

HPC Induction

Part I: Hardware

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Outline

1 What is HPC?

2 Building an HPC system

- Processors
- Memory / Data Storage
- Data Transfer / Connectivity

3 ARTEMIS Hardware



What is HPC?

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High Performance Computing (HPC) 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.

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- Requires large-scale machines and clusters (aka supercomputers) or huge distributed computing networks (cf. e.g. Einstein@Home / BOINC)
- But also requires special software to allow the components to work efficiently together (scheduling, distributed data, parallelisation, etc.)



Supercomputers & Frameworks

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A supercomputer is a computer with a high level of performance compared to a general-purpose computer. The performance of a supercomputer is commonly measured in floating-point operations per second (FLOPS) instead of million instructions per second (MIPS).



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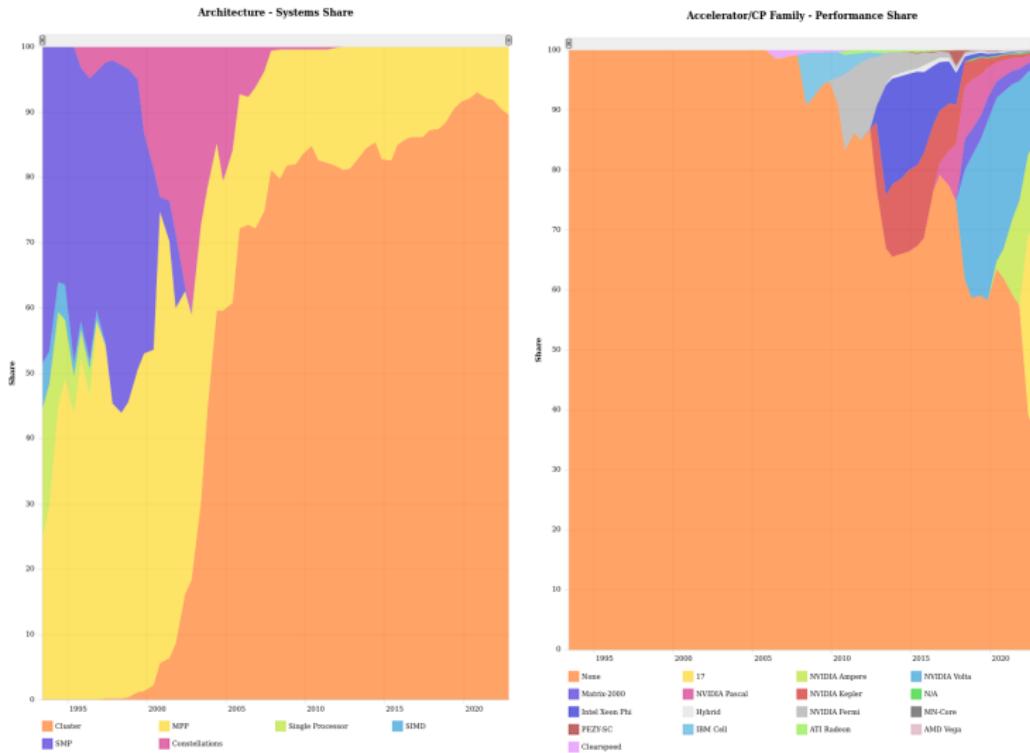
- Originally, supercomputers were big machines (SMP), often with highly specialised hardware. Nowadays, most supercomputers consists of closely inter-connected clusters (MPP) of (semi-)independent *nodes* of "off-the-shelf" hardware
- These 'servers' are hosted in so-called *data centres*



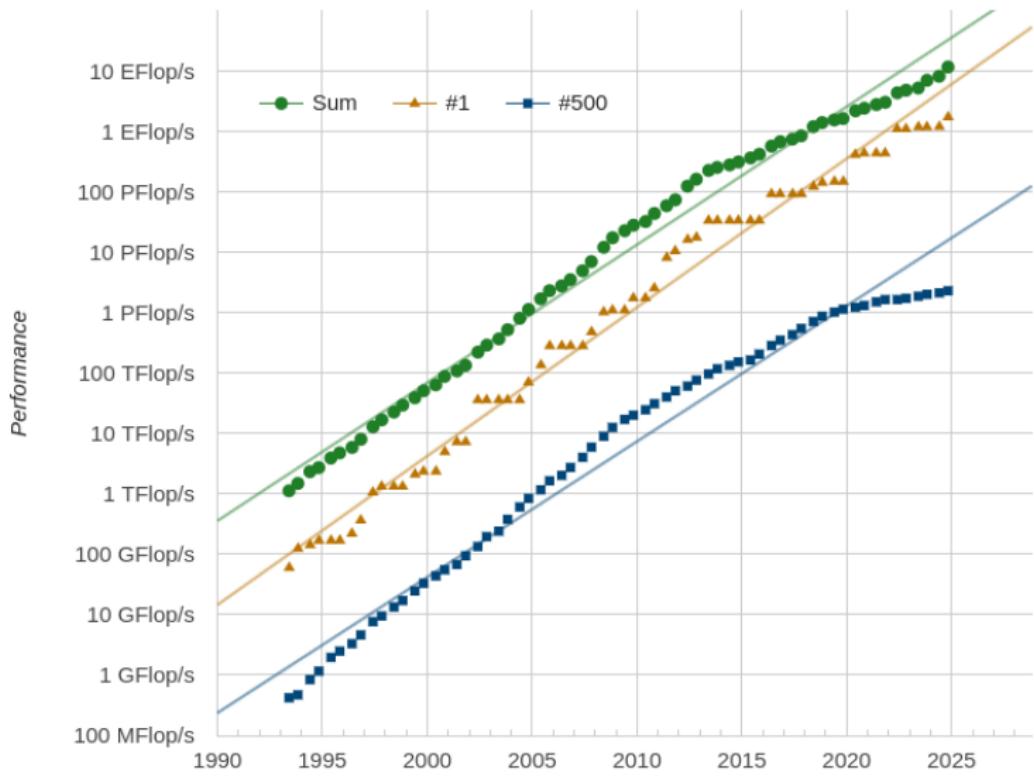
Supercomputers & Frameworks



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Supercomputers & Frameworks (cont.)



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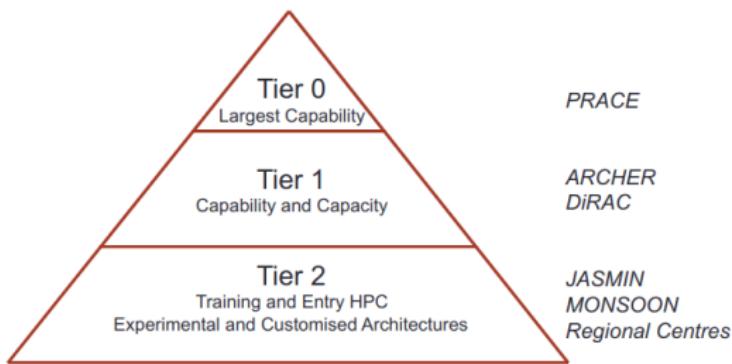
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- Commercial, shared HPC frameworks/services → e.g. Google Cloud Services, AWS
- Non-commercial/research shared HPC infrastructure → e.g. DiRAC & Archer (UK), EuroHPC (EU), usually classified in so-called Tiers



Building an HPC system

Summit Overview



Components

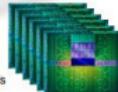
IBM POWER9

- 22 Cores
- 4 Threads/core
- NVLink



NVIDIA GV100

- 7 TF
- 16 GB @ 0.9 TB/s
- NVLink



Compute Node

- 2 x POWER9
- 6 x NVIDIA GV100
- NVMe-compatible PCIe 1600 GB SSD



- 25 GB/s EDR IB- (2 ports)
- 512 GB DRAM- (DDR4)
- 96 GB HBM- (3D Stacked)
- Coherent Shared Memory

Compute Rack

- 18 Compute Servers
- Warm water (70°F direct-cooled components)
- RDHX for air-cooled components



- 39.7 TB Memory/rack
- 55 KW max power/rack

Compute System

- 10.2 PB Total Memory
- 256 compute racks
- 4,608 compute nodes
- Mellanox EDR IB fabric
- 200 PFLOPS
- ~13 MW



GPFS File System

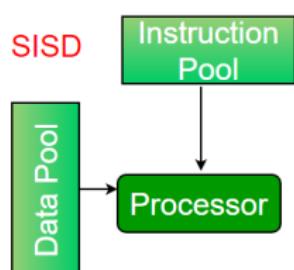
- 250 PB storage
- 2.5 TB/s read, 2.5 TB/s write



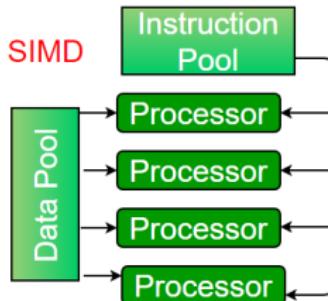
OAK RIDGE | LEADERSHIP COMPUTING FACILITY



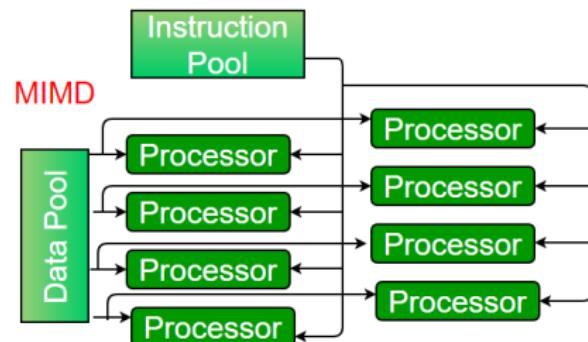
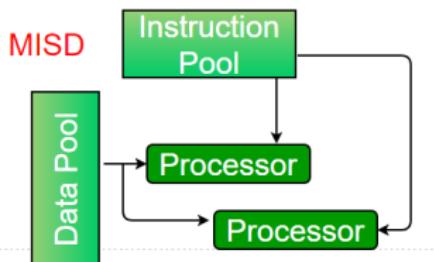
Computer Architectures - Flynn's taxonomy



classical computer



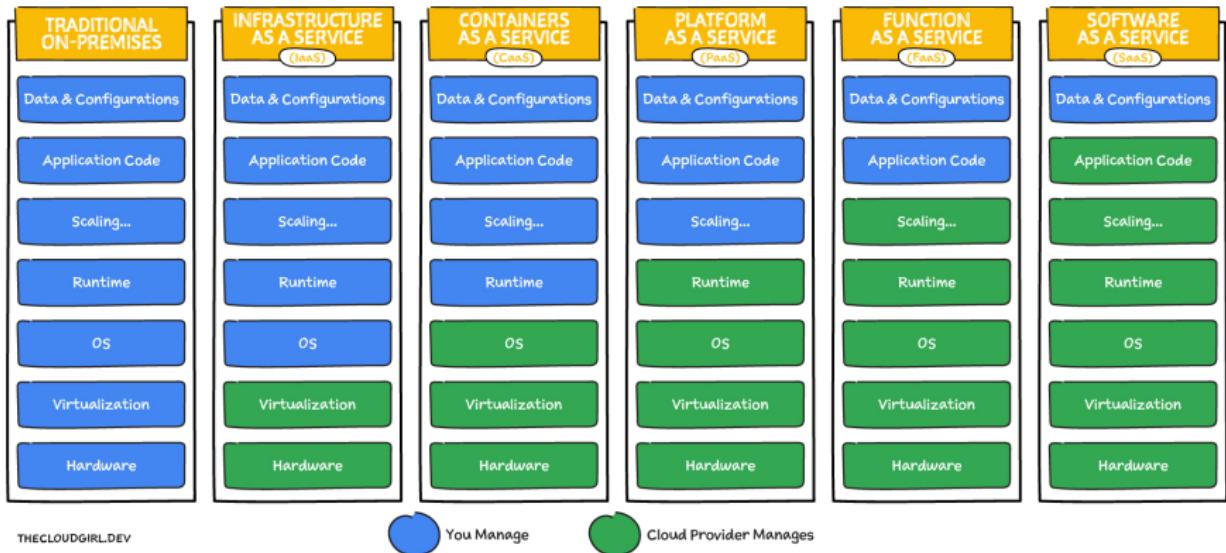
vector processing, GPUs



Multi-processing / multi-computing



Teaser: HPC as a service



HPC stack

SOFTWARE

Environments & Applications

SYSTEM SOFTWARE

Resource & Job Management

Runtime System Interprocess Comm

Operating System

VIRTUALISATION

Cloud computing / OpenStack

HARDWARE

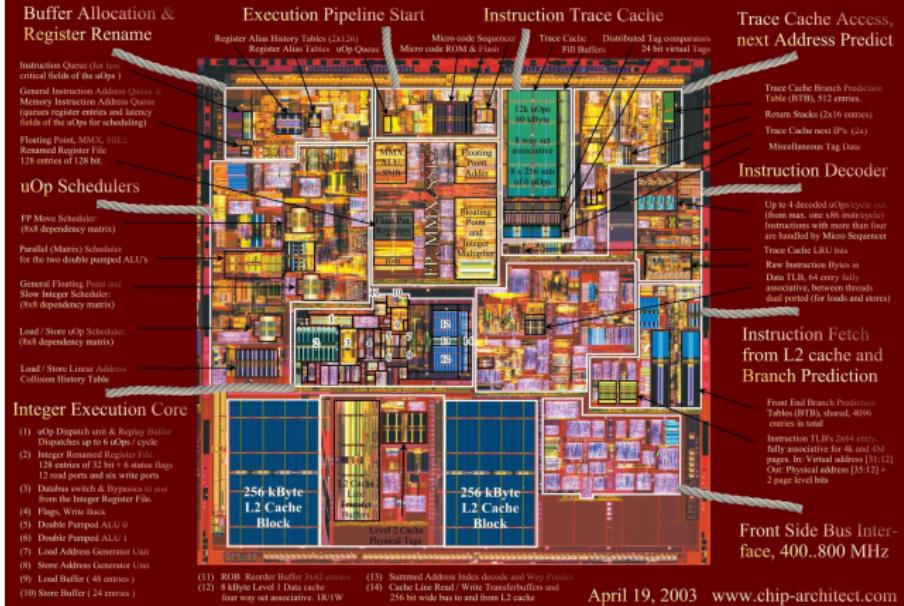
Network Interconnects

Memory & Data Storage

Processors & Accelerators

Processors

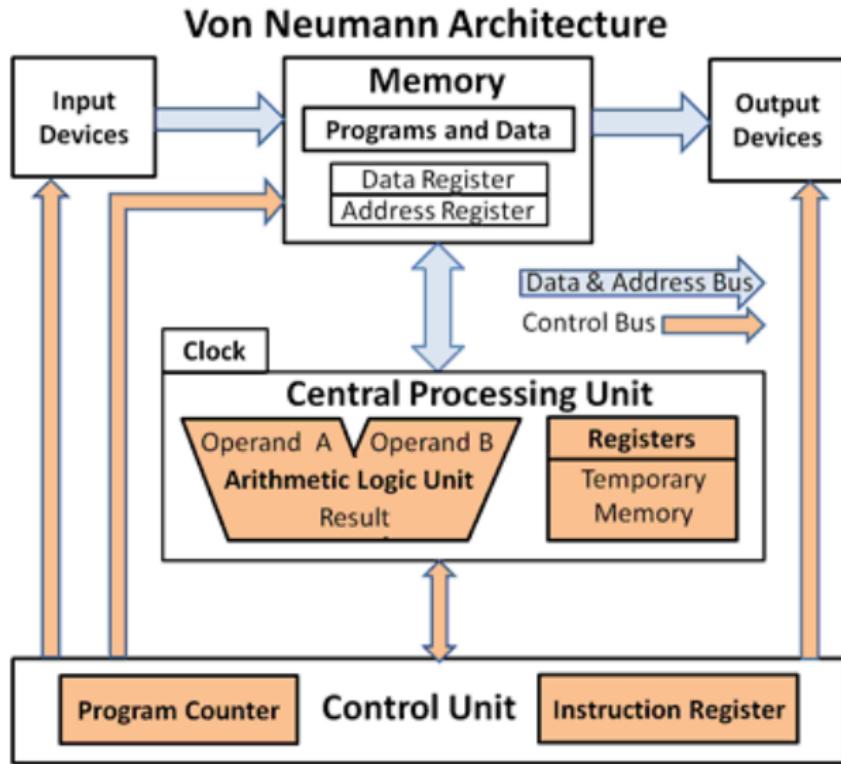
Intel Pentium 4 Northwood



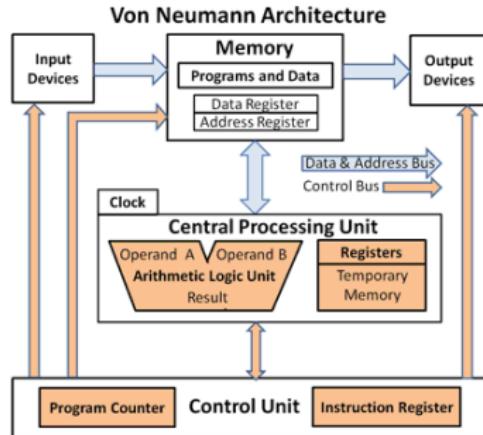
April 19, 2003 www.chip-architect.com



Processors: Basics



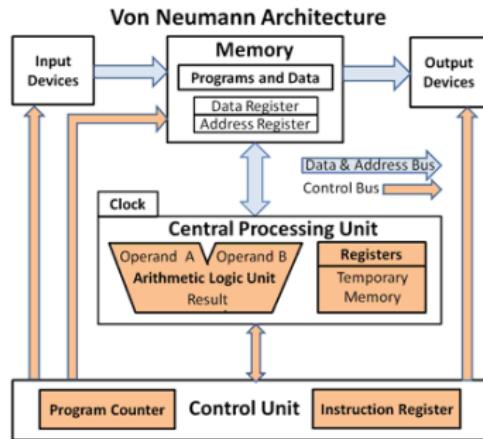
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Control Unit manages the flow and timing of data and instructions through the computer as well as the operations performed by the CPU



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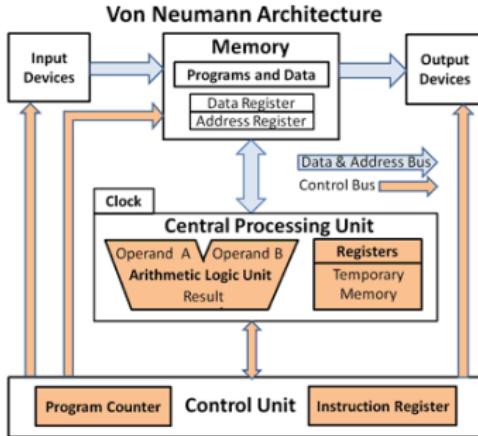


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ALU digital circuit within the processor that performs integer arithmetic and bitwise logic operations

Registers (fastest) memory to store instructions/data used by CPU in this cycle

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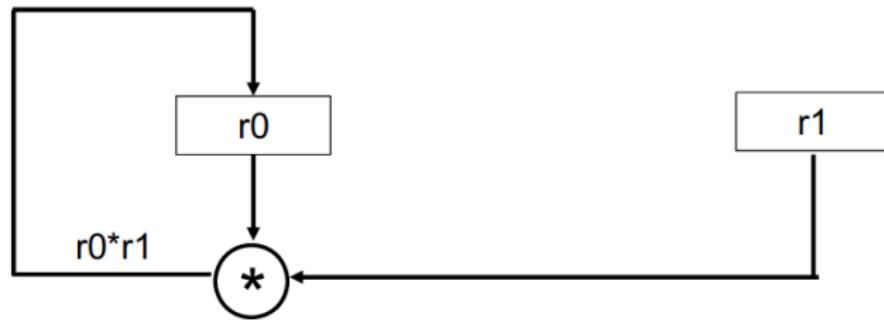
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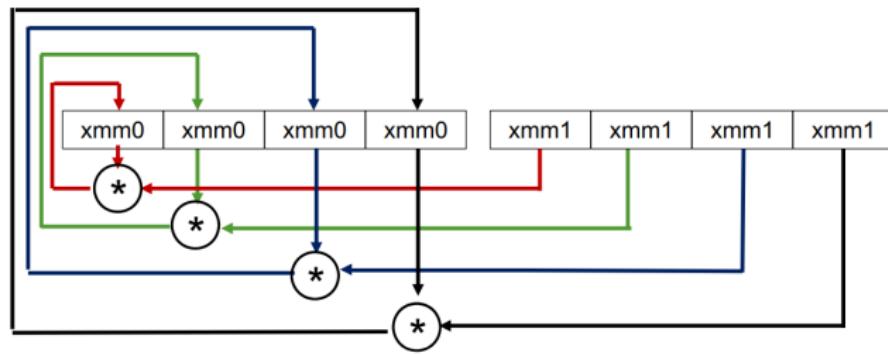
mulss r1, r0



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Processors: Supplementary instruction sets (cont.)

SSE (since Pentium 3) SIMD instruction set for SP floats;
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AVX extension to SSE extensions

AVX2 extension of SSE/AVX operations to 256 bits

AVX-512 extension of SSE/AVX operations to 512 bits (Artemis)

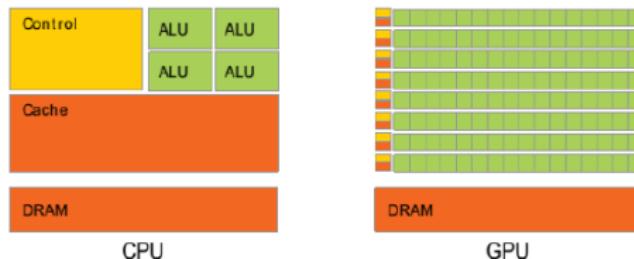
Processors: GPGPUs / SIMT

- processors with reduced instruction set (RISC) for fast execution



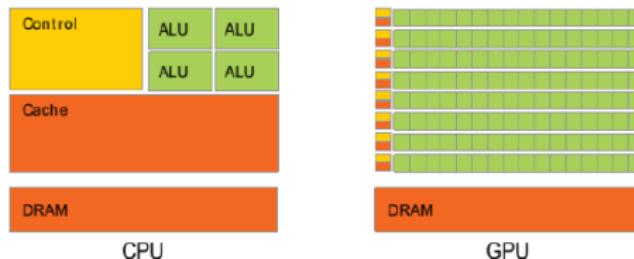
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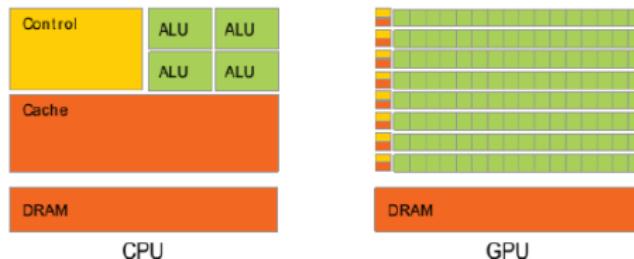


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- horrible for serial code
- require special frameworks for development: e.g. CUDA, OpenCL



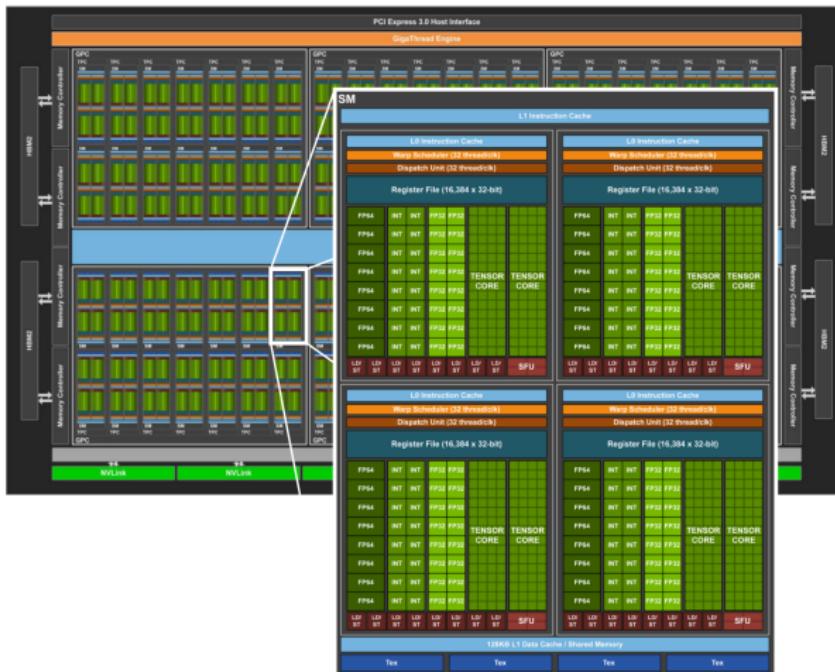
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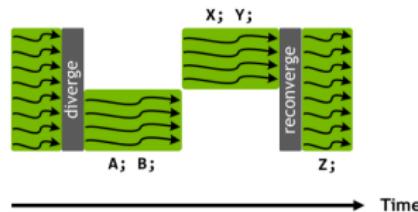
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- 192 SMs (12 GPCs)
x 128 cores per SM
= 24576 cuda cores



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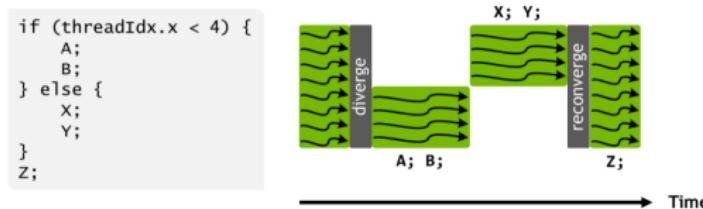
- an SIMT *thread* is a single, independent unit of execution (similar to software multithreading) and grouped into *thread blocks* of up to 1024 threads sharing the same resources of SM
- a thread block is subdivided into *warps* of 32 threads each (to be handled by processing blocks)
- one command executed at same time per warp (other threads waiting)

```
if (threadIdx.x < 4) {  
    A;  
    B;  
} else {  
    X;  
    Y;  
}  
Z;
```

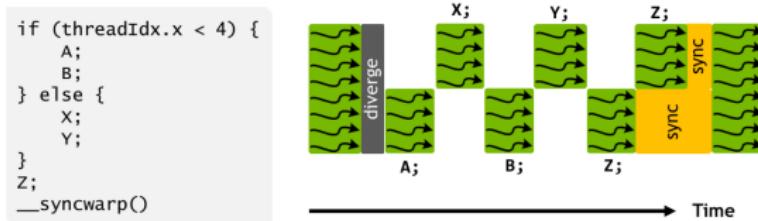


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- newer architecture (\geq Volta) allows for more complex 'divergence'



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- require special frameworks: e.g. TensorFlow for TPUs



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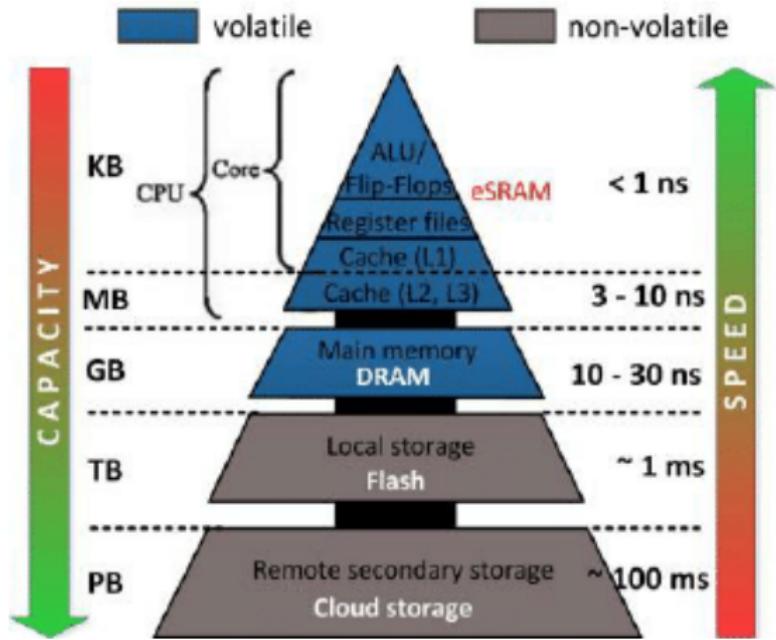
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- on OS/software level, multi-core and multi-CPU systems are equivalent



Memory / Data Storage



Memory: Hierarchy



Memory: Registers & Cache

Registers Fastest memory

(latency: 1 CPU cycle; size: $\mathcal{O}(1 \text{ kB})$)

Level 0 (some arch.) Micro operations cache

(latency: few CPU cycles; size: $\mathcal{O}(1 \text{ kB})$)

Level 1 Data & instruction caches

(latency: few CPU cycles; size: $\mathcal{O}(100 \text{ kB})$; transfer: 700 GB/s)

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Level 2 Shared data & instruction cache

(latency: few CPU cycles; size: $\mathcal{O}(1 \text{ MB})$; transfer: 200 GB/s)

Level 3 Shared cache (also with GFX)

(latency: 3-10 ns; size: few MB/core; transfer: 100 GB/s)

Level 4 (some arch.) Shared cache

(latency: 3-10 ns; size: $\mathcal{O}(100 \text{ MB})$; transfer: 40 GB/s)



Memory: Main Memory / DRAM

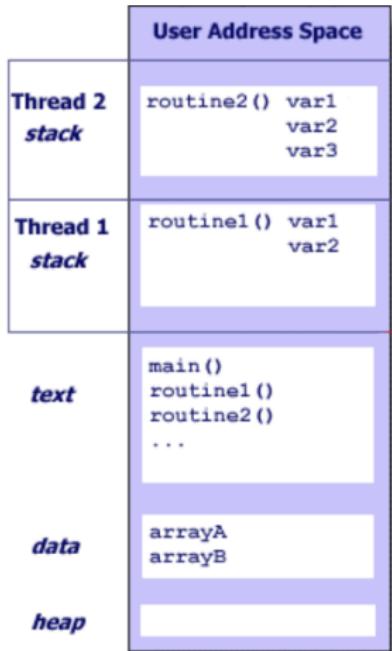
- Fast, volatile memory to hold (all) data and program code for OS and whole software application
(latency: $\mathcal{O}(10 \text{ ns})$; size: $\mathcal{O}(1 \text{ GB} - 1 \text{ TB})$;
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- Accessible/manageable via low-level programming languages (within user address space of application)



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- But may lead to horrible *thrashing* (i.e. constant swapping of pages) if e.g. a working set exceeds the main memory size



Data Storage: Types of Persistent Memory

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- Usually, data centres use a combination: SSDs for e.g. core OS files, swap space), HDDs as main data storage and tapes for backups and "cold" data



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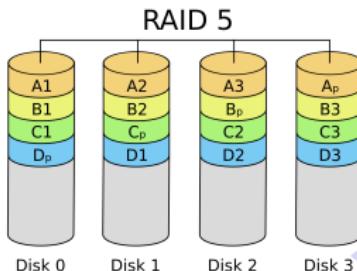
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Software e.g. via distributed file systems (cf. GFS, HDFS)

Hardware RAID - controller combines multiple physical disk drive components into one or more logical units. Depending on level used, by either mirroring whole disks (RAID 1) or spreading over multiple disk with add. parity blocks to ensure operability with (or more) discs failing (RAID 5/6)



Data Transfer / Connectivity



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- Usually data centres employ both in parallel: Ethernet for low-priority/non-critical communication (e.g. logins, remote shells) and InfiniBand for data transfers (from/to file servers or multi-processing message passing (cf. MPI) between nodes)



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 - allows for (relatively) fast data transfer between HPC data centres



Artemis Hardware

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 - ▶ 4 x 128c AMD EPYC, 1TB RAM, 2 A40 Gpu Nodes
 - ▶ 3 x 128c AMD EPYC, 512TB RAM, 2 A40 Gpu Nodes

Artemis Hardware: Storage

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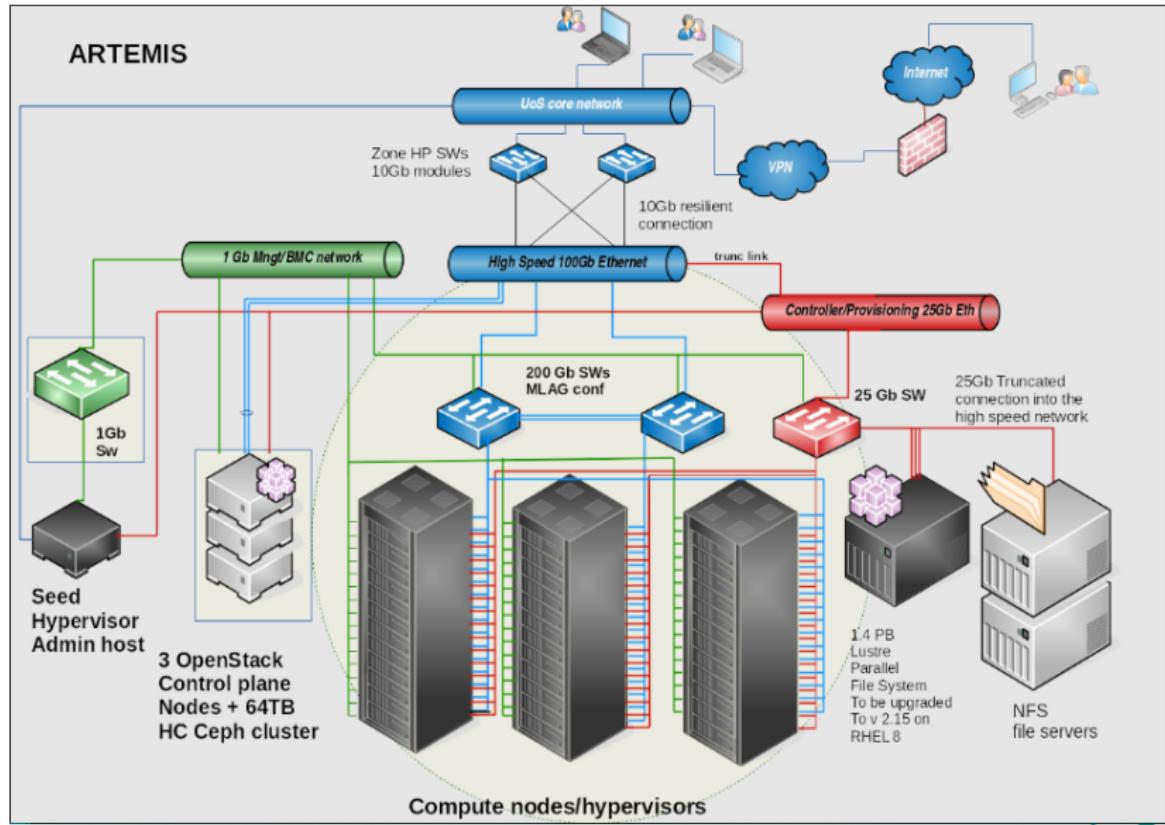
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- additionally, experimental support for google drive cloud storage

Artemis Hardware: Network



HPC stack

SOFTWARE

Environments & Applications

SYSTEM SOFTWARE

Resource & Job Management

Runtime System Interprocess Comm

Operating System

VIRTUALISATION

Cloud computing / OpenStack

HARDWARE

Network Interconnects

Memory & Data Storage

Processors & Accelerators