INTRODUCTION TO HPC
MAELSTROM BOOTCAMP JÜLICH

27 September 2022 | Dr. Andreas Herten | Forschungszentrum Jülich, MAELSTROM

Outline

*What is **HPC**?*

High Performance Computing *is computing with a powerful machine using the available resources efficiently.*

My interpretation.

Baseline

- What kind of CPU does your computer have?
  CPU generation, clock ~~speed~~ rate, number of cores, vector length

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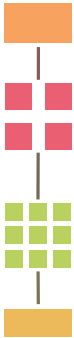

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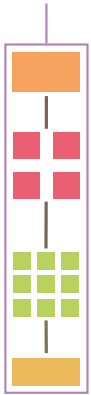
  Throughput, latency



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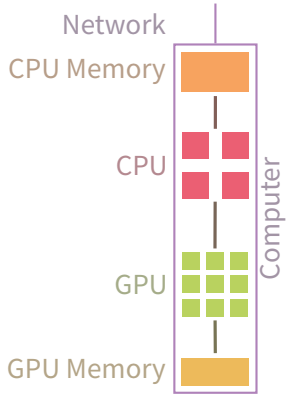
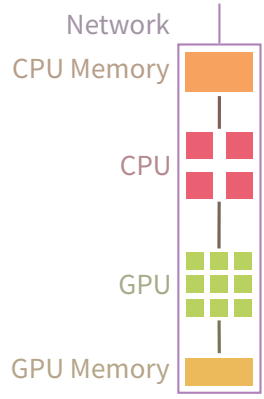
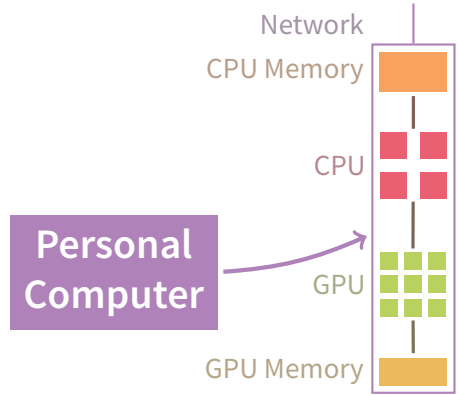



Network
CPU Memory
CPU
GPU
GPU Memory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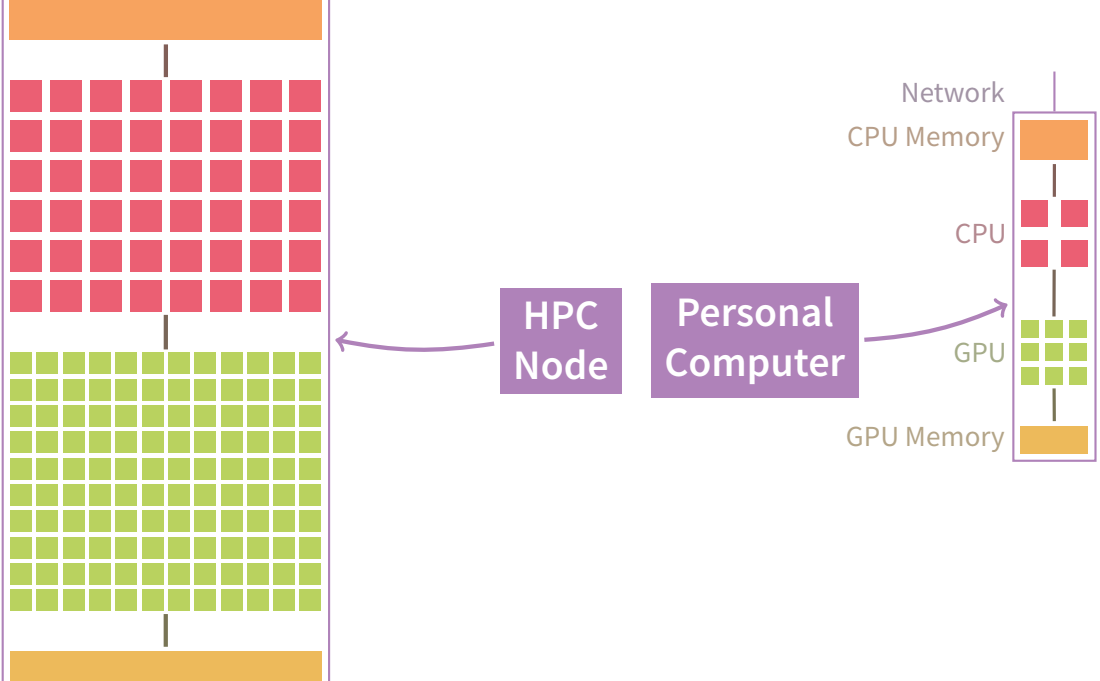
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HPC Node
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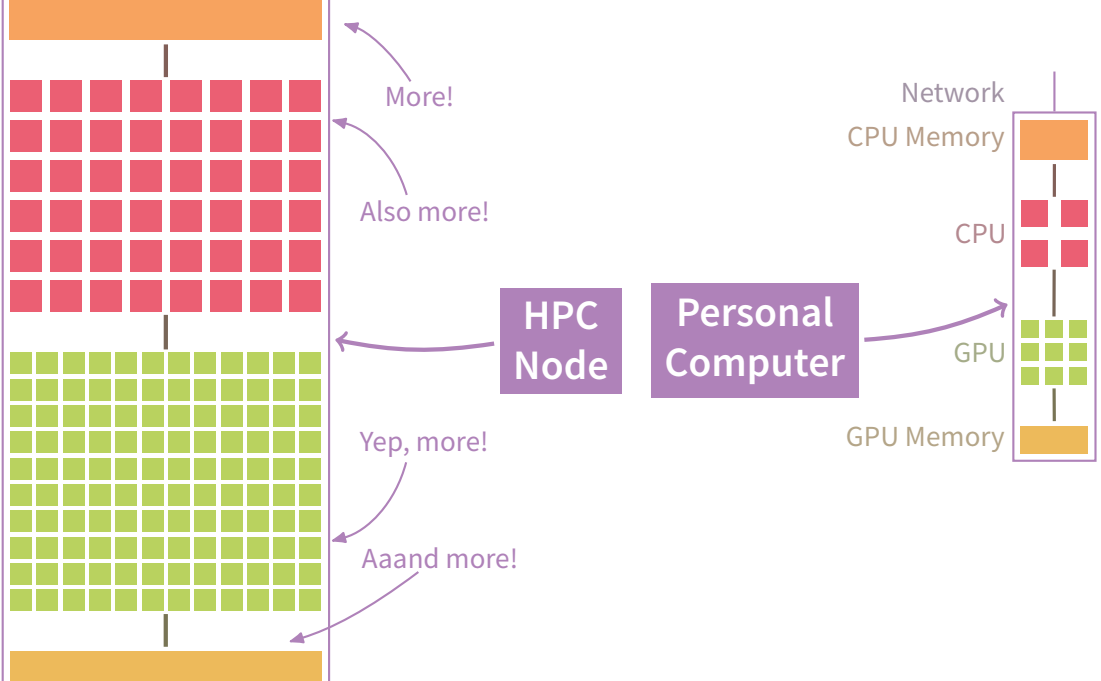
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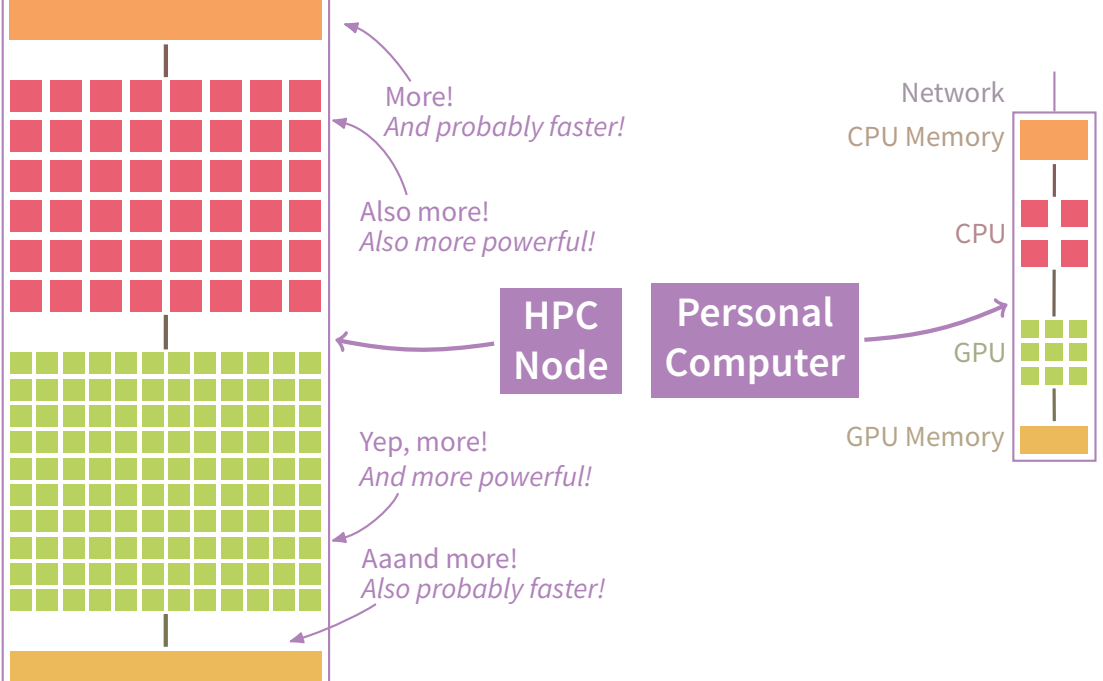
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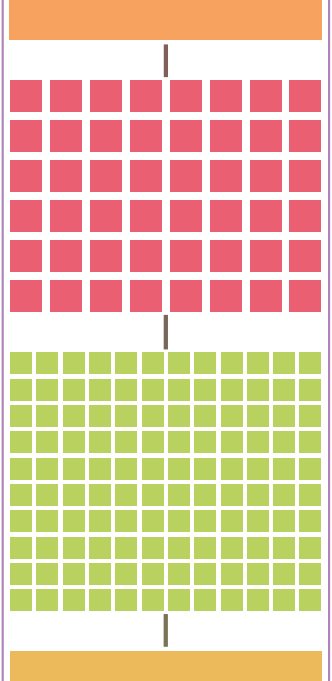
HPC
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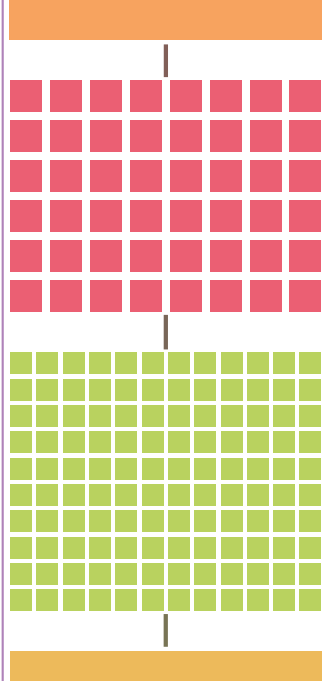
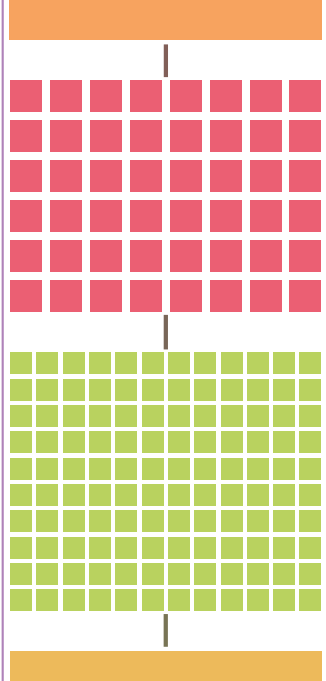


CPU 64 cores, 2.2 GHz, 2× multi-threading, large caches, advanced instructions, 220 W TDP

HPC Node

Specs based on JURECA DC



Memory 1 TB size, DDR4, 3200 MHz rate, 190 GiB/s bandwidth

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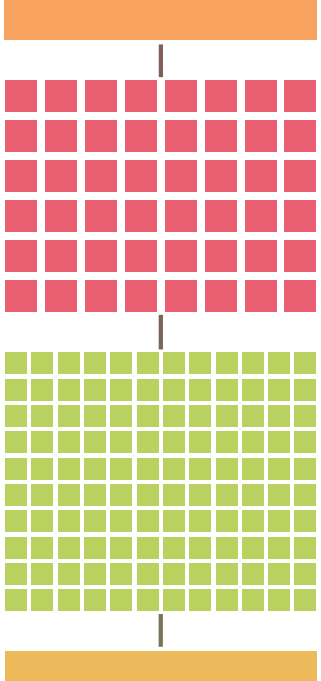

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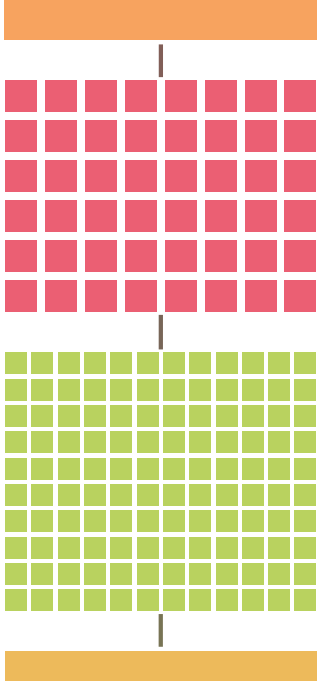

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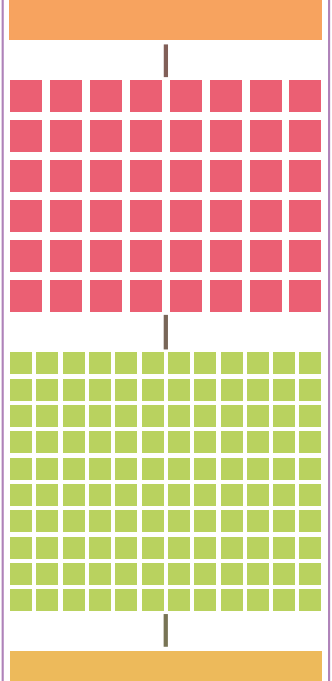
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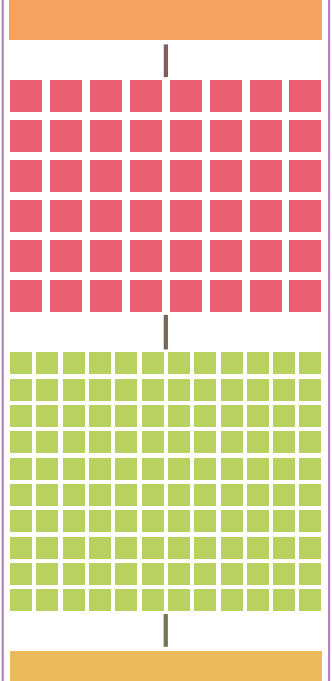

HPC Node

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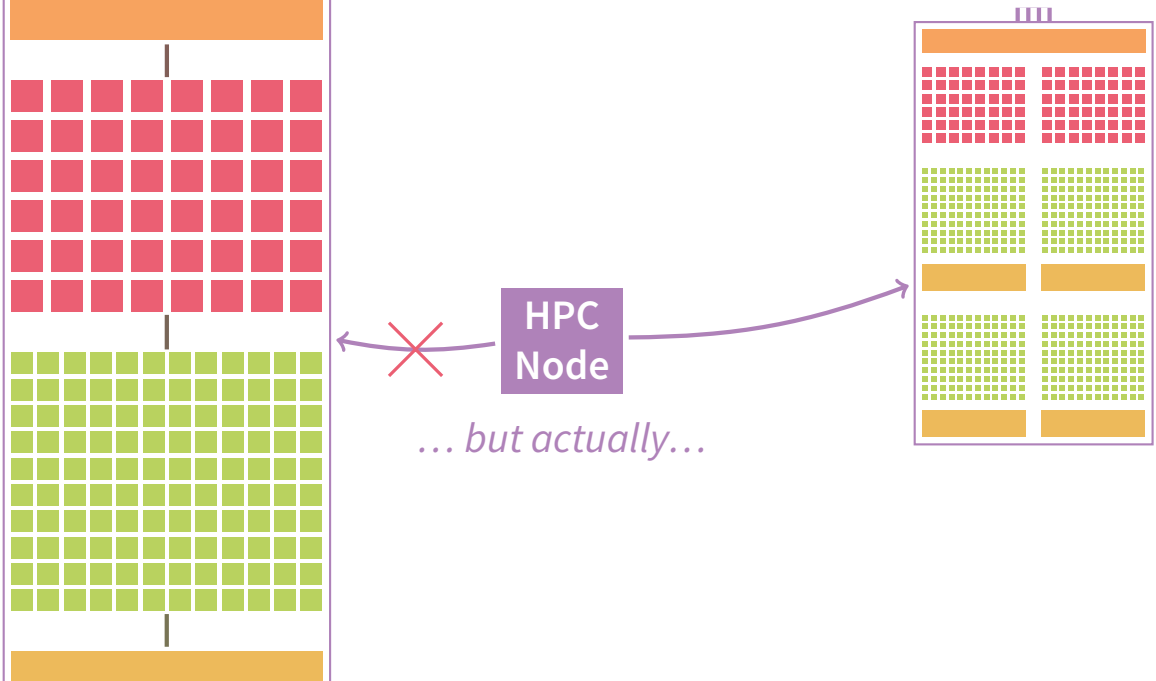
HPC
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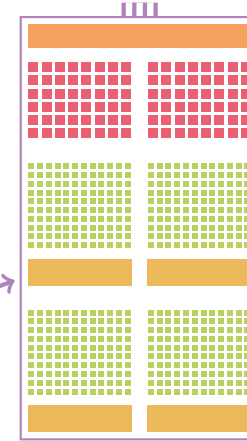
… but actually…

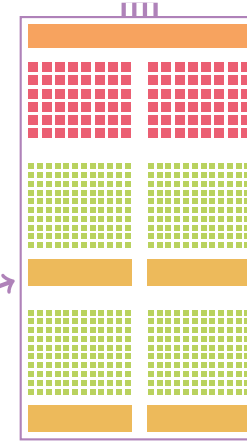
- Usually, 2 CPUs **sockets**, each with 64 cores; use mostly as one CPU with one memory
- 4 distinct GPUs, connected with each other (600 GB/s)
- 4 network connections, each 200 Gbit/s in each direction (*InfiniBand HDR-200*)

HPC Node



Specs based on JURECA DC, JUWELS

HPC Node



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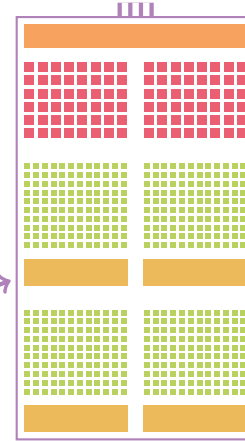
HPC Nodes



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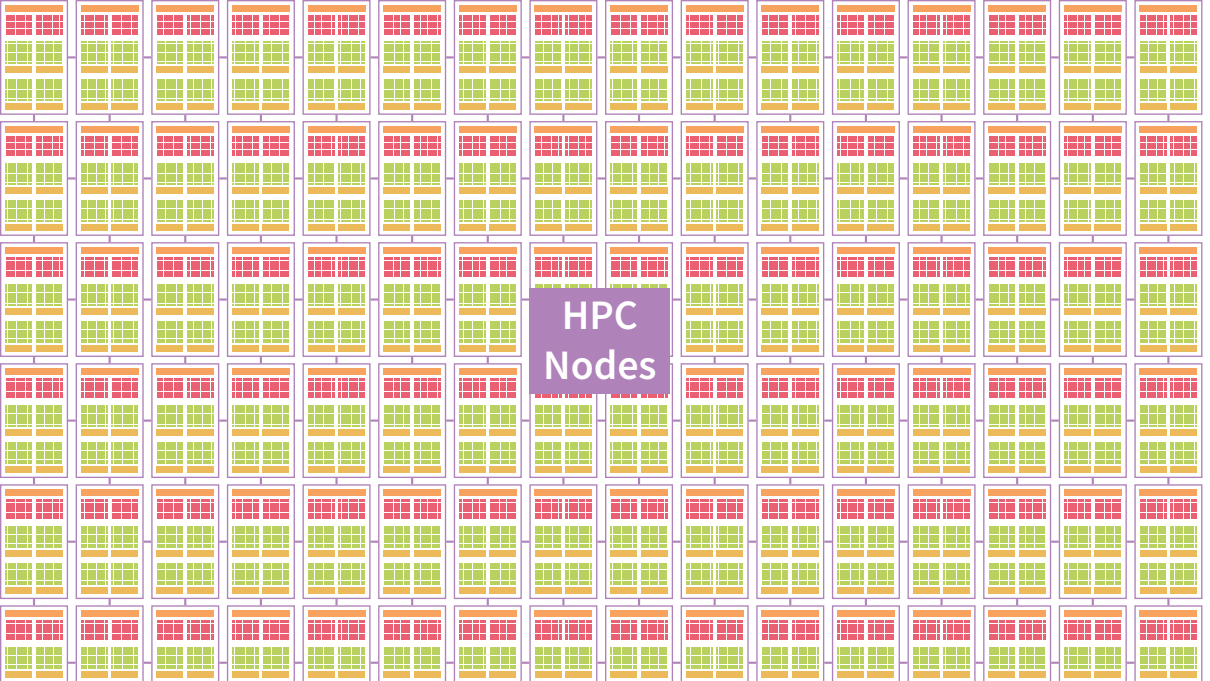
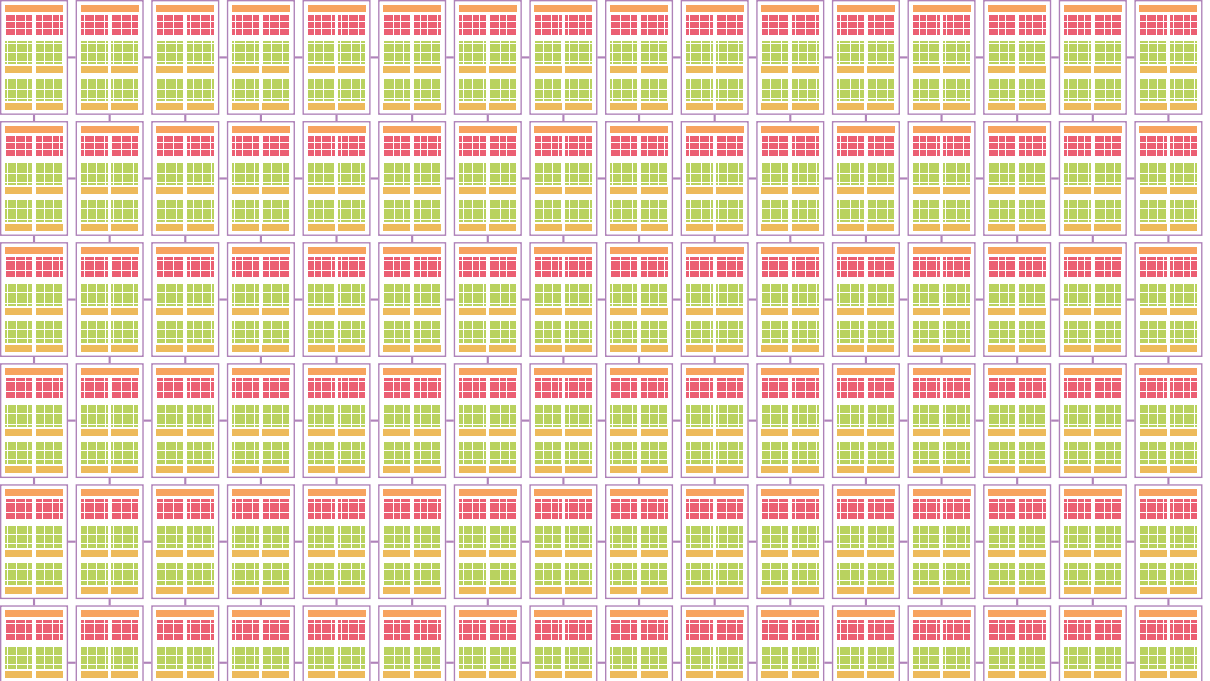
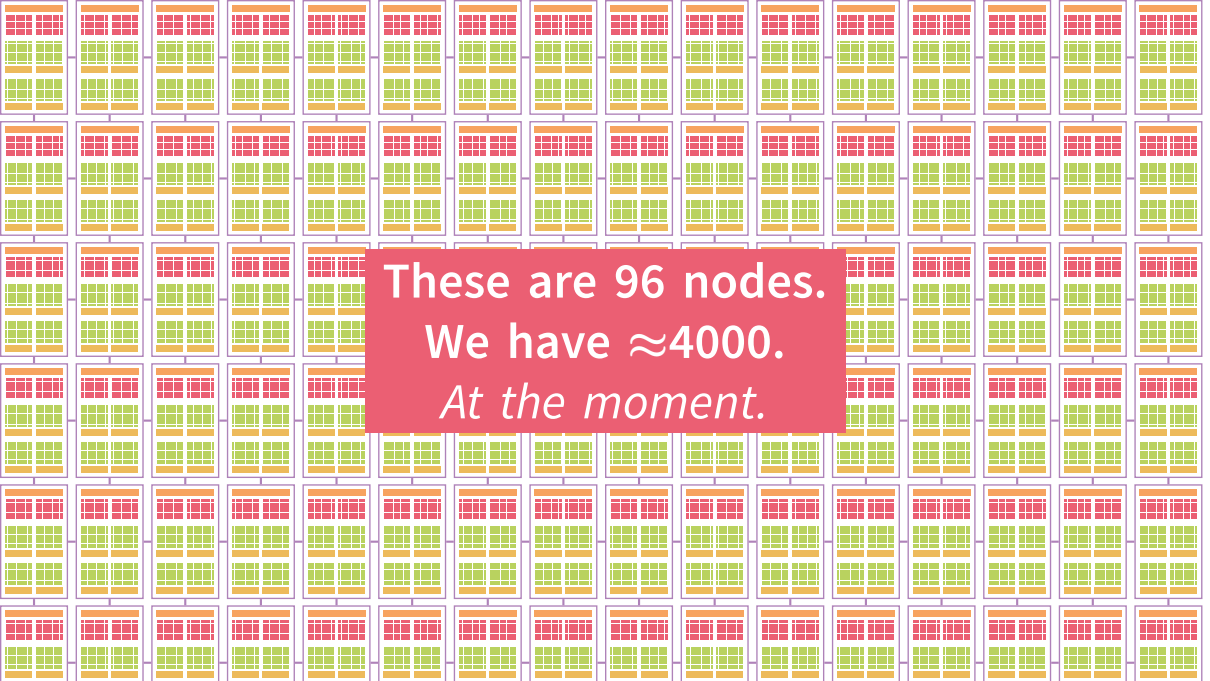

HPC
Nodes




These are 96 nodes.
We have ≈4000.
At the moment.

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Powerful Machines

Now

- Powerful nodes (large CPUs, accelerating GPUs, much memory)
- Many nodes (well-connected through high-speed interconnect)

→ **Beefed-up versions of commodity computers, with slight specializations; many**

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Past

- First computers: Supercomputers! Mainframe machines: Large installations with most powerful hardware at the time
- PC era: Even then, specialized computers, like vector machines, or many low-speed CPUs (well-connected)
- Recent history: x86, then PowerPC, then GPU accelerators, then specialized Arm CPUs

Supercomputers in Pictures

- CDC 6600 supercomputer
- Around 1965
- First supercomputer
- 3 MFLOP/s
- See Wikipedia for more
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HPC performance measured in **FLOP**/s.

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Supercomputers in Pictures

- Cray-1 supercomputer
- Around 1978
- Very successful
- 160 MFLOP/s
- Probably pictured at NERSC

Supercomputers in Pictures

- Intel XP/S 140 supercomputer
- Around 1994
- 3680 Intel i860 RISC processors; large-scale parallel system
- 143 GFLOP/s
- Picture by top500.org

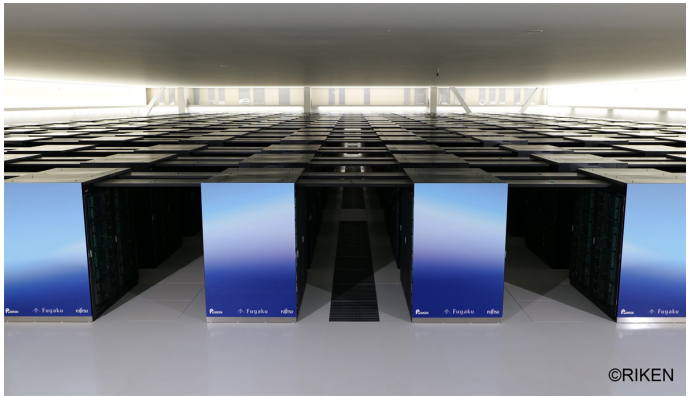
Supercomputers in Pictures

- JUGENE supercomputer
- 2008
- 294 912 PowerPC 450 cores; energy-efficient
- 800 TFLOP/s
- Picture by top500.org

Supercomputers in Pictures

- Summit supercomputer
- 2018
- 27 000 GPUs hosted by POWER9 CPUs; first #1 GPU supercomputer
- 200 PFLOP/s
- Picture by Oak Ridge National Lab

Supercomputers in Pictures



- Fugaku supercomputer
- 2020
- 7 630 848 Arm A64FX cores; #1 supercomputer
- 537 PFLOP/s
- Picture by RIKEN

JUWELS Cluster – Jülich's Scalable System

- 2500 nodes with Intel Xeon CPUs (2×24 cores)
- $46 + 10$ nodes with 4 NVIDIA Tesla V100 cards (16 GB memory)
- 10.4 (CPU) + 1.6 (GPU) PFLOP/s peak performance (Top500: #86)

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

Top500 List Nov 2021:

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

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- Over last 15 years, extended from rendering to variable computing
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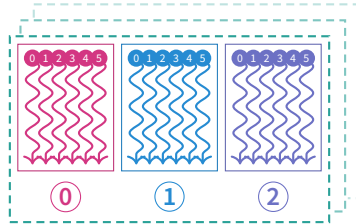

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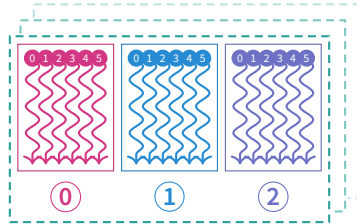

Pictures by NVIDIA [8]

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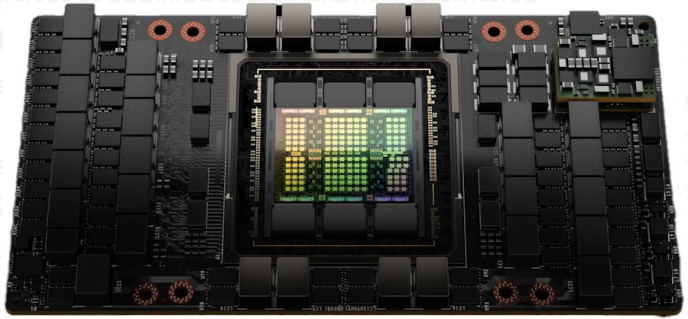

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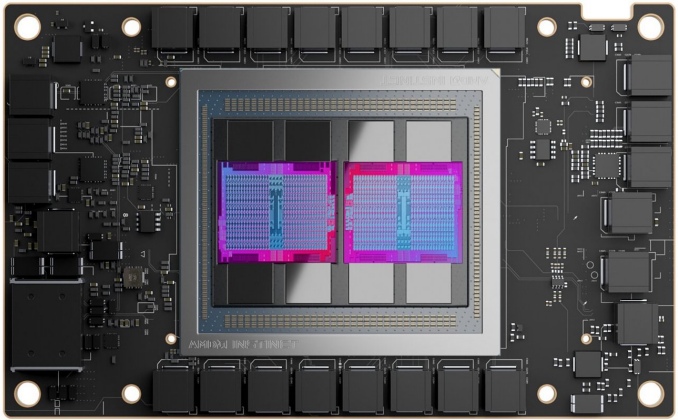

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Resource Utilization

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Exploit all capabilities of processing entity (*core*)

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Parallelize to all processing entities of node

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Parallelize to all processing entities of node

Distribute to all nodes

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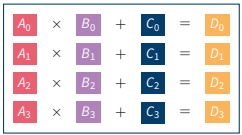

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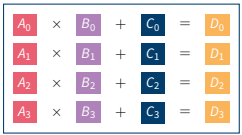

× 4 multiplications
\+ 4 additions
= 4 assignments
→ 8 instructions

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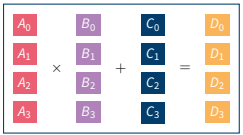

× 4 multiplications
\+ 4 additions
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→ 8 instructions

SIMD →

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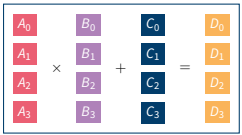

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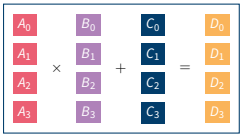

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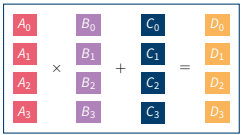

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CPU Instruction: VFMADD132PD

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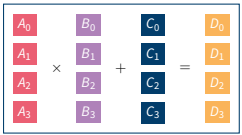

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Compiler!

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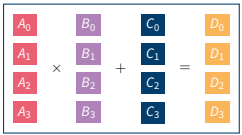

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Improve throughput!

FMA SIMD →
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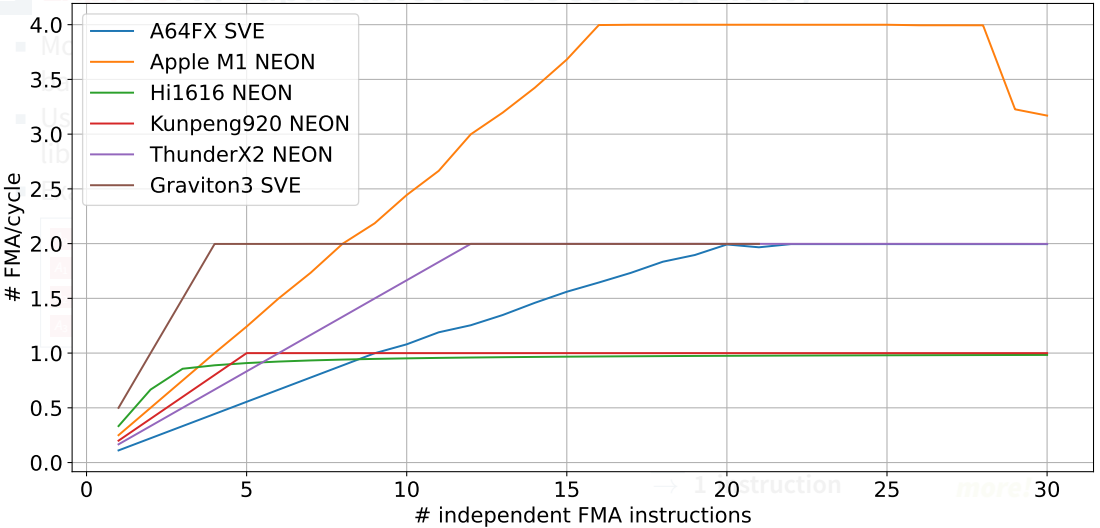
Compiler!

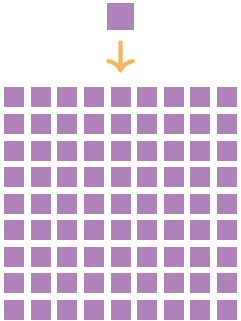
Improve throughput more!

Analysis/plot by Stepan Nassyr, 2022.



2 Parallelize to All Processing Entities of Node

- From core to cores



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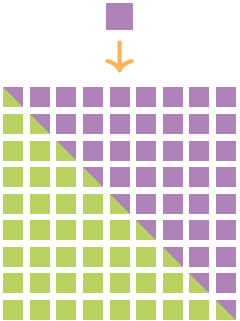
- From CPU cores to GPU *cores*



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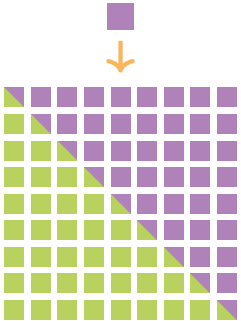

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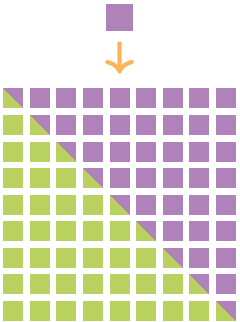
CPU Mostly through operating system capacities

- OS *threads* launched on *cores*
- Easiest threading interface: OpenMP

```
#pragma omp parallel for
for (int i = 0; i < N; i++) y[i] = x[i] * 3.14 + a[i];
```



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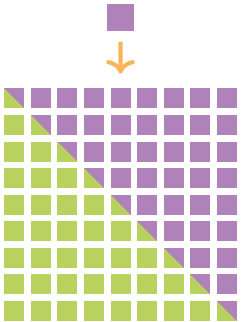

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GPU Through dedicated programming environments

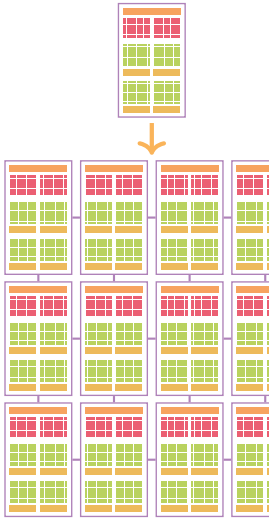
- Mostly, explicit models

```
int i = threadIdx.x + blockIdx.x * blockDim.x;
y[i] = x[i] * 3.14 + a[i];
```

- Also, higher-level models (OpenMP, OpenACC)

3 Distribute to All Nodes

- From node to node**s**



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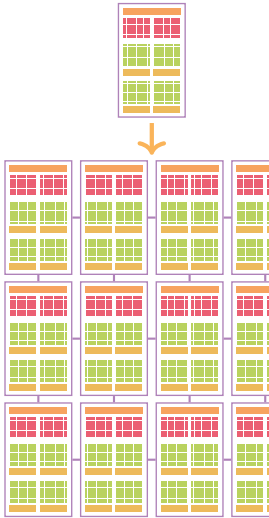
- **Distribution**: Tasks work on portion of full problem using distributed memory; *coarse-grained* split



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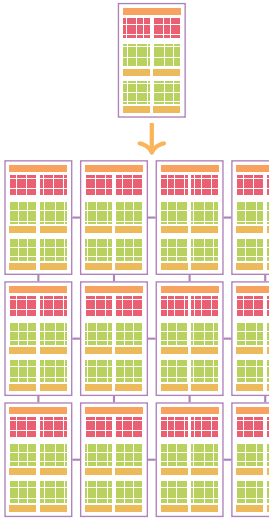
- Every task runs on own node with copy of program, defined exchange functions
- High-speed network important! GPUs directly attached to network



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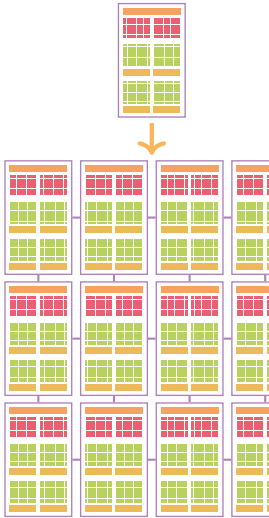
- Classical programming model: MPI

```
MPI_Comm_size(MPI_COMM_WORLD, &size);
MPI_Comm_rank(MPI_COMM_WORLD, &rank);
MPI_Send(buffer, 10, MPI_INT, 1, 555, MPI_COMM_WORLD);
MPI_Allreduce(local_sum, global_sum, 1, MPI_FLOAT, MPI_SUM,
↪    MPI_COMM_WORLD);
```



The Gateway Heroes of HPC

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Compilers

CPU GCC, LLVM, Intel, Cray

GPU + NVIDIA CUDA, NVHPC, AMD

- Long history, constantly evolving

Frameworks

MPI OpenMPI, MPICH

Threads pthreads, OpenMP

GPU CUDA, HIP, SYCL, pSTL, Kokkos

Libraries

CPU MKL, BLIS, FFTW

GPU cuBLAS, rocBLAS, cuDNN

→ TensorFlow, PyTorch, ELPA

High Performance Computing *is computing with a powerful machine using the available resources efficiently.*

My interpretation.

Conclusion

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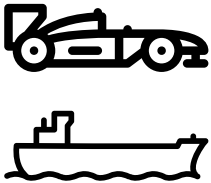
- HPC is intensive computing with largest machines
- Sometimes like Formula 1, sometimes like a tanker
- Sophisticated hardware is underlying everything, delivering up to 1.1 EFLOP/s
- Advanced software holds everything together and enables science at the frontiers



Images by lastspark and Dmitry Podluzny from Noun Project.

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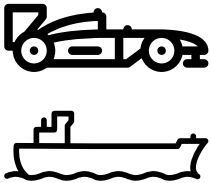

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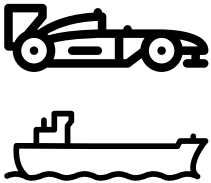

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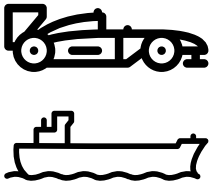
- We are hiring!
  go.fzj.de/jsc-jobs



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Thank you for your attention!

a.herten@fz-juelich.de

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Appendix

Appendix

- License
- References

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References: Images, Graphics I

[1] Forschungszentrum Jülich GmbH (Ralf-Uwe Limbach). *JUWELS Booster*.

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