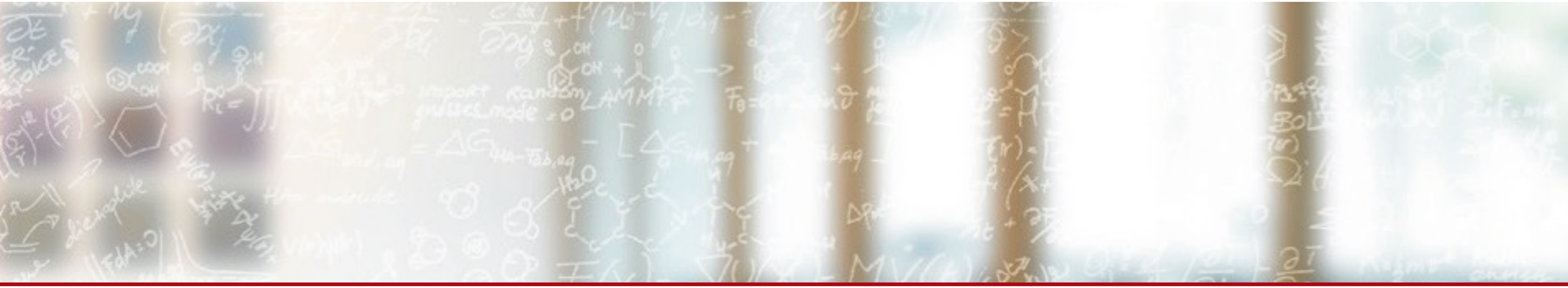
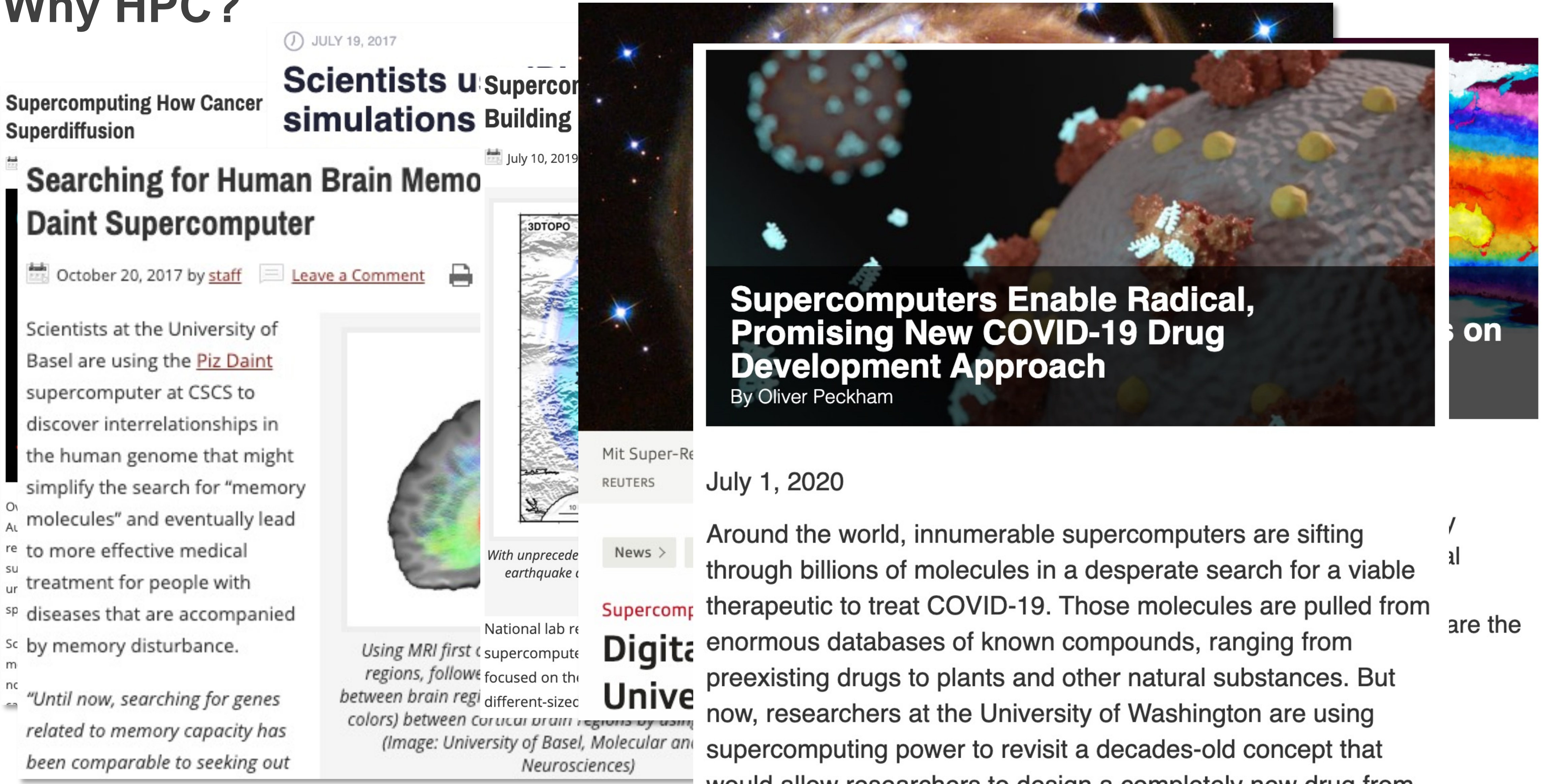


Introduction to High Performance Computing

CSCS-USI Summer School 2021
Vasileios Karakasis, CSCS
July 19, 2021

https://github.com/eth-cscs/SummerSchool2021

Why HPC?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July 10, 2019
Searching for Human Brain Memo
Daint Supercomputer
October 20, 2017 by staff
Leave a Comment
Scientists at the University of Basel are using the Piz Daint supercomputer at CSCS to discover interrelationships in the human genome that might simplify the search for “memory molecules” and eventually lead to more effective medical treatment for people with diseases that are accompanied by memory disturbance.
“Until now, searching for genes related to memory capacity has been comparable to seeking out
Using MRI first
regions, followe
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(Image: University of Basel, Molecular and
Neurosciences)
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Supercomputers Enable Radical, Promising New COVID-19 Drug Development Approach
By Oliver Peckham
July 1, 2020
Around the world, innumerable supercomputers are sifting through billions of molecules in a desperate search for a viable therapeutic to treat COVID-19. Those molecules are pulled from enormous databases of known compounds, ranging from preexisting drugs to plants and other natural substances. But now, researchers at the University of Washington are using supercomputing power to revisit a decades-old concept that would allow researchers to design a completely new drug from
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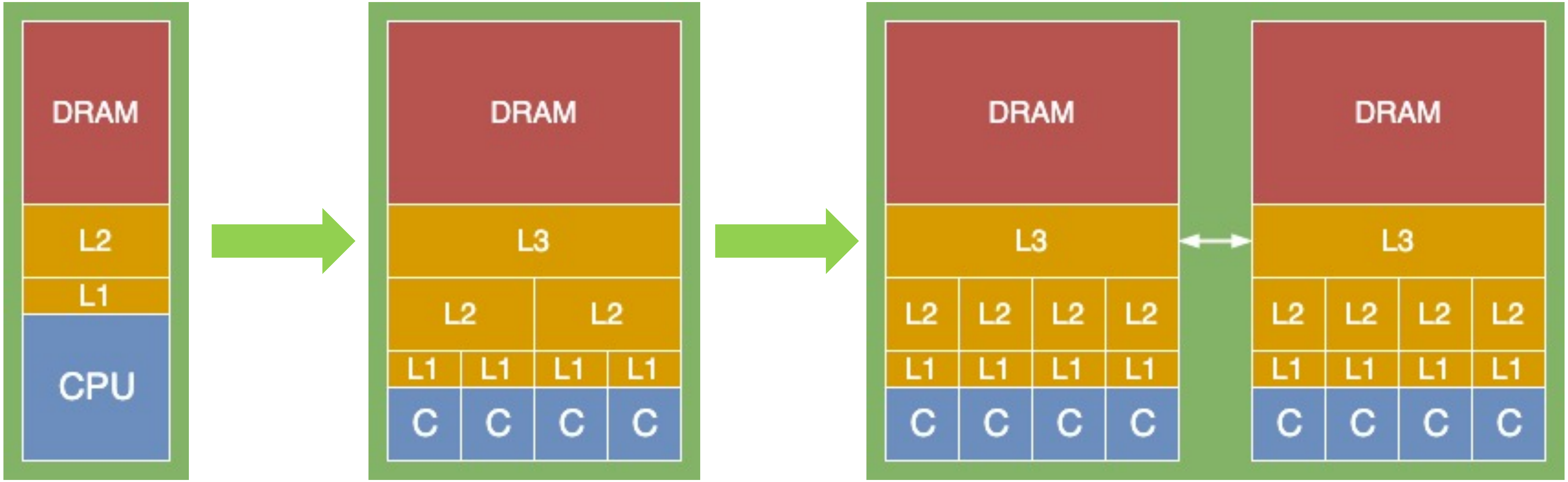
Why HPC?

- Complex workloads
  - Computationally intensive algorithms
  - Latency-sensitive, high communication needs
  - Heavy post-processing of data
  - Machine learning and AI
  - Demanding visualization processes
- Huge amounts of data
  - Efficient stage-in and stage-out of data
  - Checkpointing
  - Parallel reading and writing to filesystem at high speeds

- Sophisticated solutions are required; No. 1 requirement is **high performance**
  - Processors and memory subsystem
  - Interconnection networks and communication protocols
  - Storage and filesystems
  - Libraries, Software, Applications

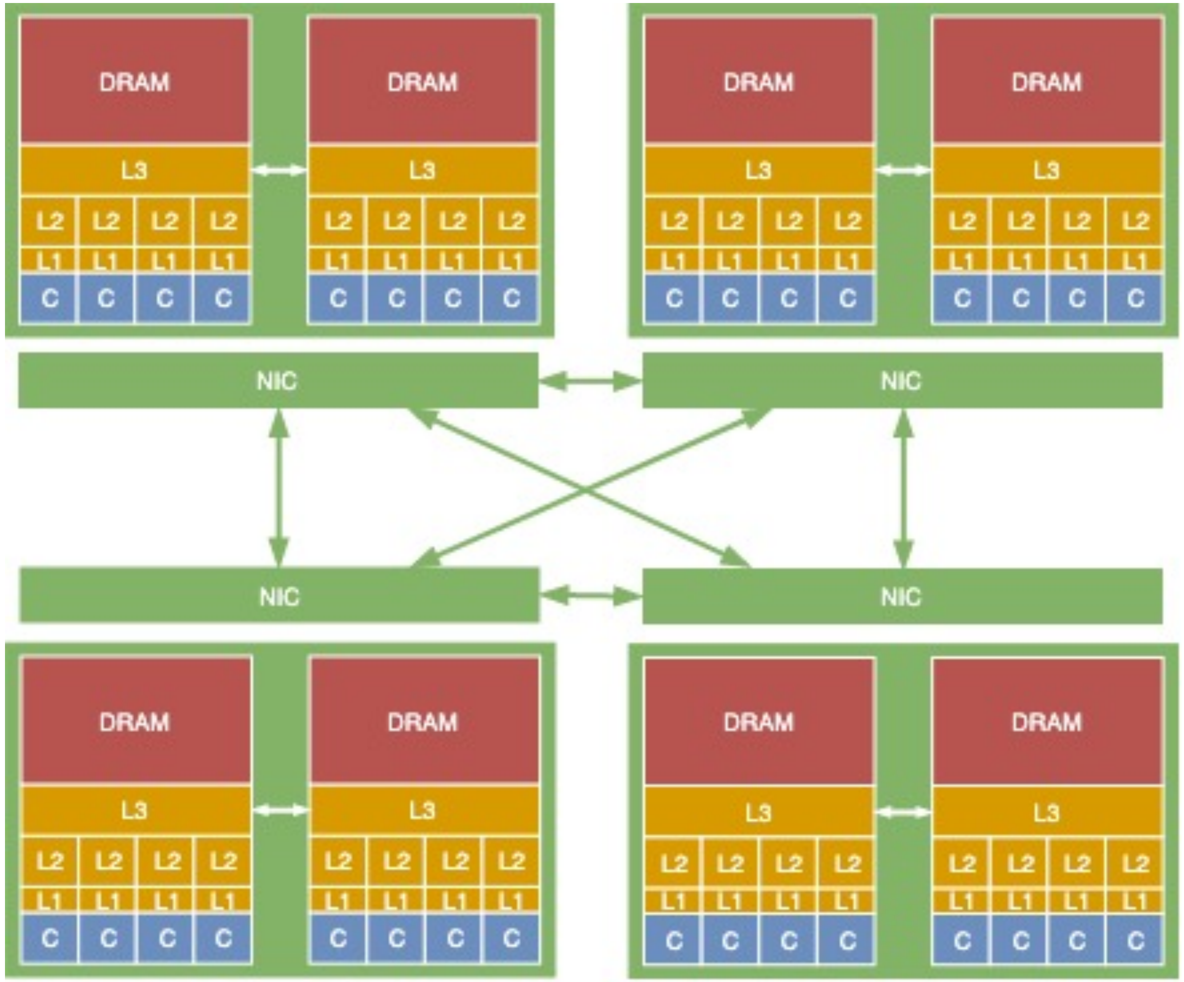
Building blocks for HPC systems: the CPU



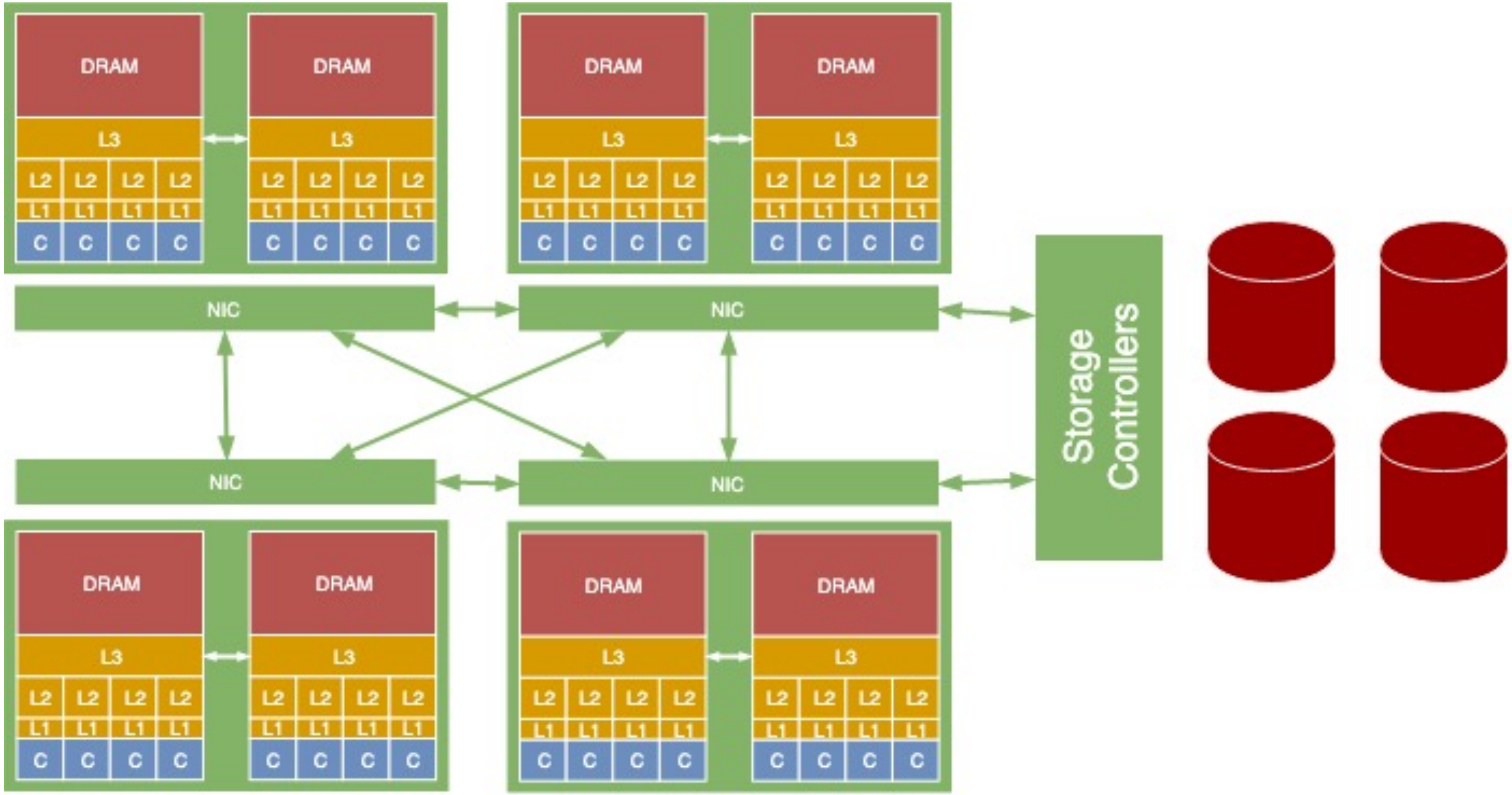
Single-core | Multicore SMP | Multicore NUMA

SMP: Symmetric Multi-Processor
NUMA: Non-Uniform Memory Access

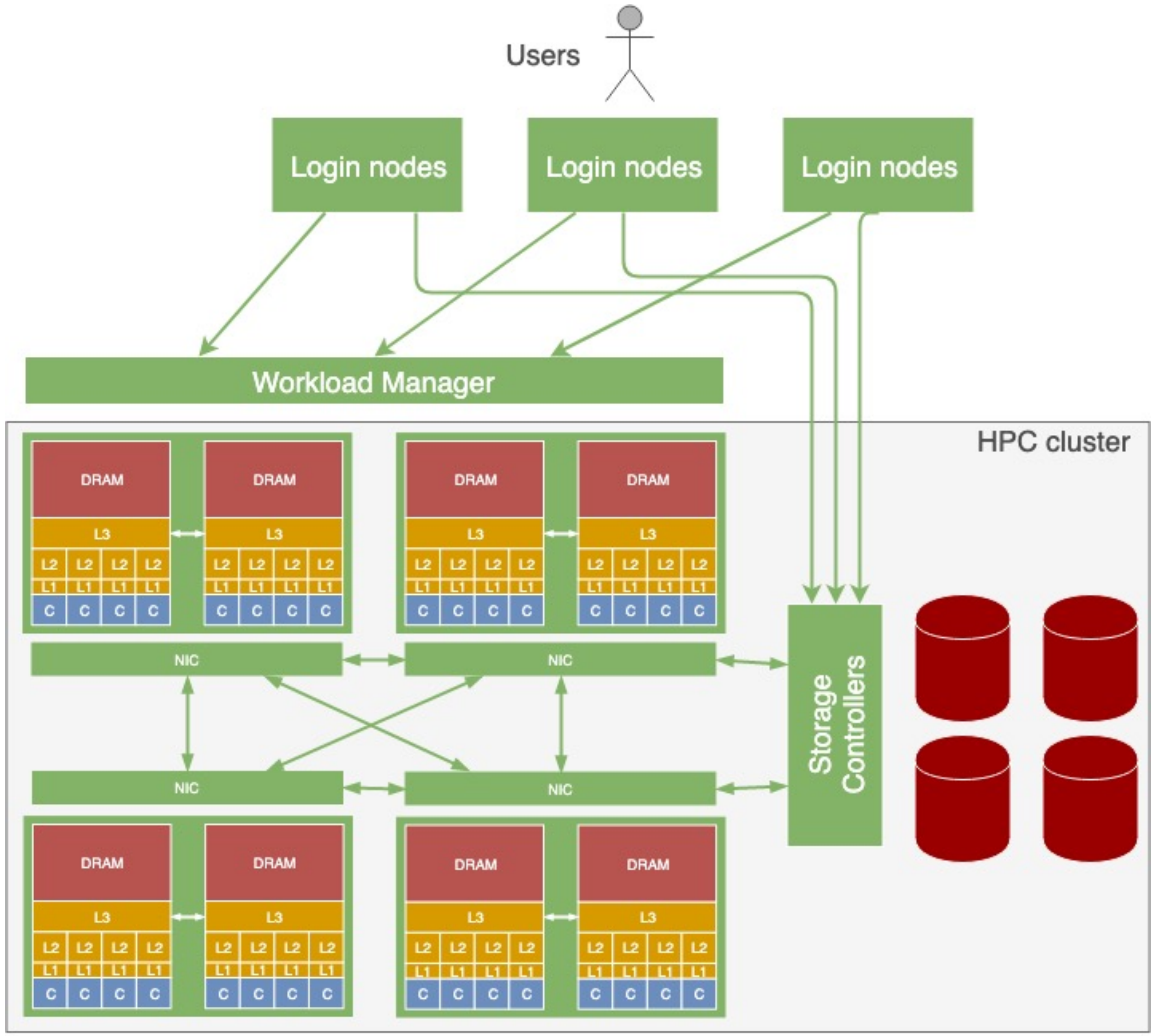
Building blocks for HPC systems: the network



Building blocks for HPC systems: the storage



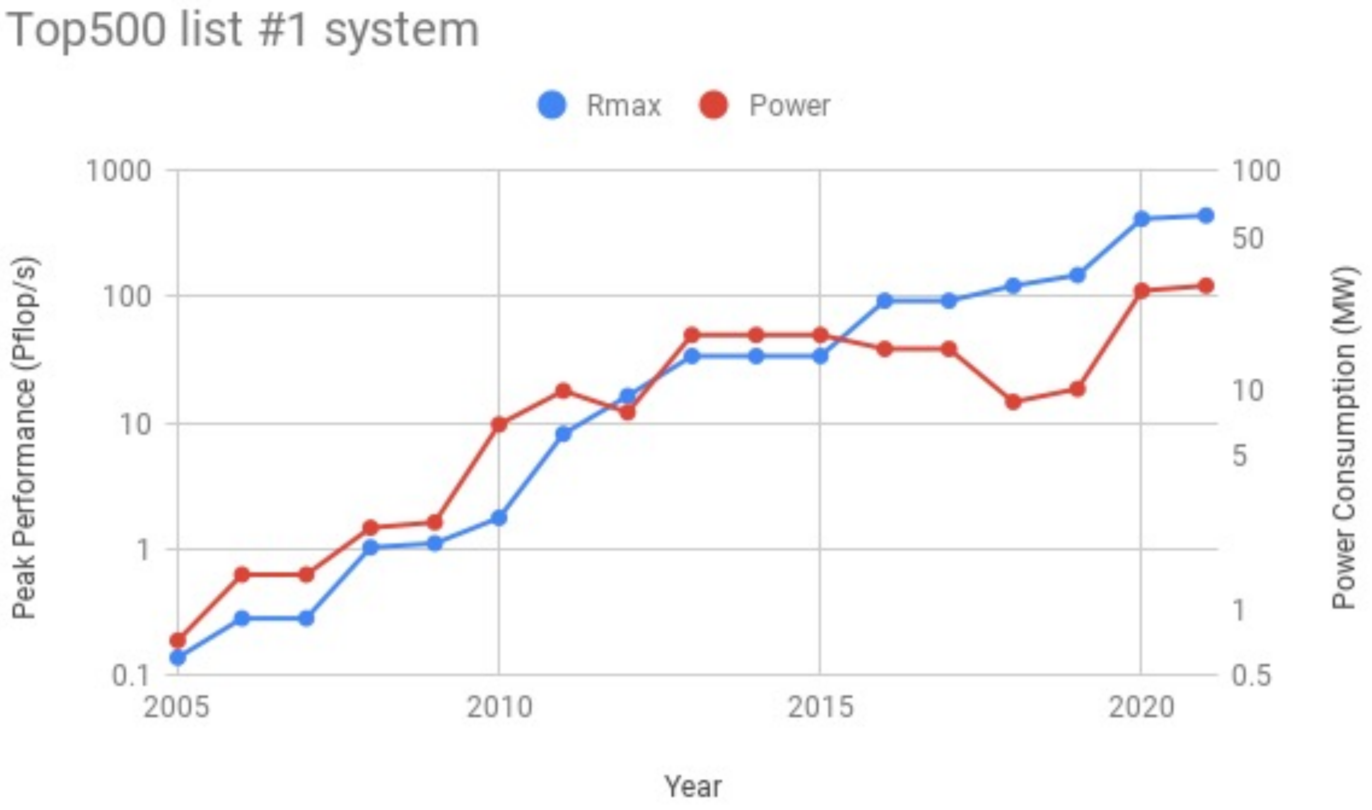
Building blocks for HPC systems: login nodes & workload manager



Issues and limitations

- HPC systems are expensive!
  - Power costs
  - Cooling and infrastructural costs
  - Technology costs
    - High-end processors
    - Fast, low-latency networks
    - Fast storage
    - ...

Performance and power consumption evolution

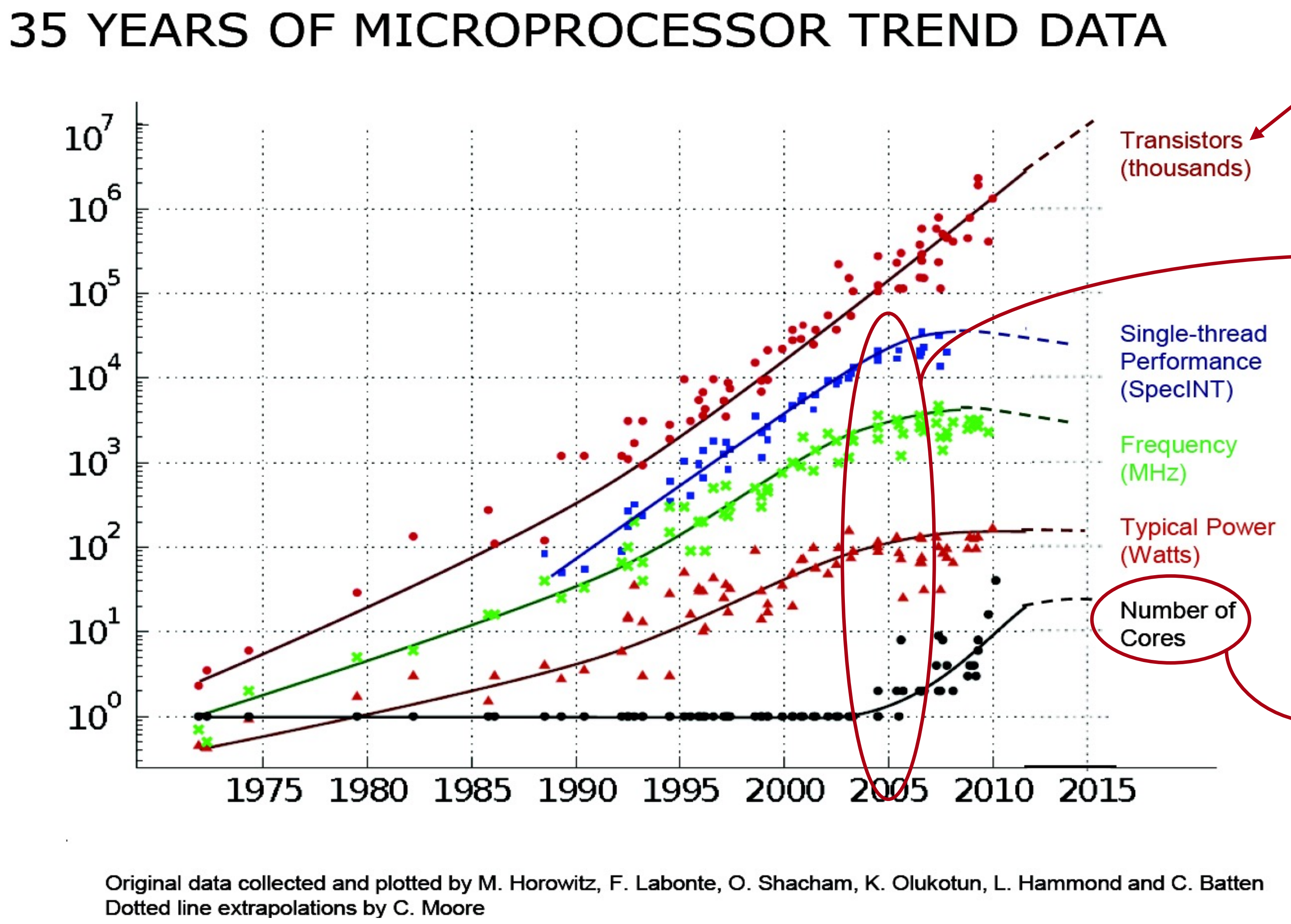


Power consumption has been following closely the exponential growth in performance, but at a lower rate.

Exascale is now before us!

- Already reached in AI workloads

How did we reach here?



Transistor count doubles every 18 months, Moore's Law

The Power Wall

- Power dissipation of single-core processors becomes prohibitive
- The "Free Performance Lunch" of frequency scaling is over!

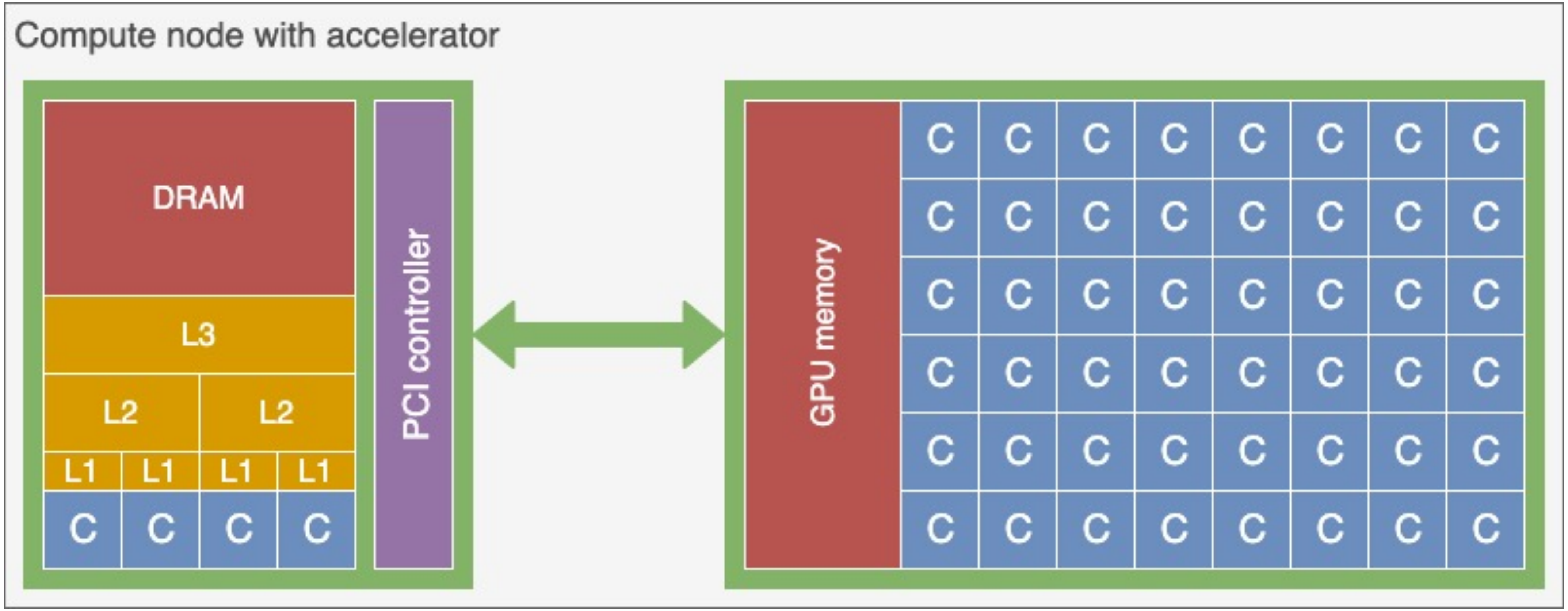
Performance can only grow through node-level parallelism!

Beyond multicores

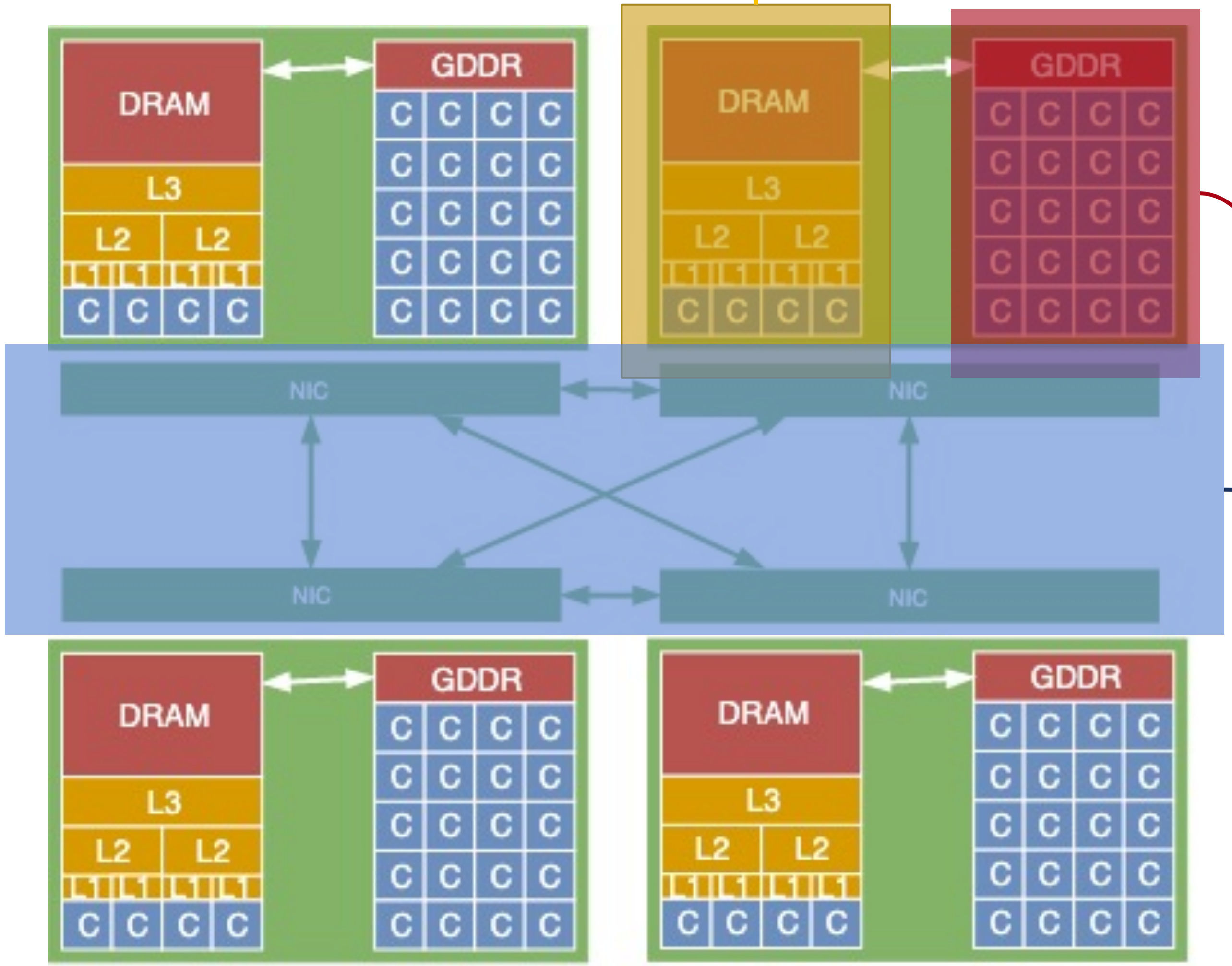
- Multicores have limitations
  - Fat cores (branch prediction, out-of-order execution, large caches)
    - Optimized for latency and multiprocessing
  - Still high frequencies
  - Still high power consumption
  - But programming is easy; matches better our brain’s serial way of thinking

- Accelerators are taking the opposite direction
  - Low frequencies, thus lower power consumption
  - Die area dedicated to processing units rather than control or caches
  - Suitable for very specific workloads; not for general-purpose tasks
  - Programming not so straightforward; we must think “parallel” now

Accelerators in a HPC system



How do we program for HPC?



Shared memory: OpenMP, Task-based, POSIX threads, etc.

GPUs: CUDA, OpenACC, OpenMP, OpenCL, etc.

Distributed memory: MPI, Fortran coarrays, UPC, Charm++, etc.

Piz Daint

- Cray XC40/XC50 system
  - Top500: #15 in the world, #4 in Europe
- 5320 XC50 nodes
  - 1x 12-core Haswell (64 GB DRAM) + 1x Nvidia Tesla P100 (Pascal) GPU (16 GB HBM2)
- 1813 XC40 nodes
  - 2x 18-core Broadwell (64/128 GB DRAM)
- Dragonfly network + Aries routing
- Filesystems
  - 8.8 PB Lustre filesystem for scratch data
  - GPFS for users home and long-term data

Energy efficiency of accelerators and specialized processors

Rank	Top500 rank	System	Rmax (Tflop/s)	Power (kW)	Efficiency (Gflops/W)
1	335	**MN-3** - MN-Core Server, Xeon Platinum 8260M 24C 2.4GHz, Preferred Networks MN-Core, MN-Core DirectConnect,	1,822	61	29.700
2	22	**HiPerGator AI** - NVIDIA DGX A100, AMD EPYC 7742 64C 2.25GHz, NVIDIA A100, Infiniband HDR, Nvidia University of Florida	17,200	583	29.521
3	100	**Wilkes-3** - PowerEdge XE8545, AMD EPYC 7763 64C 2.45GHz, NVIDIA A100 80GB, Infiniband HDR200 dual rail, Dell EMC University of Cambridge	4,124	147	28.144

Green500 list, June 2021

Summary

- HPC has an important societal impact
- Very high complexity at all levels of integration; from the infrastructure up to the software stack
- Learning how to efficiently use and program such a system can open new horizons to research

Q & A