DISTRIBUTED GPU PROGRAMMING FOR EXASCALE

SC23 TUTORIAL *SESSION 1*

13 November 2023 | Andreas Herten | Jülich Supercomputing Centre, Forschungszentrum Jülich

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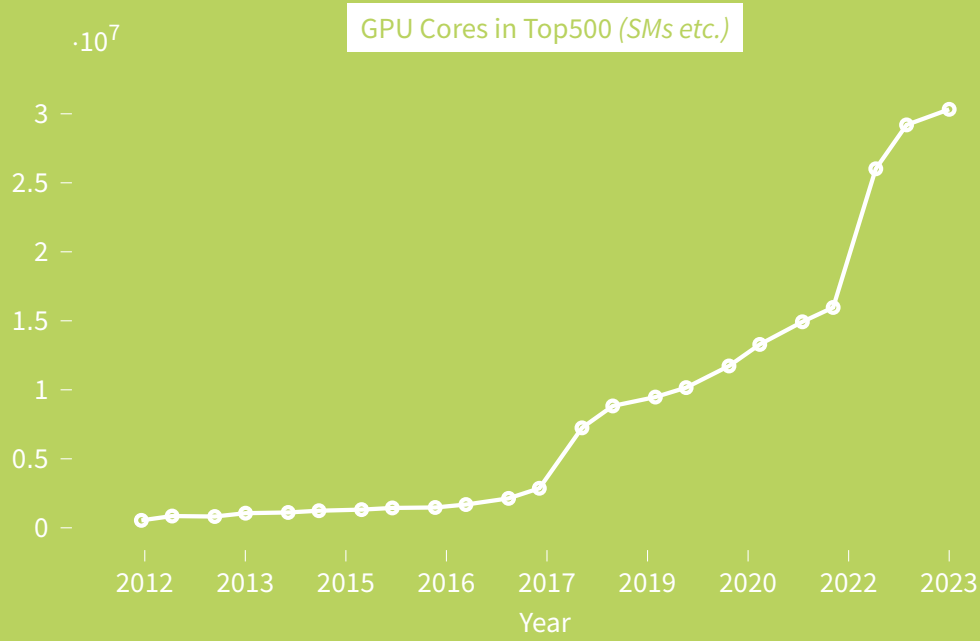
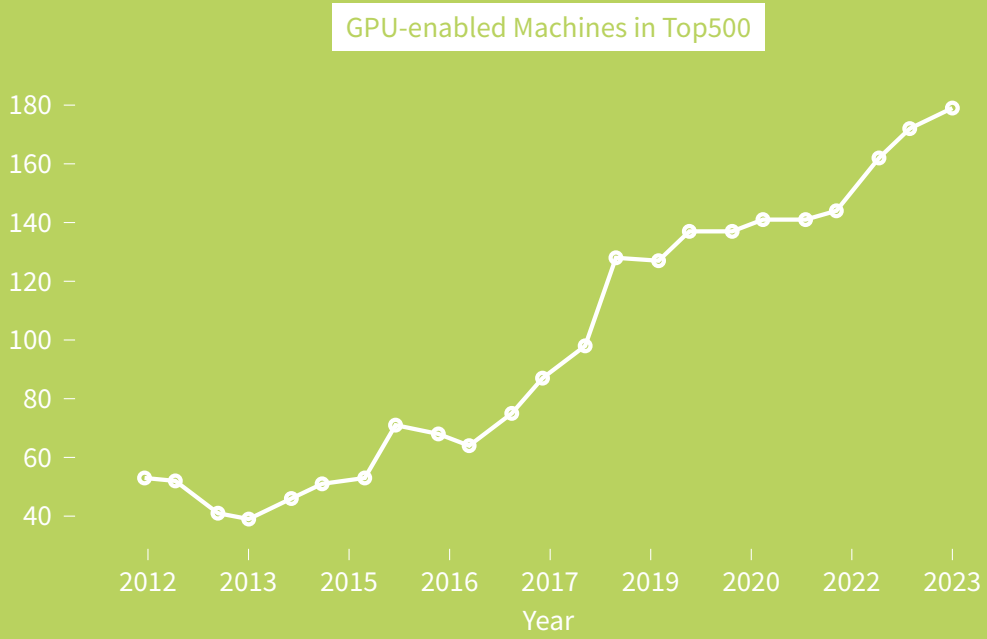
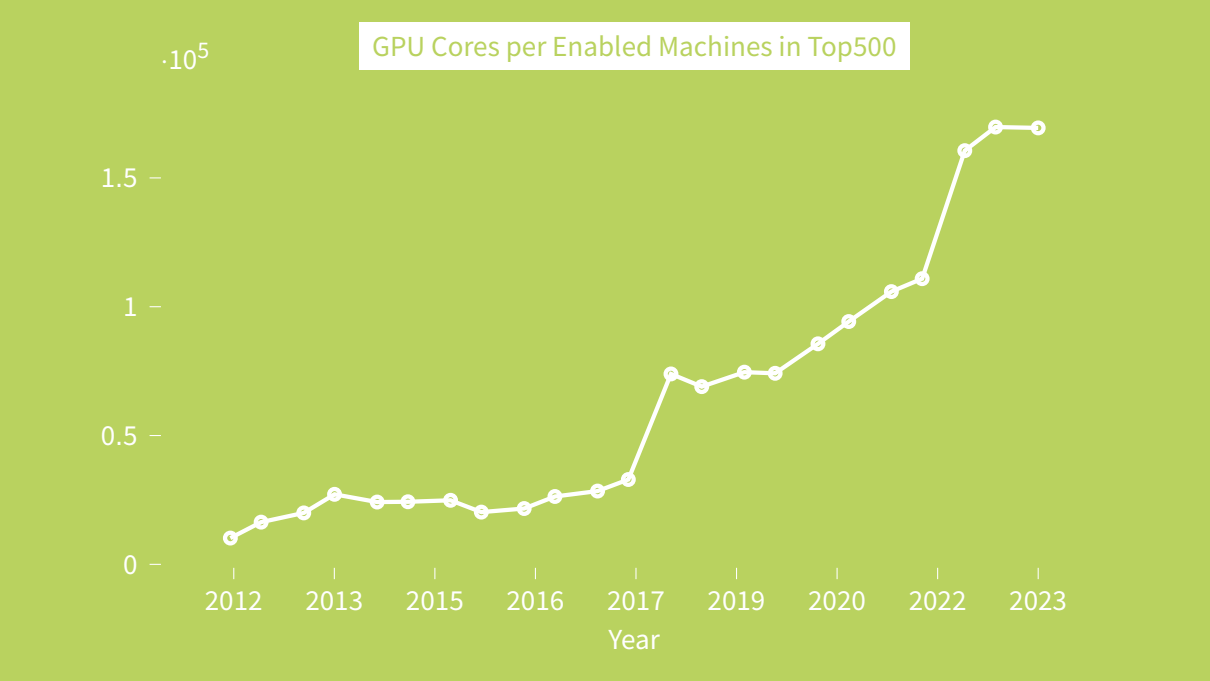
Welcome to

Efficient Distributed GPU Programming for Exascale,

an *SC23 Tutorial*


GPU Cores in Top500 (SMs etc.)
·10^7
3
2.5
2
1.5
1
0.5
0
2012
2013
2015
2016
2017
2019
2020
2022
2023
Year


GPU-enabled Machines in Top500
180
160
140
120
100
80
60
40
2012
2013
2015
2016
2017
2019
2020
2022
2023
Year


GPU Cores per Enabled Machines in Top500
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1.5
1
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2012
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State of the GPUnion

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

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  - 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 EFLOP/S, 2022
32 % of all installed GPU cores in Frontier!
Rendering by ORNL

[A]: AMD, [I]: Intel, [N]: NVIDIA

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- Last decade
  - More and more GPUs installed in HPC machines
  - More and more HPC machines with GPUs
  - M[illegible]
- Future
  - G[illegible]
  - → Ev[illegible]
  - Pre-Exascale systems: LUMI[A], Leonardo[N]; JUWELS Booster[N], Perlmutter[N]
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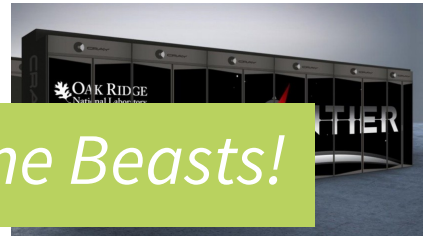
We help to Tame the Beasts!



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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	Tutorial Overview, Introduction to System
	Onboarding	*Accessing JUWELS Booster*
2L	Lecture	Introduction to MPI-Distributed Computing with GPUs
3H	Hands-On	Multi-GPU Parallelization
		10:00 - 10:30: Coffee Break
4L	Lecture	Performance and Debugging Tools
5L	Lecture	Optimization Techniques for Multi-GPU Applications
6H	Hands-On	Overlap Communication and Computation with MPI
		12:00 - 13:30: Lunch Break
7L	Lecture	Overview of NCCL and NVSHMEM in MPI Programs
8H	Hands-On	Using NCCL and NVSHMEM
		15:00 - 15:30: Coffee Break
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

Hello from Europe

Simon Garcia
Scalable Computer Architectures
Sandia National Laboratories

Andreas Herten
Accelerating Devices Lab
Jülich Supercomputing Centre

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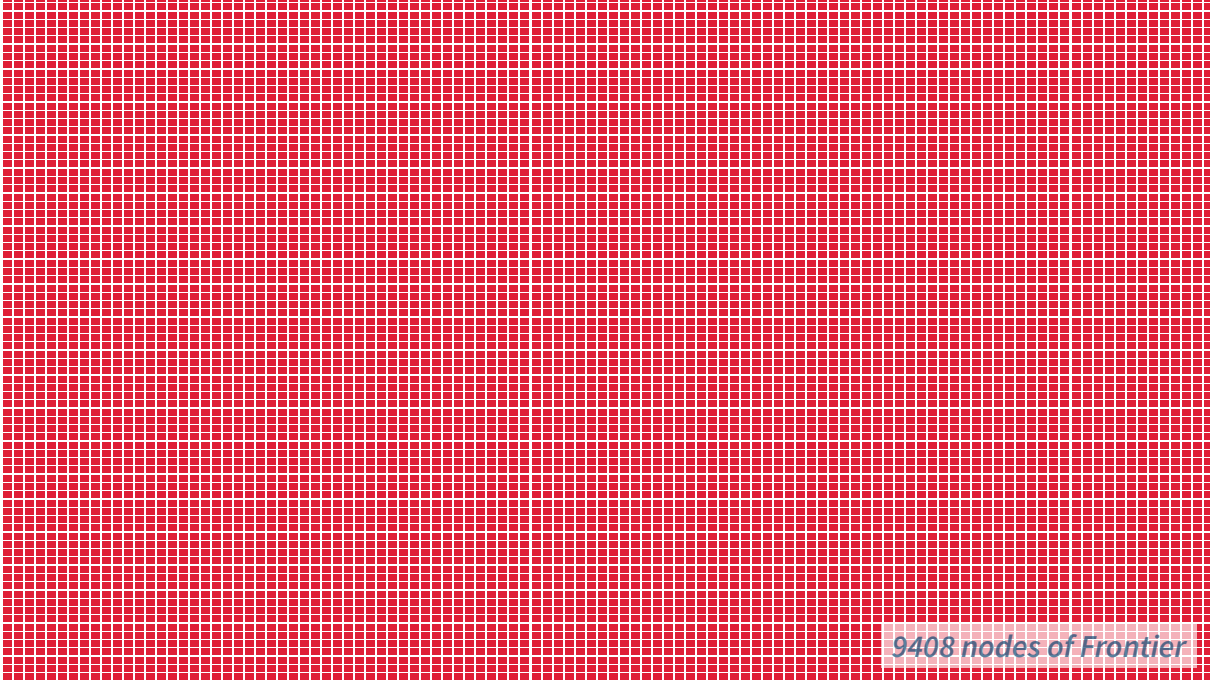
DevTech Compute
NVIDIA

Jiri Kraus
DevTech Compute
NVIDIA

Lena Oden
Prof. for Computer Engineering
University Hagen

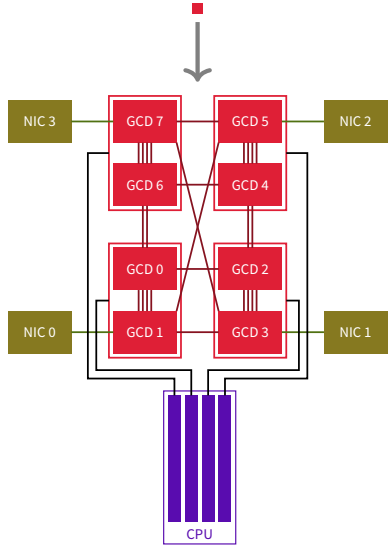
TAs
Chelsea John

Exascale GPU Systems


9408 nodes of Frontier

Frontier

Frontier



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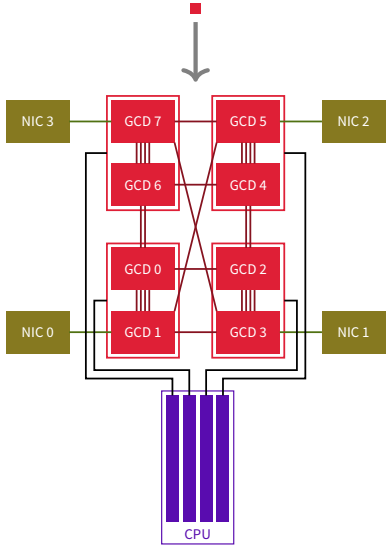
Frontier

- 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



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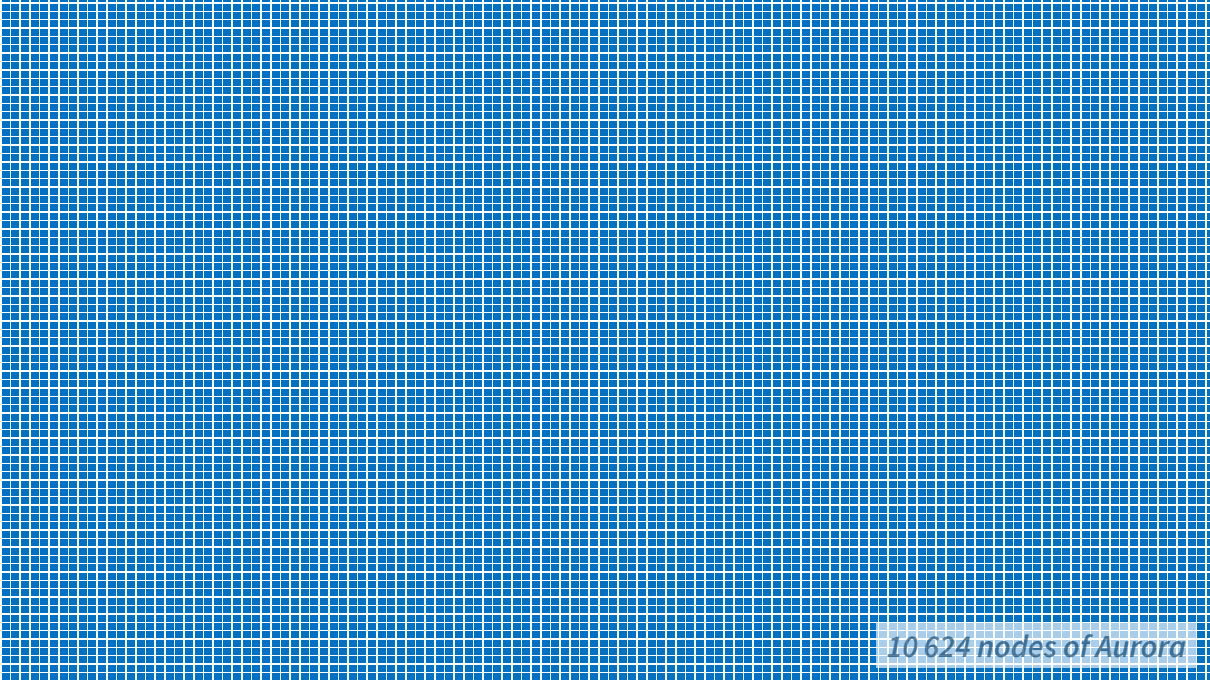
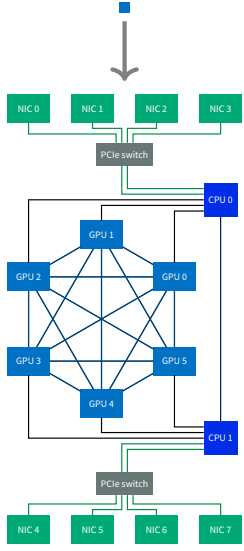

10 624 nodes of Aurora

Aurora

Aurora



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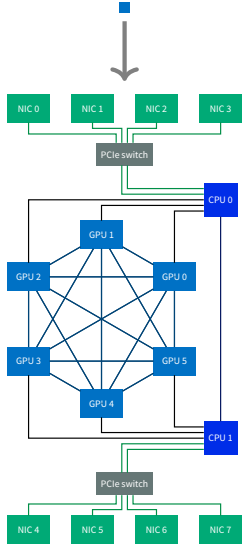
Aurora

- At Argonne National Lab, US
- First 2 EFLOP/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



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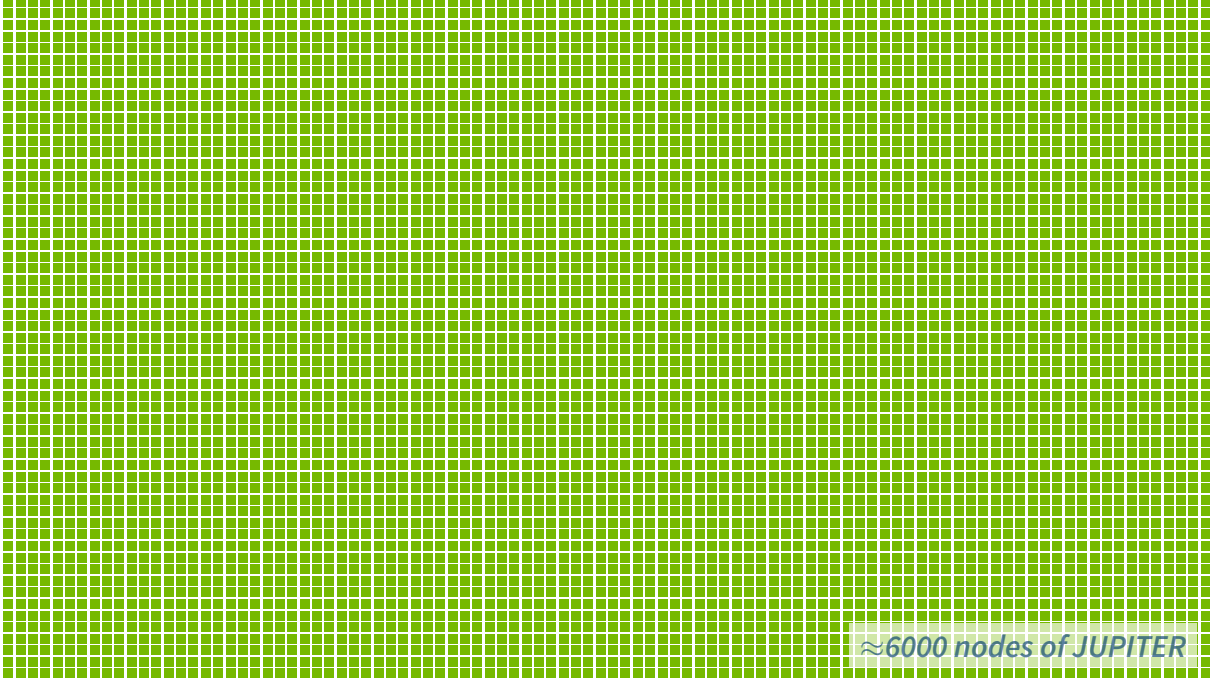
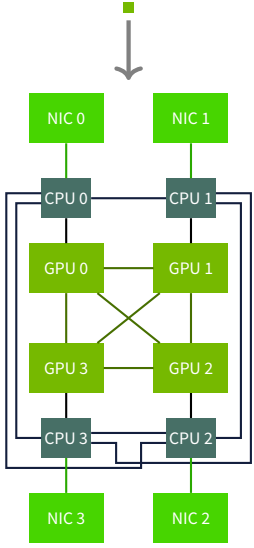

≈6000 nodes of JUPITER

JUPITER

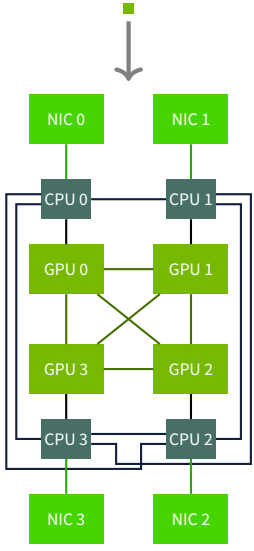
JUPITER



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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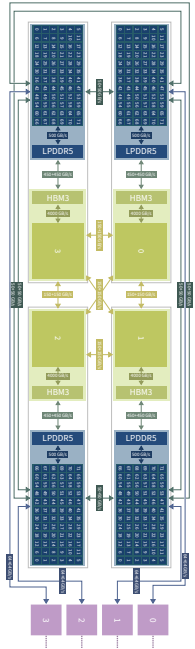

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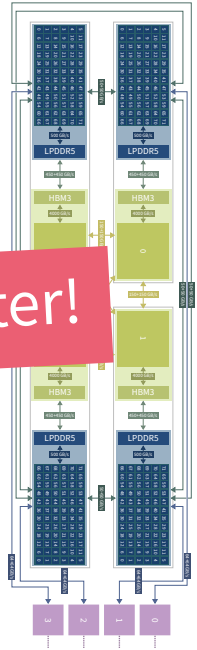
Today: JUWELS Booster!



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 *FP64:* 9.7 TFLOP/s, 40 GB memory)
- InfiniBand DragonFly+ HDR-200 network; 4 × 200 Gbit/s per node

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Top500 List Nov 2020:

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

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JUWELS Booster Overview

Node Configuration

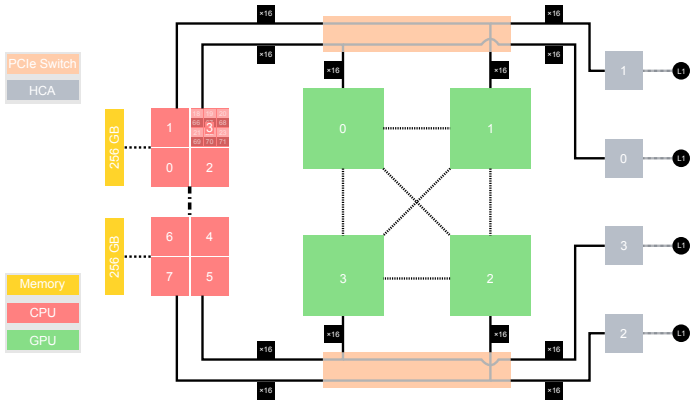
Arch Atos Bull Sequana XH2000

CPU $2 \times$ AMD EPYC 7402:
$2_{\text{Socket}} \times 24_{\text{Core}} \times 2_{\text{SMT}}$,
2×256 GB DDR4-3200 RAM;
NPS-4

GPU $4 \times$ NVIDIA A100 40 GB, NVLink3

HCA $4 \times$ Mellanox HDR200
(200 Gbit/s) InfiniBand ConnectX 6

etc $2 \times$ PCIe Gen 4 switch



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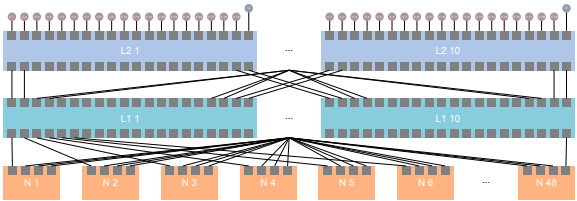
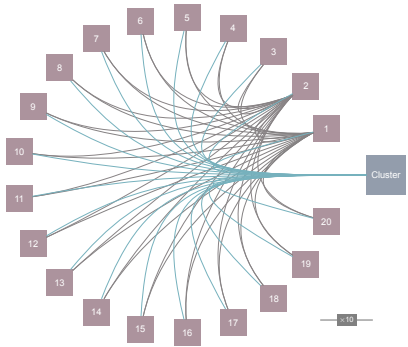
JUWELS Booster Overview

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

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AMD EPYC Rome

Some Processor Basics

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

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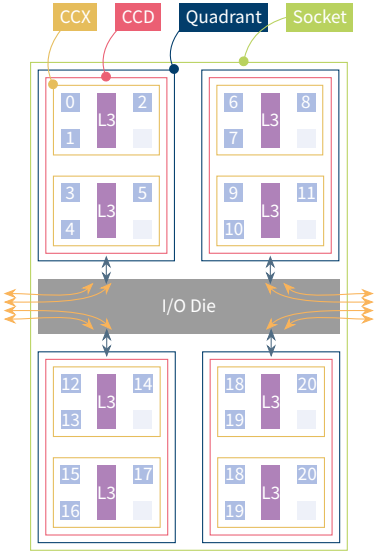
3 cores	Core-Complex (CCX), shared L3 *(max 4 cores)*
2 CCXs	Core Complex Die (CCD)
1 CCD	1 quadrant *(max 2 CCDs per quadrant)*
4 quadrants	1 socket; NPS-4: 4 NUMA domains per socket
2 sockets	1 node *(only 1 shown)*
I/O Die	Connections between quadrants and outside
RAM	8 memory channels, 2 per quadrant



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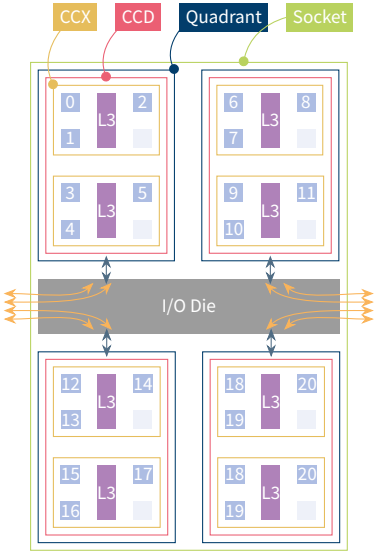
$\Rightarrow$ **Complex topology!**



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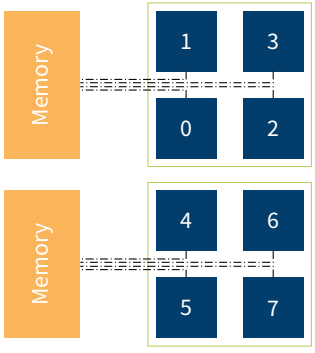
NUMA Overview

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



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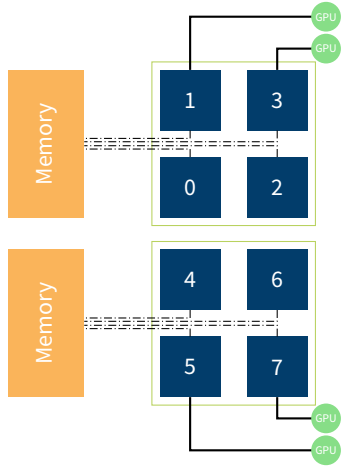

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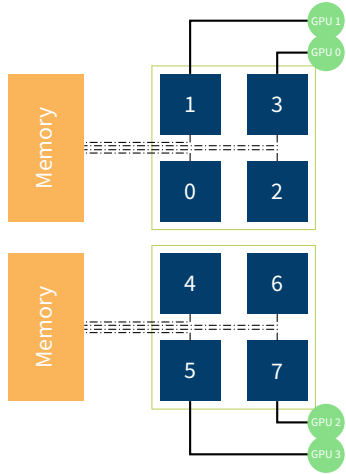
- Complete affinity table

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



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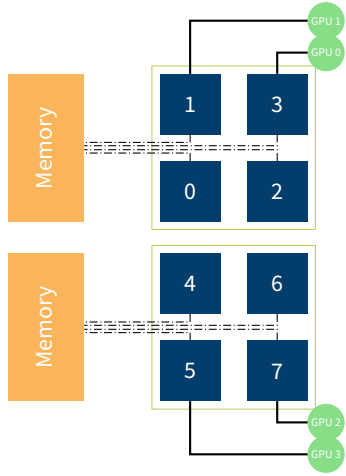
3	5	3	3

→ Slurm configured to automatically use best topology



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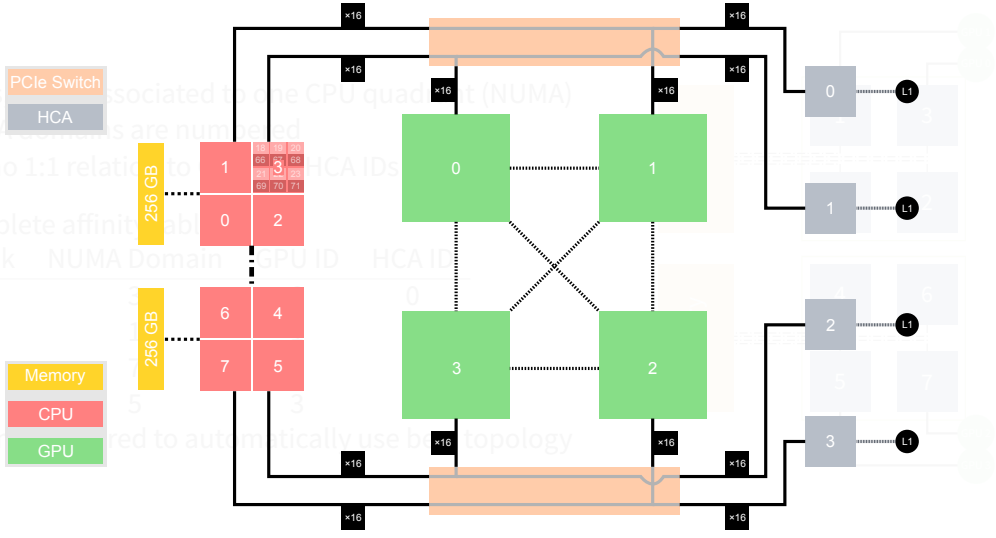


DragonFly+ Topology

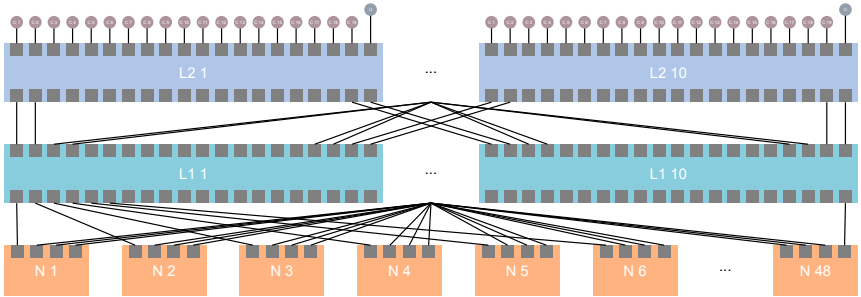
Overview

- 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)*



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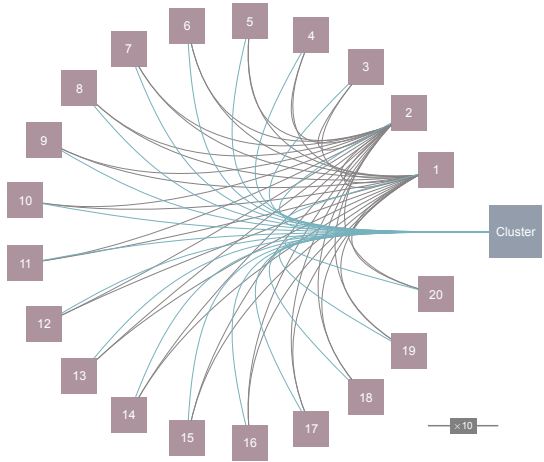
DragonFly+ Topology

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:

$$\mathcal{B}(N) = \lfloor (N/2)^2 \rfloor \times (10 \times \mathrm{bw}_1)$$



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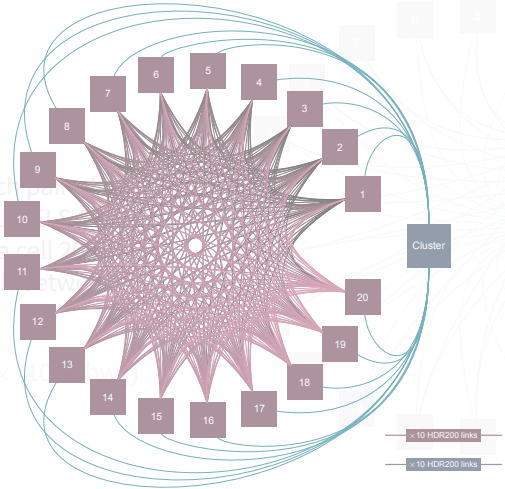
DragonFly+ Topology

Intra-Cell Topology

- Inter-cell: 20 cells
  - 10 links between each
  - 10 links per cell to JU
  - Filesystem access via cell
  - Bi-section bandwidth between cells:

$$B(N) = \lfloor (N/2)^2 \rfloor \times 10$$



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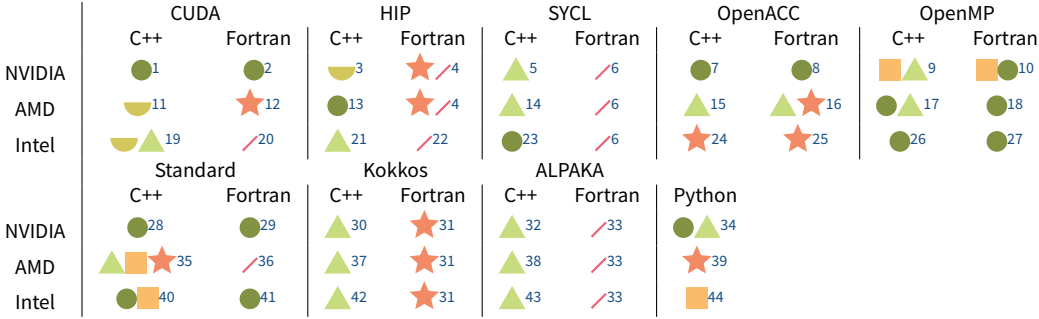
Vendors, Models

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

- Full vendor support
- Indirect, but comprehensive support, by vendor
- Vendor support, but not (yet) entirely comprehensive
- Comprehensive support, but not by vendor
- Limited, probably indirect
- Vendor support, but not (yet) support – but at least some
- No direct support available
- C++ C++ (sometimes also C)
- Fortran Fortran



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

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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

Summary and Conclusions

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Thank you for your attention!

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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++.