

Who I am

- PhD in Experimental High Energy Physics @ University of Milan (Italy), 2007
 - Working at the BaBar experiment @ SLAC laboratory (Menlo Park, CA)
- Since then, I have been working in High Performance Computing (HPC)
 - Numerical algorithms, optimizations, parallelization, computing devices...







2015-2016



2016-2018

Hewlett Packard Enterprise

2018-∞

2009-2012



CSCS

2012-2014

Centro Svizzero di Calcolo Scientifico Swiss National Supercomputing Centre







HPE HPC/AI EMEA Research Lab (part of the HP Labs)



Partnering with leading organizations in the EMEA region to advance supercomputing R&D

Our Role

Deep technical collaboration with industry, academia, and public sector

- Long term technical relationships surrounding research, co-design, and operational support
- Focus on new technologies, driving HPE products
- Create reusable PoCs & European IP

Research Interests

- HPC, Cloud, AI, Quantum
- Data movement, analysis, and workflows
- Heterogeneous computing and novel accelerators
- Programming languages and models
- Compilers and mathematical optimisation
- Performance portability, security, and containerisation
- Energy efficiency and sustainability

Engagement Models

- Centres of Excellence
- Advanced Collaboration Centres
- Value-add projects
- Joint-funded research projects
- Nationally/internationally funded research projects
- Ph.D. and Placements

https://www.hpe.com/emea_europe/en/compute/hpc/emea-research-lab.html



Disclaimer

 I'm speaking solely for myself, not for my company or as a formal representative of my company

 Spoiler Alert: This is NOT a technical presentation (at least as I could image)

the 10-Megabyte Computer System COMPLETE New From IMSA . 28-Amp Power Supply . 12" Monitor 10 Megabyte Hard Disk . Standard Intelligent 62-Key . 51/4" Dual-Density Floppy Disk Back-up **ASCII** Keyboard (Optional 8-Bit Microprocessor Intelligent 86-Key ASCII (Optional 16-bit Microprocessor) Extended Keyboard) · Memory-Mapped Video Display Board 132-Column Dot-Matrix Printer Disk Controller . CP/M* Operating System Standard 64K RAM You Read It Right ... (Optional 256K RAM) 10-Slot S-100 Motherboard All for \$5995! IMSAI...Thinking ahead for the 80's Computer Division of the Fischer-Freitas Corporation 415/635-7615 910 81st Avenue, Bldg. 14 . Oakland, CA 94621 is a trademark of Digital Research. Imsai is a trademark of the Fischer-Freitas Corporation

Outline

- Introduction
 - HPC and Supercomputing
 - Performance trend over the years
- The Exascale Era of Computing
 - Hardware and Software challenges
- Conclusion



Introduction

Where is the 'any' key?

- Homer Simpson (in response to the message "Press any key", E7 S7)

High Performance Computing

• "High Performance Computing most generally refers to the practice of aggregating computing power in a way that delivers much higher performance than one could get out of a typical desktop computer or workstation in order to solve large problems in science, engineering, or business."

https://insidehpc.com/hpc-basic-training/what-is-hpc/

- Several performance metrics can be optimized
 - Latency: faster and faster application execution
 - Throughput: more and more work done
 - Energy: consume less energy to carry out a given task (Sustainable HPC)
- HPC is everywhere there is a computing system!



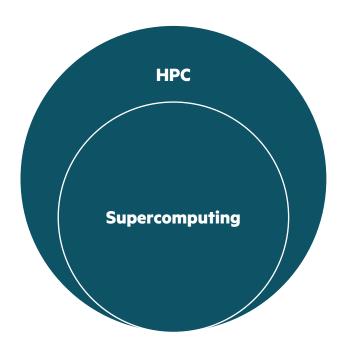






Supercomputing

- Supercomputing uses HPC techniques to build a single tightly-coupled system
 - A (complex and expensive) system which acts as a whole to perform an HPC single simulation
 - Write software that can take advantage of the supercomputer performance,
 e.g. employing parallel execution
- All system hardware/software aspects are important:
 - Select best microprocessor and accelerator
 - Surround it with a bandwidth-rich environment: local memory, interconnection network
 - Scale the system
 - Provide scalable programming and performance tools
 - Provide scalable I/O
 - Eliminate operating system interference (OS jitter)
 - Design in reliability and resiliency
 - Provide scalable system management



"Anyone can build a fast CPU.

The trick is to build a fast system."

— Seymour Cray

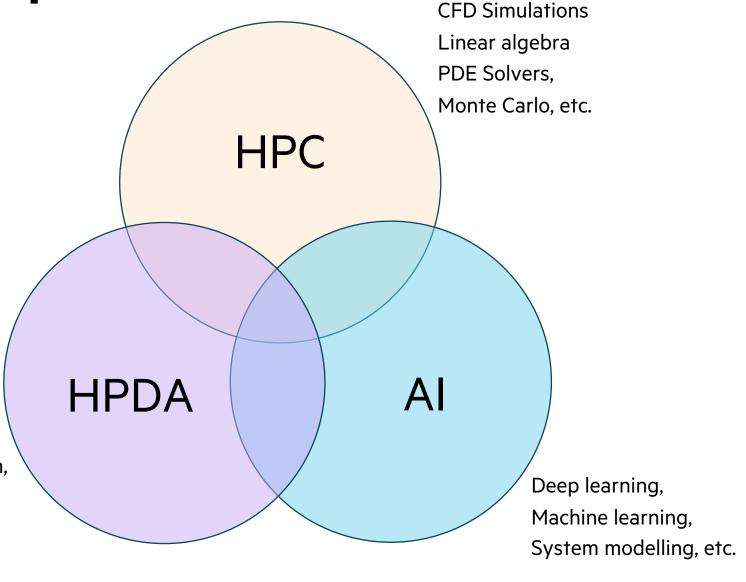


Focus on Intensive Numerical Computations

 Traditionally, HPC has been embraced by research scientists who needed to perform complex mathematical calculations, which requires intensive numerical computations (Floating-Point operations, Flop)

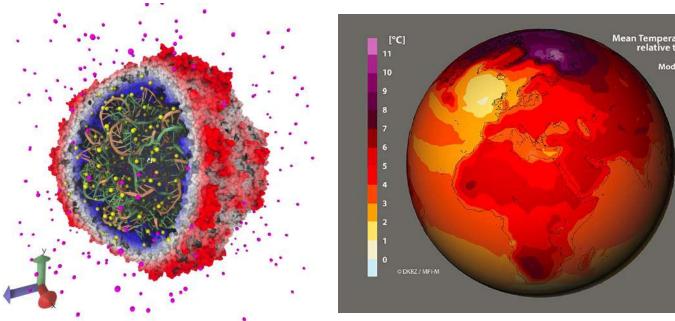
- Double-precision (DP) operations
- Nowadays HPC is gaining the attention of a wider number of enterprises spanning an array of fields
 - Not discussed in the rest of the presentation (lack of time)

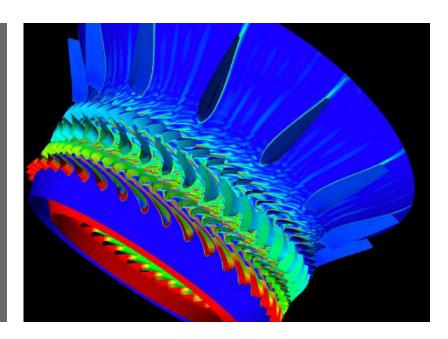
Monitoring, classification, anomaly detection, hypothesis testing, clustering, optimization, signal processing, etc.



Why we need (more and more) Supercomputing

- Simulation is the third pillar of the science research (with experiment and theory)
 - Quantum mechanics, weather forecasting, climate research, oil and gas exploration, cosmology, biology, fluid dynamics, ...
 - More and more complex systems to study





Recent convergence of Artificial Intelligence and Supercomputing



RCP 8.5

Supercomputers

#3 pencils and quadrille pads.

 Seymour Cray (when asked what CAD tools he used to design the Cray-1 supercomputer), 1980

The Beginning

- The first supercomputer (1964): CDC6600
 - Realized by Seymour Cray (1925-1996),
 the father of supercomputing
 - Single CPU@10MHz, 1-3 MFlop/s
 - 8 M\$ cost (~60M\$ in today's money)

- In 1972 Cray started his own company and released the first supercomputer in 1976: Cray-1
 - Fastest system for 5 years, 10x faster than competing systems
 - Single processor @80MHz, 160 MFlop/s
 - 5-8 M\$ (~25M\$ in today's money)





The Cray Era: Vector Processors

1982

A single instruction can operate on one-dimensional arrays of data called *vectors*, at the same time

1988

• Cray X-MP

- First multi-processors supercomputer, 2 vector processors @105MHz, up to 400 MFlop/s
- 16 MB memory

• Cray Y-MP

- 2, 4, or 8 vector processors @167MHz, 333 MFlop/s each (up to 2.6GFlop/s)
- Up to 512 MB memory

1991

Cray C90

• 3x faster than Y-MP vector processor, 2x more processors, i.e. up to 15.6GFlop/s





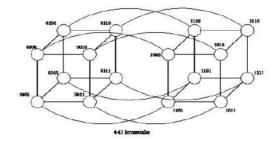
Massively Parallel Era (>1990)

- Vector processing did not allow to scaling to hundred processors systems
 - Custom processors were not feasible
- Shift towards commodity-based processors, i.e. PC technology
 - The attack of Killer Micros, Eugene Brook's talk at Supercomputing 90
 - Mainly driven by cost computing went mainstream
- Thousands of "small" (and relatively "cheap") compute units (nodes) connected together
 - "If you were plowing a field, which would you rather use: two strong oxen or 1,024 chickens?", Seymour Cray's joke
 - Distributed memory: each node has its own memory attached
 - Use special networks to connects nodes



Network Complexity

- nD Hypercube
 - Number of outgoing ports scales with the log of the machine size
 - Difficult to scale out



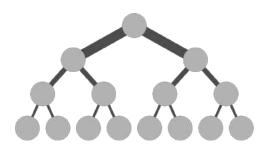
- nD Torus
 - Nearest neighbor



- Dragonfly
 - Hierarchical design
 - All-to-all connectivity between groups



- Fat Tree
 - Increases bandwidth for the higher levels of the tree

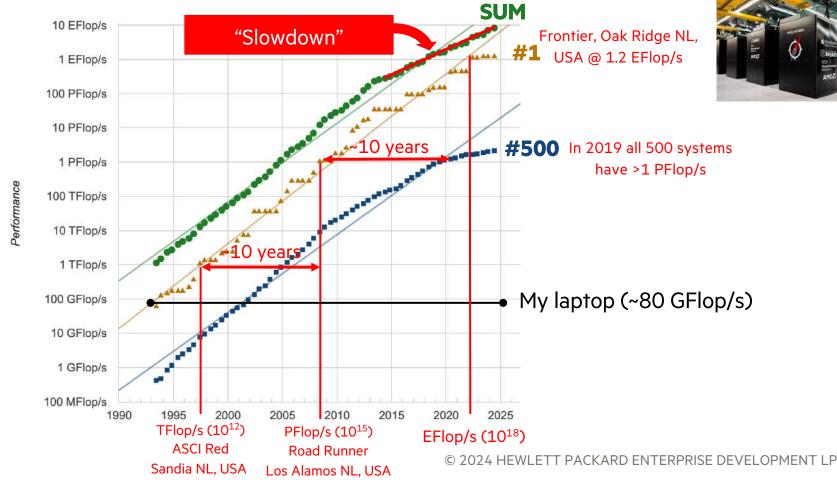


Challenging task

- Connect thousands of nodes
- Topology mapping of the application
- Hardware instability

Performance Trend

- Top500.org: list of the 500 fastest supercomputers (update twice a year)
 - Ranking based on the (historical) HPL benchmark (DP Flop/s)
 - Numerical linear algebra solver (compute intensive)



Top-10 list

| Rank | System | Cores | Rmax (PFlop/s) | Rpeak (PFlop/s) | Power (kW) |
|------|--|-----------|-------------------|--------------------|---------------|
| 1 | Frontier - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE D0E/SC/Oak Ridge National Laboratory United States | 8,699,904 | 1,206.00 | 1,714.81 | 22,786 |
| 2 | Aurora - HPE Cray EX - Intel Exascale Compute Blade, Xeon CPU Max 9470 52C 2.4GHz, Intel Data Center GPU Max, Slingshot-11, Intel D0E/SC/Argonne National Laboratory United States | 9,264,128 | 1,012.00 | 1,980.01 | 38,698 |
| 3 | Eagle - Microsoft NDv5, Xeon Platinum 8480C 48C 2GHz, NVIDIA H100, NVIDIA Infiniband NDR, Microsoft Azure Microsoft Azure United States | 2,073,600 | 561.20 | 846.84 | |
| 4 | Supercomputer Fugaku - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan | 7,630,848 | 442.01 | 537.21 | 29,899 |
| 5 | LUMI - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE EuroHPC/CSC Finland | 2,752,704 | 379.70 | 531.51 | 7,107 |
| | 1 st System in Eu | ırope (| since 20 |)22), | |

Same HPE Cray system as Frontier

- Rmax: HPL benchmark performance
- Rpeak: theoretical aggregate max performance
- Rmax/Rpeak: performance efficiency (%)
- Rmax/Power: energy efficiency (GFlop/s/W)

| 6 | Alps - HPE Cray EX254n, NVIDIA Grace 72C 3.1GHz, NVIDIA GH200 Superchip, Slingshot-11, HPE Swiss National Supercomputing Centre [CSCS] Switzerland | 1,305,600 | 270.00 | 353.75 | 5,194 |
|----|--|-------------------------|--------------------|--------|--------|
| 7 | Leonardo - BullSequana XH2000, Xeon Platinum 8358 32C 2.6GHz, NVIDIA A100 SXM4 64 GB, Quad-rail NVIDIA HDR100 Infiniband, EVIDEN EuroHPC/CINECA Italy | 1,824,768 n in Italy | 241.20 (since 2 | 306.31 | 7,494 |
| 8 | MareNostrum 5 ACC - BullSequana XH3000, Xeon Platinum 8460Y+ 32C 2.3GHz, NVIDIA H100 64GB, Infiniband NDR, EVIDEN EuroHPC/BSC Spain | 663,040 | 175.30 | 249.44 | 4,159 |
| 9 | Summit - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM DOE/SC/Oak Ridge National Laboratory United States | 2,414,592 | 148.60 | 200.79 | 10,096 |
| 10 | Eos NVIDIA DGX SuperPOD - NVIDIA DGX H100, Xeon Platinum 8480C 56C 3.8GHz, NVIDIA H100, Infiniband NDR400, Nvidia NVIDIA Corporation United States | 485,888 | 121.40 | 188.65 | |

Energy Concern

- **Top500.org/green500:** list of the 500 most energy efficient supercomputers
 - Still based on HPL benchmark, now focusing on energy efficiency
- Frontier test system at the 7th position
- Clear pattern appears: all efficient systems have Graphics Processor Units (GPU) coprocessors!

| Rank | TOP500 Rank | System | Cores | Rmax (PFlop/s) | Power (kW) | Energy Efficience (GFlops/watts) |
|------|----------------|---|---------|-------------------|---------------|-------------------------------------|
| 1 | 189 | JEDI - BullSequana XH3000, Grace Hopper Superchip 72C 3GHz, NVIDIA GH200 Superchip, Quad-Rail NVIDIA InfiniBand NDR200, ParTec/EVIDEN EuroHPC/FZJ Germany | 19,584 | 4.50 | 67 | 72.733 |
| 2 | 128 | Isambard-AI phase 1 - HPE Cray EX254n, NVIDIA Grace 72C 3.1GHz, NVIDIA GH200 Superchip, Slingshot-11, HPE University of Bristol United Kingdom | 34,272 | 7.42 | 117 | 68.835 |
| 3 | 55 | Hetios GPU - HPE Cray EX254n, NVIDIA Grace 72C 3.1GHz, NVIDIA GH200 Superchip, Slingshot-11, HPE Cyfronet Poland | 89,760 | 19.14 | 317 | 66.948 |
| 6 | 329 | Henri - ThinkSystem SR670 V2, Intel Xeon Platinum 8362 32C 2.8GHz, NVIDIA H100 80GB PCIe, Infiniband HDR, Lenovo Flatiron Institute United States | 8,288 | 2.88 | 44 | 65.396 |
| i | 71 | preAlps - HPE Cray EX254n, NVIDIA Grace 72C 3.1GHz, NVIDIA GH200 Superchip, Slingshot-11, HPE Swiss National Supercomputing Centre (CSCS) Switzerland | 81,600 | 15.47 | 240 | 64.381 |
| i | 299 | HoreKa-Teal - ThinkSystem SD665-N V3, AMD EPYC 9354 32C 3.25GHz, Nvidia H100 94Gb SXM5, Infiniband NDR200, Lenovo Karlsruher Institut für Technologie (KIT) Germany | 13,616 | 3.12 | 50 | 62.964 |
| 7 | 54 | Frontier TDS - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot- 11, HPE DOE/SC/Oak Ridge National Laboratory United States | 120,832 | 19.20 | 309 | 62.684 |

The Exascale Era of Computing

In the future, computers may weigh no more than 1.5 tons.

- Popular mechanics, 1949

Exascale Estimates

- After the first Petascale system came online (2009), people started to discuss about an Exascale system
 - The International Exascale Software Project (IESP)
- The IESP Roadmap was published in 2011
 - Dongarra J., Beckman P., et al. The International Exascale Software Roadmap. International Journal of High Performance Computer Applications, 25(1), 2011

| | 2009 | Pre-exascale | Exascale estimates | |
|-------------------------------|--------|--------------|--------------------|-------------------|
| System peak (PFlop/s) | 2 | 100-200 | 1000 | |
| Power (MW) | 6 | ~ 15 | ~ 20 | DOE Constraint |
| Node concurrency | 12 | O(100) | O(1k-10k) | Constraint |
| System size (nodes) | 18,700 | >50,000 | O(100k-1M) | |
| Mean time to interrupt (days) | >1 | O(1) | O(0.1) | |

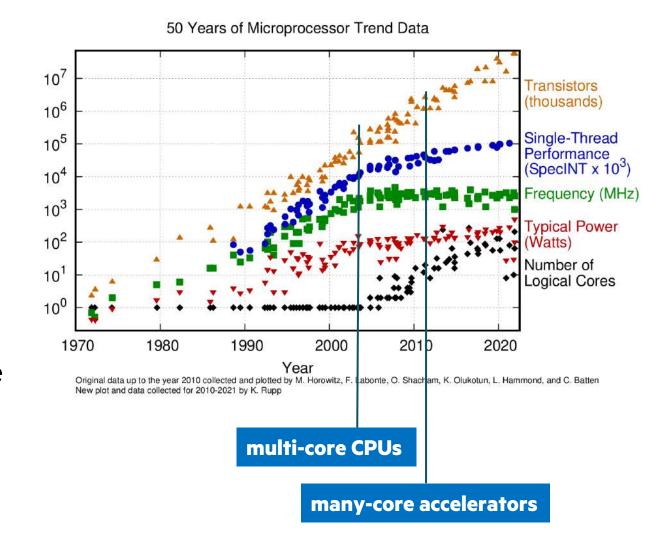
Source: https://www.hpcwire.com/2021/07/14/frontier-to-meet-20mw-exascale-power-target-set-by-darpa-in-2008/



Technology Trend

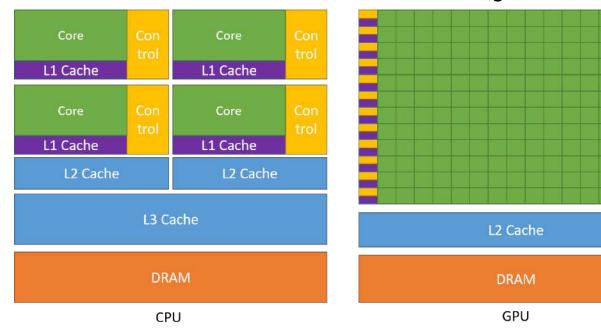
- Moore's law has been driven the performance improvement in the last 50 years
 - 3nm in current production (well, this dimension is meaningless...)
 - Current model up to ~1nm (?), probably another 4
 years before reaching this limit

- Power density wall: hard to increase performance per core without large energy investment (Dennard scaling)
 - Multi-core CPUs (>2004)
 - Many-core accelerators, eg. GPUs (>2012)



Accelerators

- Specialized parallel hardware for floating point operations
 - Based on massive parallel architectures
 - Co-processors for traditional CPUs (which are used for generic workloads)
 - GPUs have been the most common accelerators during the last few years

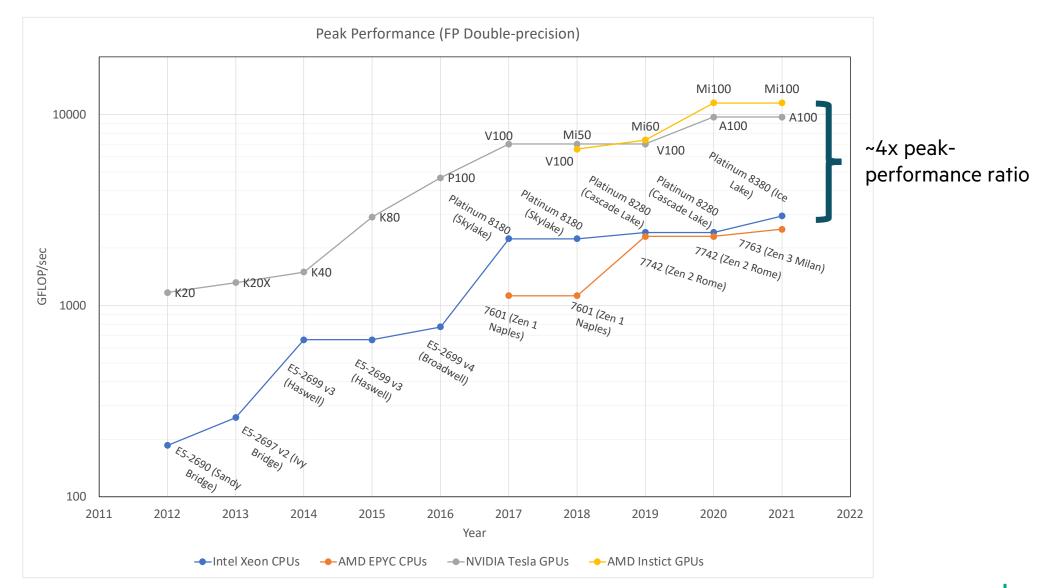


Source: CUDA C++
Programming Guide

- Low compute density
- Large caches
- Optimized for serial operations
- Latency optimized

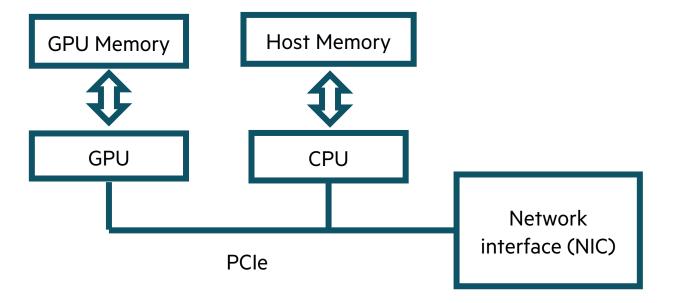
- High compute density
- High computations per Memory Access
- Built for parallel operations
- Throughput optimized

CPU VS GPU Performance Trend



Typical node layout: Single GPU

- GPU connected to CPU via PCIe
 - GPU and Host memory do not share the same address space
 - Must copy data from/to the host memory to/from the GPU (device) memory



AMD Mi250 GPU: Chiplet Multichip Architecture

Extend chips complexity

- Monolithic chips: all components into a single printed piece of silicon
- Chiplets break things up into smaller components that are then combined into a larger processor via an interposed in a single package
 - Mix-and-match "LEGO-like" assembly
 - → Reduce costs
- AMD using this approach on the Zen CPUs and Mi250 GPUs



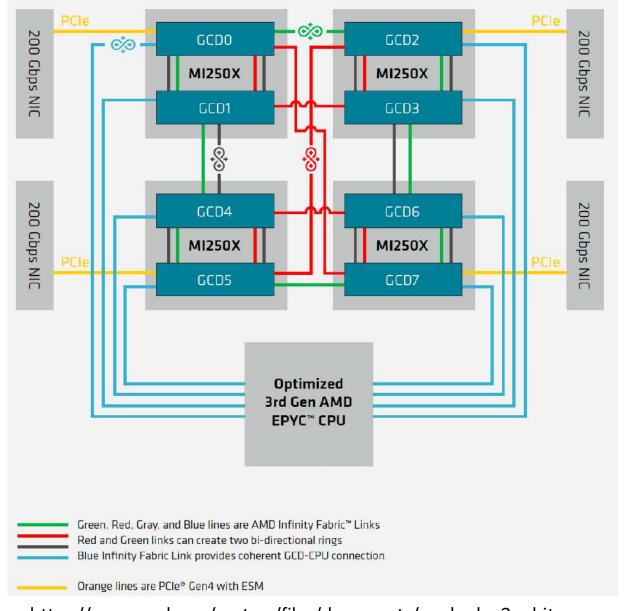
4 links for fast GCDs connection (up to 400GB/s of bidirectional bandwidth)

Source

Source: https://www.amd.com/en/technologies/cdna2

HPE-AMD Multi-GPUs Node Layout

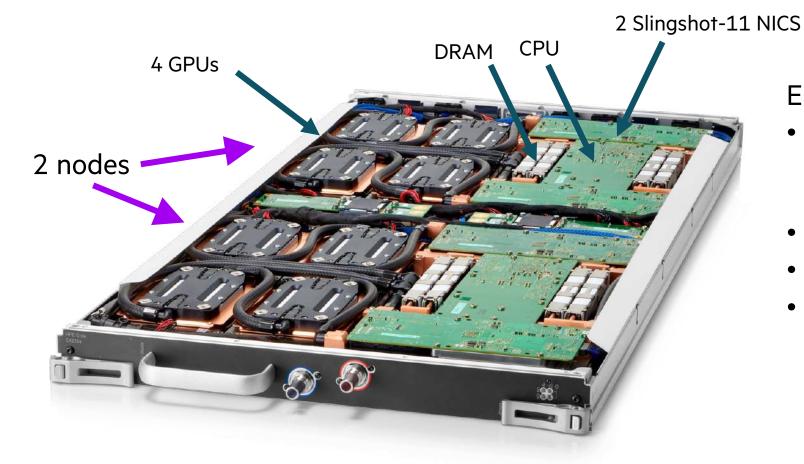
- Fast connections between GPUs, CPU-GPUs, GPU-NICs
- AMD node layout: 4 Mi250 GPUs
- Mi250 specs:
 - 110 Compute Units (CU) per each die = 220 CUs
 - 64 SIMD threads per each CU = 14080 Stream Processors
 - Peak FP64/FP32 Vector: 47.9 TFLOPS
 - Peak FP64/FP32 Matrix: 95.7 TFLOPS
 - Total L2 cache: 8 MB per each die (64kB per CU)
 - Frequency: up to 1700 MHz
 - Max power: up to 560 Watts



Source: https://www.amd.com/system/files/documents/amd-cdna2-white-paper.pdf



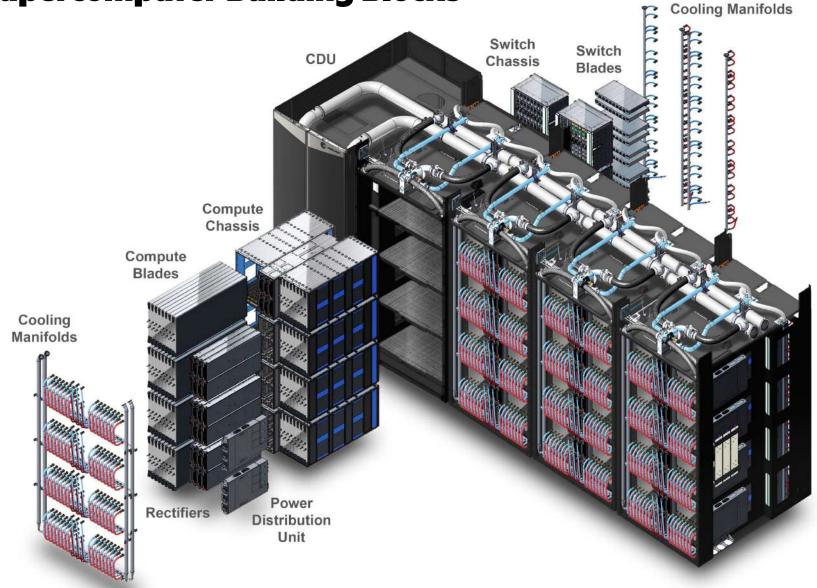
Frontier Compute Blade Architecture



Each node:

- AMD EPYC 7A53 "Optimized 3rd Gen EPYC" 64-Core Processor, 2.00 GHz
- 512 GB DDR4 memory
- 4x AMD MI-250X GPU
- Each GPU connected to a Slingshot 200Gb/s NIC (Dragonfly topology)

Frontier Supercomputer Building Blocks



Frontier in Numbers



- •#1 in the world @ 1.2 EFlop/s
- •74 HPE Cray EX cabinets
- 9,408 AMD EPYC CPUs,37,632 AMD GPUs,37,632 Slingshot NICs
- •700 petabytes of storage capacity
- 90 miles of HPE
 Slingshot networking
 cables

Exascale Estimates VS Frontier Numbers

| | 2009 | Pre-exascale | Exascale estimates | Frontier |
|-------------------------------|--------|--------------|-----------------------|-----------------------------|
| System peak (PFlop/s) | 2 | 100-200 | 1000 | 1206 |
| Power (MW) | 6 | ~ 15 | ~ 20 | 22.786 (<20 MW per exaflop) |
| Node concurrency | 12 | O(100) | O(1k-10k) | O(100k) |
| System size (nodes) | 18,700 | >50,000 | O(100k-1M) | 9,408 |
| Mean time to interrupt (days) | >1 | 0(1) | O(0.1) | O(0.3) |

Source: https://www.hpcwire.com/2021/07/14/frontier-to-meet-20mw-exascale-power-target-set-by-darpa-in-2008/

Quoting Al Geist (ORNL): "In the end, what we found out was that exascale didn't require this exotic technology that came out in the 2008 report. We didn't need special architectures, we didn't even need new programming paradigms. It turned out to be very incremental steps, not a giant leap like we thought it was going to take to get to Frontier."



Programming Models

If you build it, they will come.

- Quote from the Field of Dreams movie (1989)

We got the Fantastic Powerful Hardware...

What could go wrong?





Baby Is Given Fresh Air in Window Cage

BABIES of flat and tenement dwellers, whose tiny lungs have been forced to breathe stale and overheated air, are offered relief by the recent English invention pictured above. A large metal crate is attached to the outside of the window by two stout iron poles. A baby basket can easily be lowered inside. If insects are likely to trouble the child, the crate can be screened.

Software Complexity: A Long Story

Hardware > Software

- Reach peak performance
- Several level of parallelism
 - Intra-cores, intra-nodes, inter-nodes
 - Accelerators
- Memory access
 - Various level of memories with different speeds and sizes
 - Flop/s are for free, memory speed can be the ultimate limit
- Mixed-precision computations
- Erratic hardware

Software Hardware

- Auto-tuning
 - Rewriting code for each system generation is not an option!
- Parallel programming paradigms
 - E.g. Message Passing, Threading, Tasking
- New algorithms
- Legacy code
 - Yes, the old good Fortran
- New languages and programming models
- Static versus dynamic parallelism
 - Runtime scheduling

This is just the beginning of the story... very challenging!



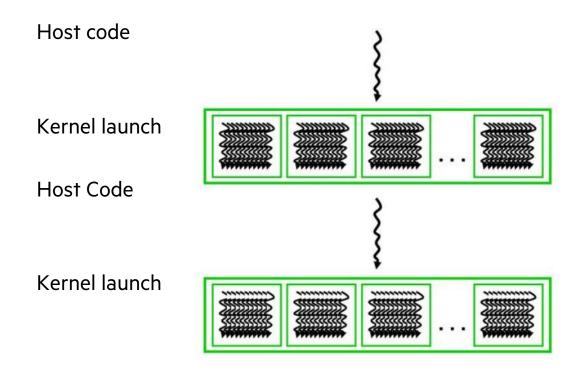
Parallel Programming Models: Short Overview

- Multi-processes
 - Suitable for distributed-memory systems (e.g. on multi-nodes)
 - Message Passing Model: MPI
 - Partitioned Global Address Space (PGAS): SHMEM, Coarrays, UPC, Chapel, GASPI
- Multi-threaded
 - Suitable for shared-memory systems (e.g. on multi-cores)
 - Direct parallelism: Pthreads, std::threads
 - Directive based: OpenMP
 - Programming languages: C++ Parallel STL
 - Via parallel libraries: HPX, TBB, C++ Parallel STL Executors
- Accelerator execution (via GPUs)
 - Code regions are **offloaded** from a host CPU to be computed on an accelerator
 - Portability across AMD, NVIDIA, Intel GPUs
- Hybrid model: mixing all the above



GPU Offload execution

- Code regions are **offloaded** from a host CPU to be computed on an accelerator
 - Kernel execution
- Keep latency sensitive work on the CPU (host)
- Memory management via copies (host-to-device, device-to-host, device-to-device)



Programming considerations

- GPU model requires many small tasks executing a kernel
 - Can replace iterations of a CPU loop with a GPU kernel call
 - -Would it be better to port 10 iterations with 1M instructions each or 1M iterations with 10 instructions each?
- Need to adapt CPU code to run on the GPU
 - Programming patterns, eg. reduction
 - Decompose your problem in hierarchical thread/grid model
 - Manage data transfers between CPU and GPU memories
 - -Data movement can easily become the bottleneck for performance
 - -Try to reduce data movement, eg. reusing data
 - -Hide latency by overlapping data movement with communications
 - Keep reusing data on the GPU to reach high an efficient use of the hardware (occupancy)
- Usually, after a first porting of the code to GPU, performance tunings is required to reach good performance



Accelerate applications

Accelerated Libraries

- The easiest solution, just link the library to your application without in-depth knowledge of GPU programming
- Many libraries are optimized by GPU vendors, eg. algebra libraries

Directive based methods

- Add acceleration to your existing code (C, C++, Fortran)
- Can reach good performance with somehow minimal code changes
- OpenACC, OpenMP

Programming Languages

- Maximum flexibility, require in-depth knowledge of GPU programming and code rewriting (especially for Fortran)
- Kokkos, RAJA, CUDA, HIP, OpenCL, SYCL

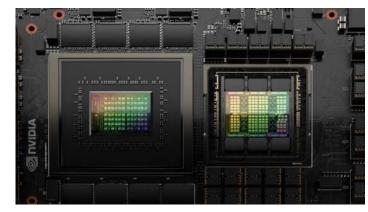
Conclusion

I don't know what the language of the year 2000 will look like, but I know it will be called Fortran.

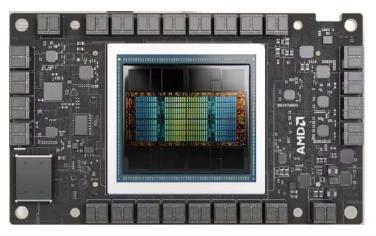
- CA Hoare, 1982

The Take-home Message

- Accelerators and more accelerators
 - GPUs and more GPUs
 - NVIDIA Grace-Hopper: Jupiter, the 1st European Exascale system (end of 2024)
 - AMD Mi300: El-Capitan (USA), target 2 EFlop/s (end of 2024)
- Need to adapt algorithms/code to run on the GPUs
 - Offload model
 - Optimize code for data-movement and occupancy
- Programming models: choose the model that best fits your requirements
 - Do not forget portability in the long run



NVIDIA Grace-Hopper Superchip (source: https://www.nvidia.com/en-us/data-center/grace-hopper-superchip/)



AMD Mi300X (source:

https://www.amd.com/en/products/accelerators/instinct/mi300/mi300x.html

One Slide Summary

HPC is there to stay for a long time

- Exascale mission accomplished, Zettascale next...
- Pushing technology to the limit, hardware and software

Exascale and beyond will enhance computing systems at all scales

- Affordable petascale systems?
- Golden age of HPC software developers, very exciting

Traditionally HPC can learn a lot from emerging applications (and vice versa)

• In primis machine learning and data science

Major cloud vendors provide HPC infrastructures to experiment with

 HPC on Demand, assuming you don't want to buy a supercomputer or apply for accessing to a supercomputer center...

Secondments @ HPE

- Reconfigurable hardware, namely FPGA, as an accelerator
 - Adapt the hardware to your software
- GPU application porting
- Quantum Computing applications
- Al applications
- Data-driven workflow optimization
- Data movement cost models / benchmarking
- Presenting and accessing memory efficiently
- Memory abstraction frameworks
- Tiling abstractions
- High-level workflow managers
- C/C++/Fortran-related compiler tools
- Performance-portable application containerization

Contact me if you are interested!



Questions?

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(Some) GPU Programming Models Portability



Level of control

CUDA / ROCM

- CUDA is targeting NIVIDA GPUs only
 - https://docs.nvidia.com/cuda/cuda-c-programming-guide/index.html
 - Hardware co-design, full control of the hardware features
 - Only a main compiler, proprietary
 - -C/C++ extension
 - Quite long history (>10 years)
 - Well supported, rich set of tools and libraries
 - Large community adoption and experience
- ROCM is targeting AMD GPUs
 - Analogous to CUDA-NVIDIA, but
 - Open-source at https://github.com/RadeonOpenCompute
 - -LLVM/Clang based compiler, full compatibility with C/C++
 - Increasing tools and libraries availability

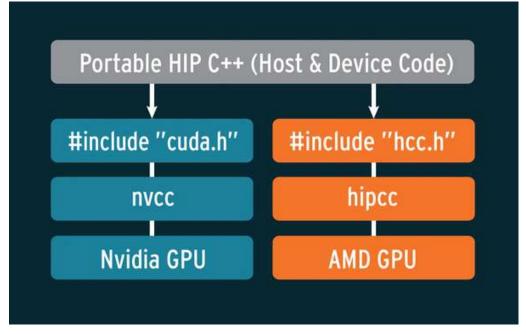






HIP (Heterogeneous Interface for Portability)

- C++ runtime API and kernel language
- Supported by AMD
 - https://github.com/ROCm-Developer-Tools/HIP
- Provide access to NVIDIA and AMD GPUs



Source: https://www.admin-magazine.com/HPC/Articles/Porting-CUDA-to-HIP

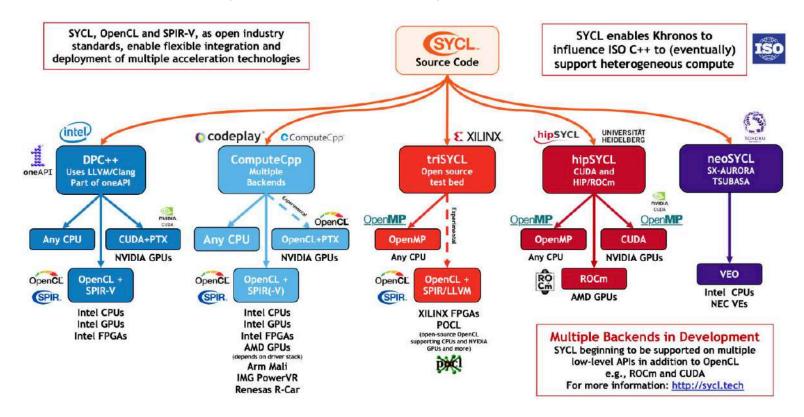
- Syntactically similar to CUDA
 - Most CUDA API calls can be converted in place: replace 'cuda' with 'hip'
 - Supports a strong subset of CUDA runtime functionality
 - You can "hipify" an existing CUDA code (https://github.com/ROCm-Developer-Tools/HIPIFY)
 - Eg. source-to-source conversion (hipify-perl)



SYCL



- C++ Single-source Heterogeneous Programming for Acceleration Offload
 - Standard from the Khronos Group, https://www.khronos.org/sycl/
 - SYCL 2020 is the latest revision, more info at https://sycl.tech/
- Several backends available (SYCL implementation ecosystem)



KOKKOS/RAJA

- Kokkos and RAJA provide portability to C++ programs via backends
 - Based on lambdas and templates
 - Cross-platform abstraction layers targeting all major HPC platforms (CPU, GPUs)
 - Big US labs and projects to support them
 - https://github.com/kokkos/
 - https://github.com/LLNL/RAJA
- Kokkos provides memory abstraction via "view" datatype
 - Separation of concerns between "where data is stored" and "where code is run"
 - Default memory and execution space selected at compile time

```
int n = 100000;
Kokkos::View<double *> a("a", n), b("b", n);
// Fill a and b - not shown
Kokkos:parallel_for(n, KOKKOS_LAMDA(size_t const i) { a(i) += b(i); });
```

 Similarly, RAJA insulates application loop kernels from underlying architecture and programming model-specific implementation details







OpenMP



- De-facto standard for Shared-Memory Parallelization (OpenMP 1.0, 1997)
 - Directives-based (pragma's) approach
 - Easily add to an existing code, minimal disruption
- OpenMP 4.0 (2013) includes initial support for accelerators
 - Significant revisions/extensions in 4.5 (2015), 5.0 (2018), 5.1 (2020), 5.2 (2021)

All vendors committed to supporting OpenMP offload



C++



- C++17 introduced several parallel algorithms (Parallel STL)
 - Extended in C++20, C++23 and beyond (executors)
 - See < numeric>, < algorithm>, < execution>
- Compiler support for GPU accelerated is emerging
 - Evolving support as part of the C++ standard
- Portability will be guarantee as part of the C++ standard
 - Can run on CPUs and GPUs
 - Interesting option in the long run