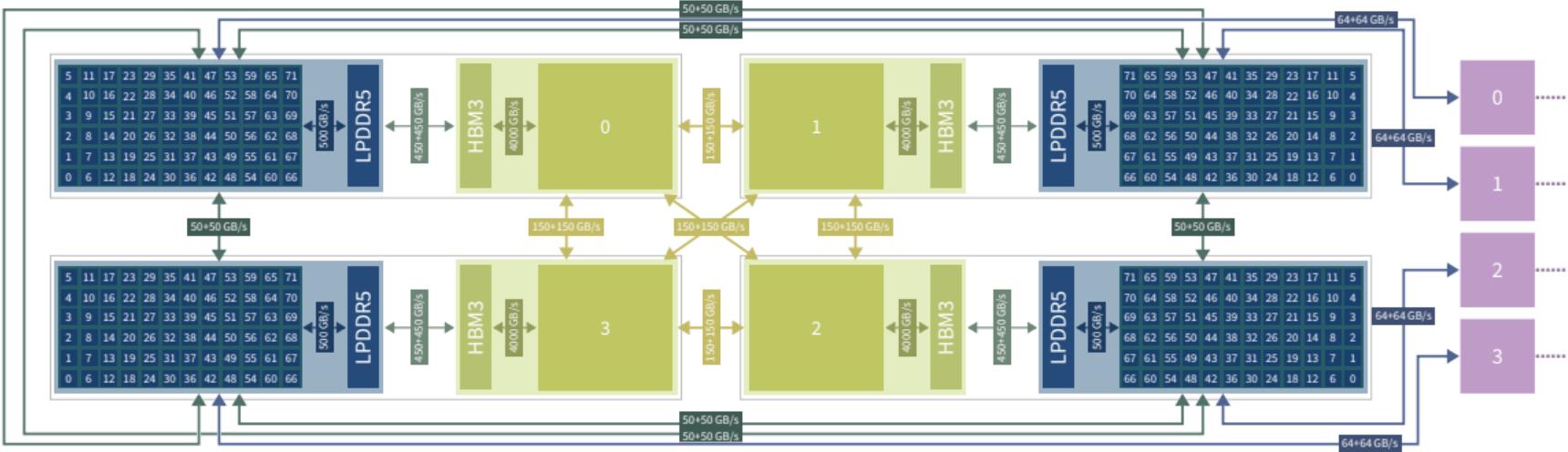
Today: ⚡ JUPITER!

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System: JUPITER Booster

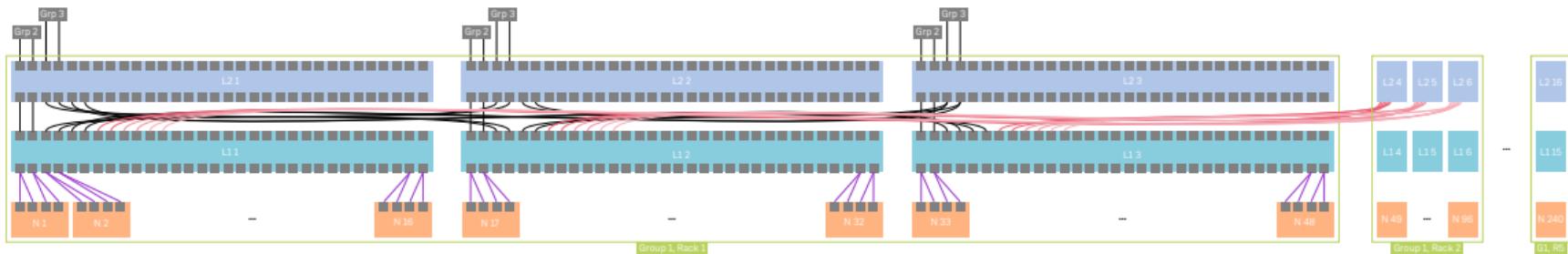
Node Topology



- 4 GH200 superchips, each 120 GB LPDDR5X & 96 GB HBM3 memory → 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!

JUPITER Booster System Topology

- 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

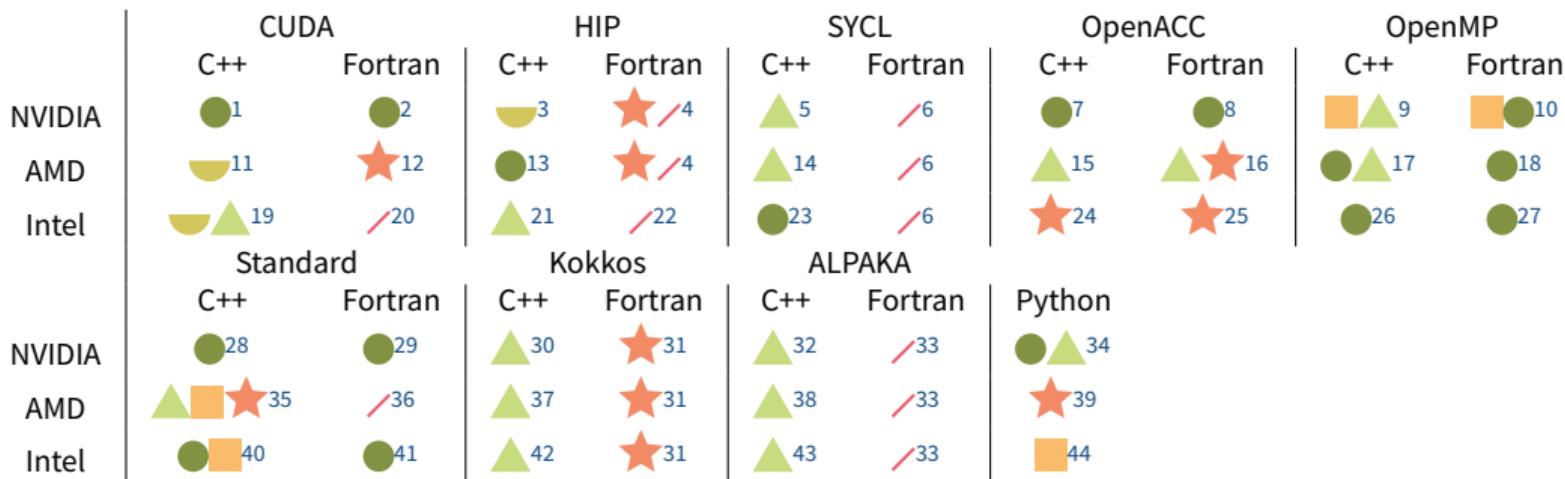
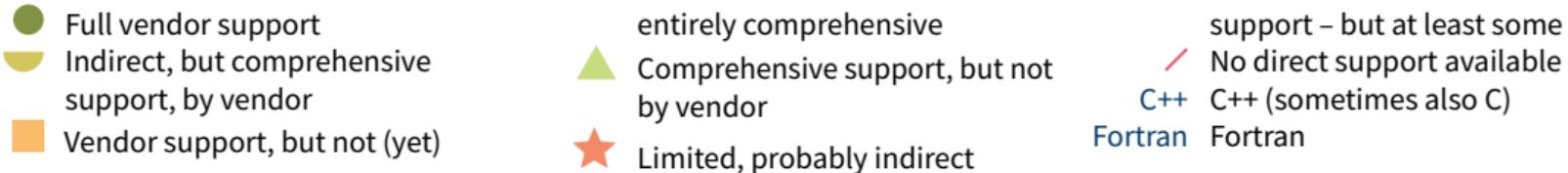


Vendors, Models

GPU Vendors in Tutorial

- First Exascale machine: Frontier, with **AMD** GPUs!
- This tutorial: **NVIDIA** examples
 - We have most experience with NVIDIA
 - **JUPITER**: NVIDIA GPUs
- **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 (first EU Exascale system)
- 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++.