CSCS
Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

ETH zürich

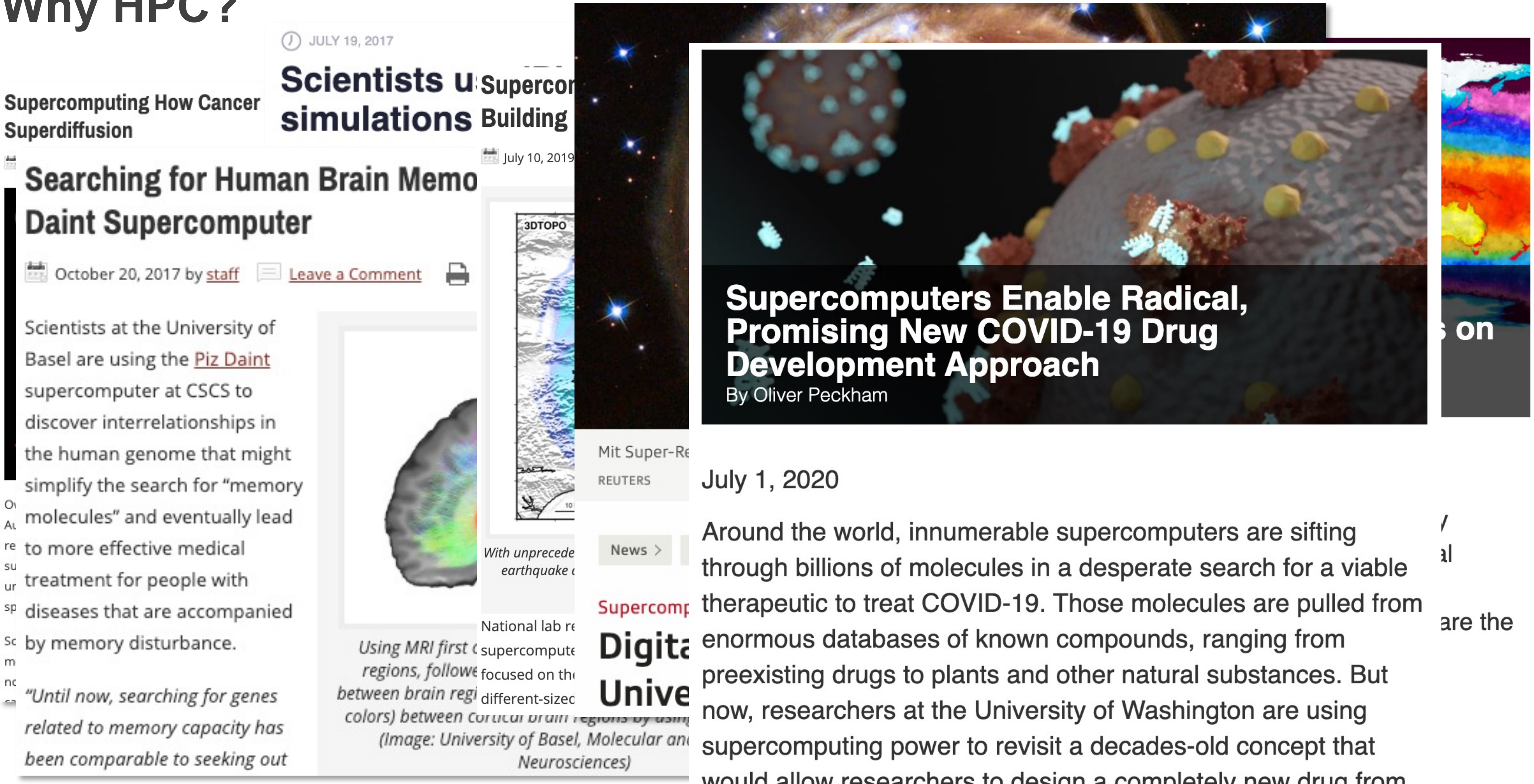
Introduction to High Performance Computing

CSCS-USI HPC/Data Analytics Summer University 2022

Vasileios Karakasis, CSCS
July 11, 2022

https://github.com/eth-cscs/SummerUniversity2022

Why HPC?



Supercomputing How Cancer Superdiffusion

JULY 19, 2017

Scientists u[...] simulations

Supercom[...] Building

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[...] between brain regi[...] colors) between cortical brain regions by usin[...] (Image: University of Basel, Molecular and [...] Neurosciences)

With unprecede[...] earthquake [...]

National lab re[...] supercompute[...] focused on th[...] different-sized[...]

Mit Super-Re[...]

REUTERS

News >

Supercomp[...]

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Supercomputers Enable Radical, Promising New COVID-19 Drug Development Approach

By Oliver Peckham

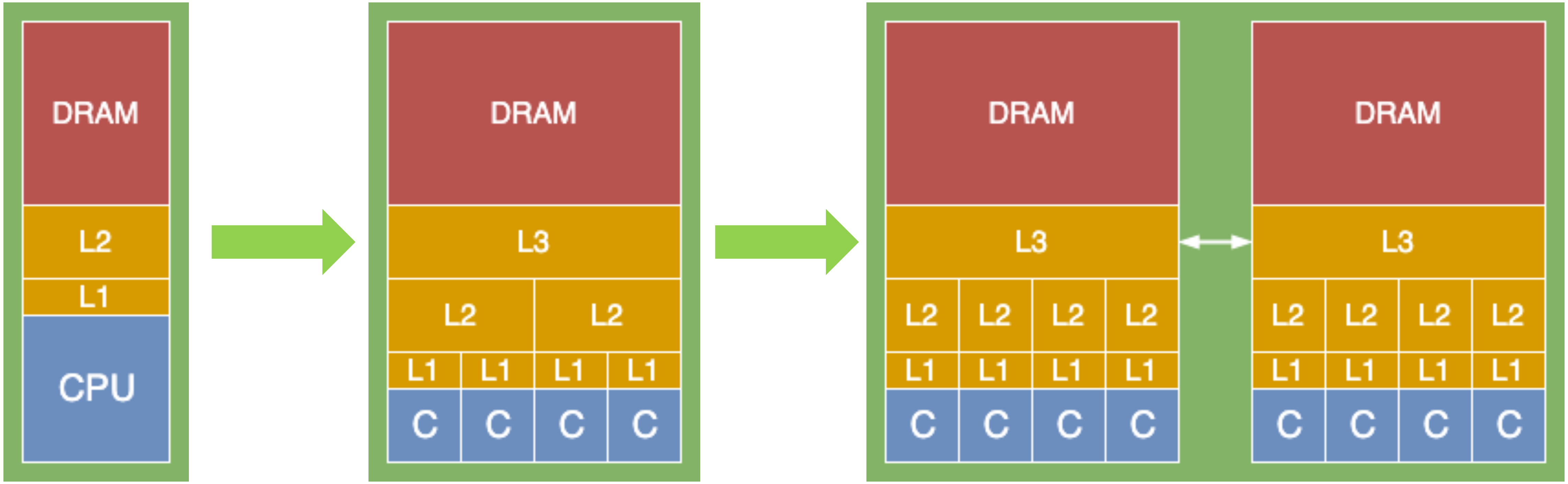
July 1, 2020

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

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



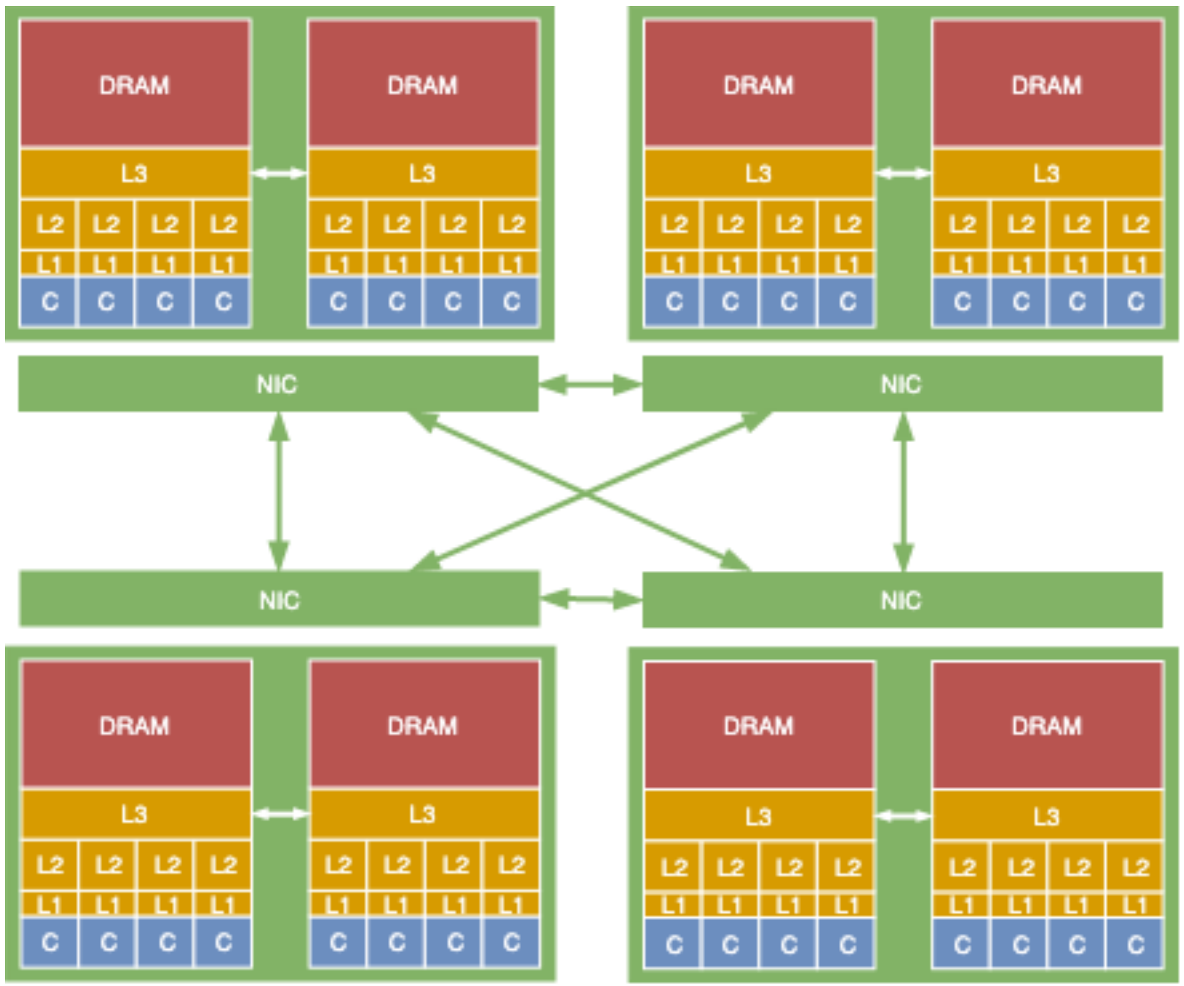
Single-core

Multicore SMP

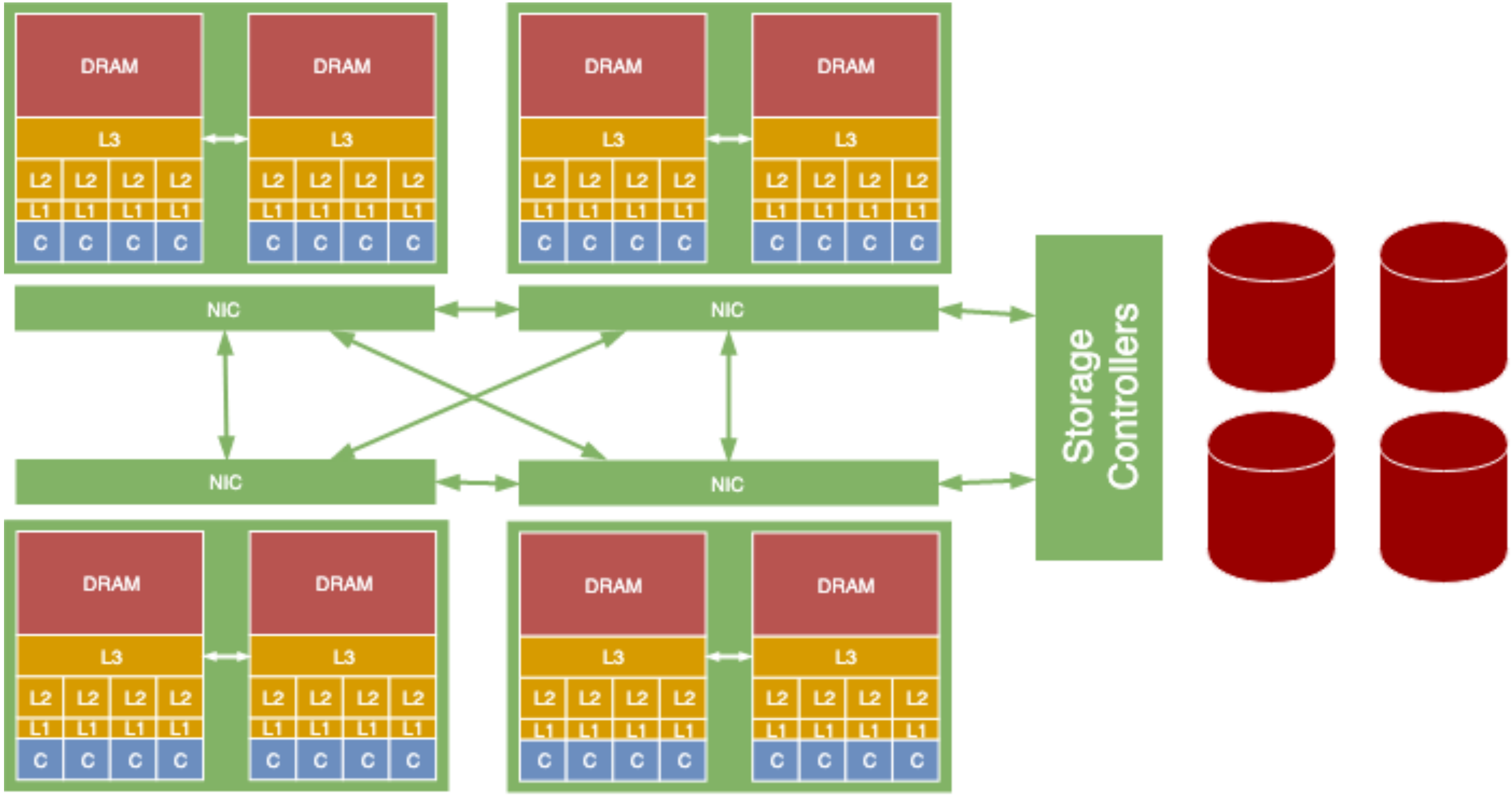
Multicore NUMA

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

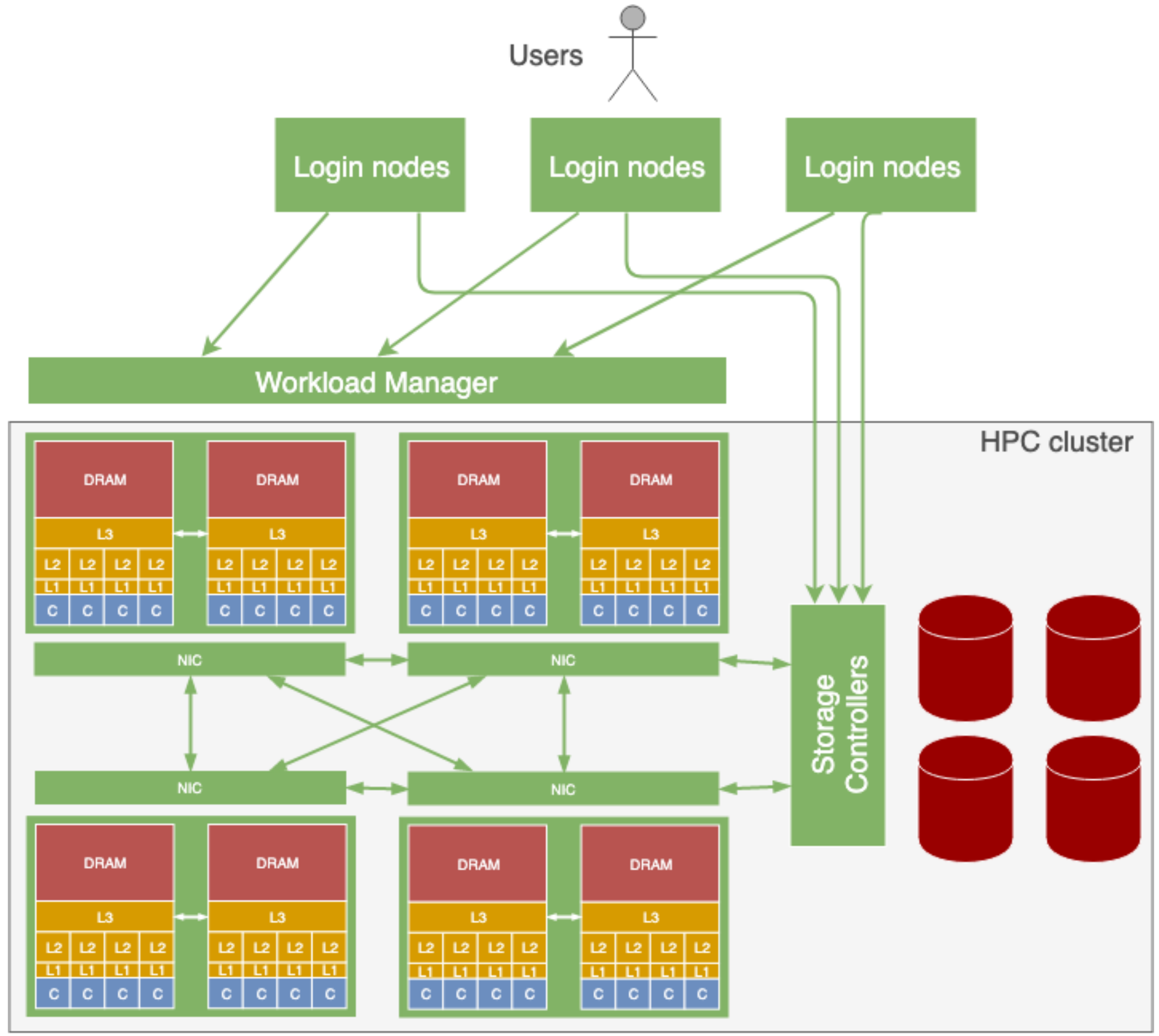
Building blocks for HPC systems: the network



Building blocks for HPC systems: the storage



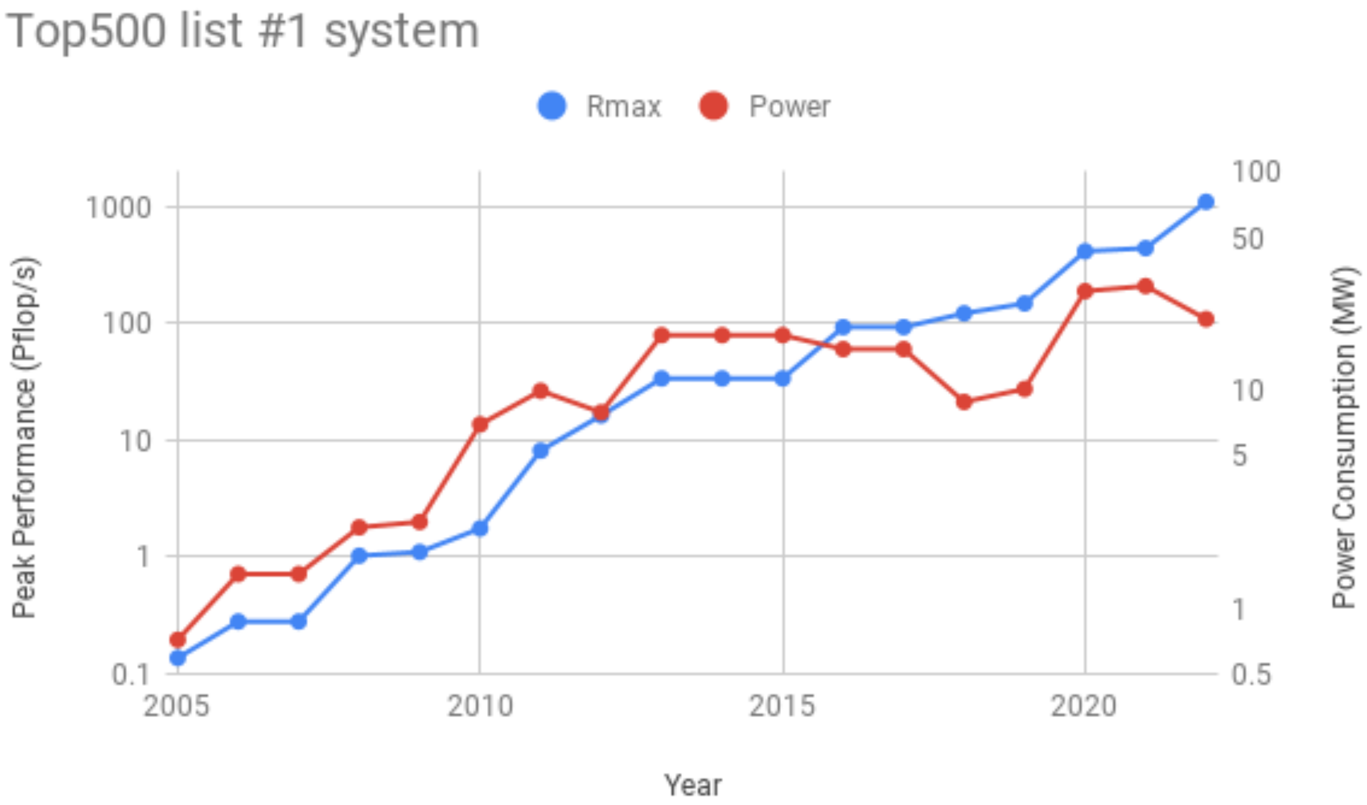
Building blocks for HPC systems: login nodes & workload manager



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

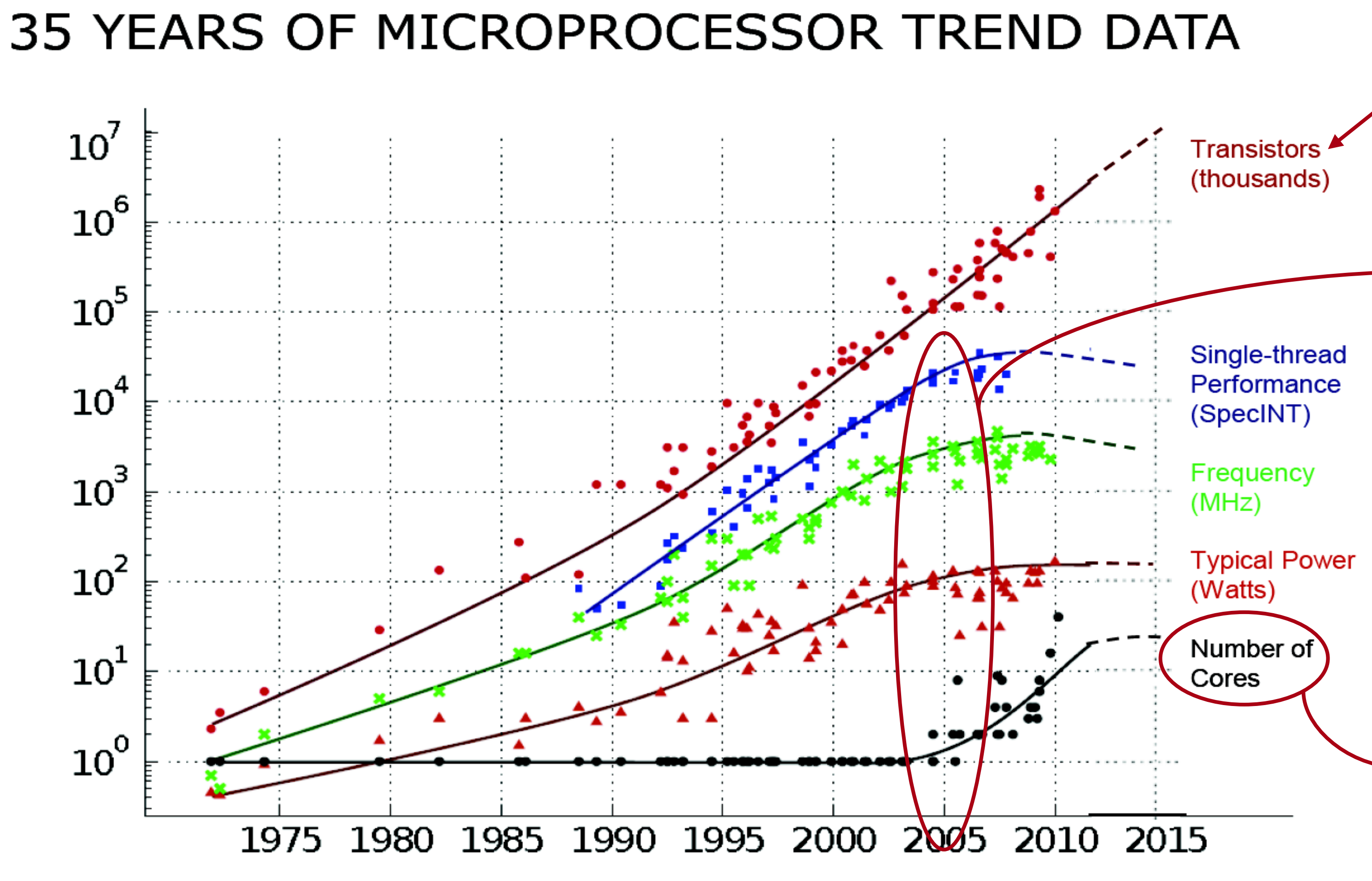


Power consumption has been following closely the exponential growth in performance, but at a lower rate.

Exascale is now reached!

- Sustained exascale performance in the HPL benchmark

How did we reach here?



Original data collected and plotted by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond and C. Batten
Dotted line extrapolations by C. Moore

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!

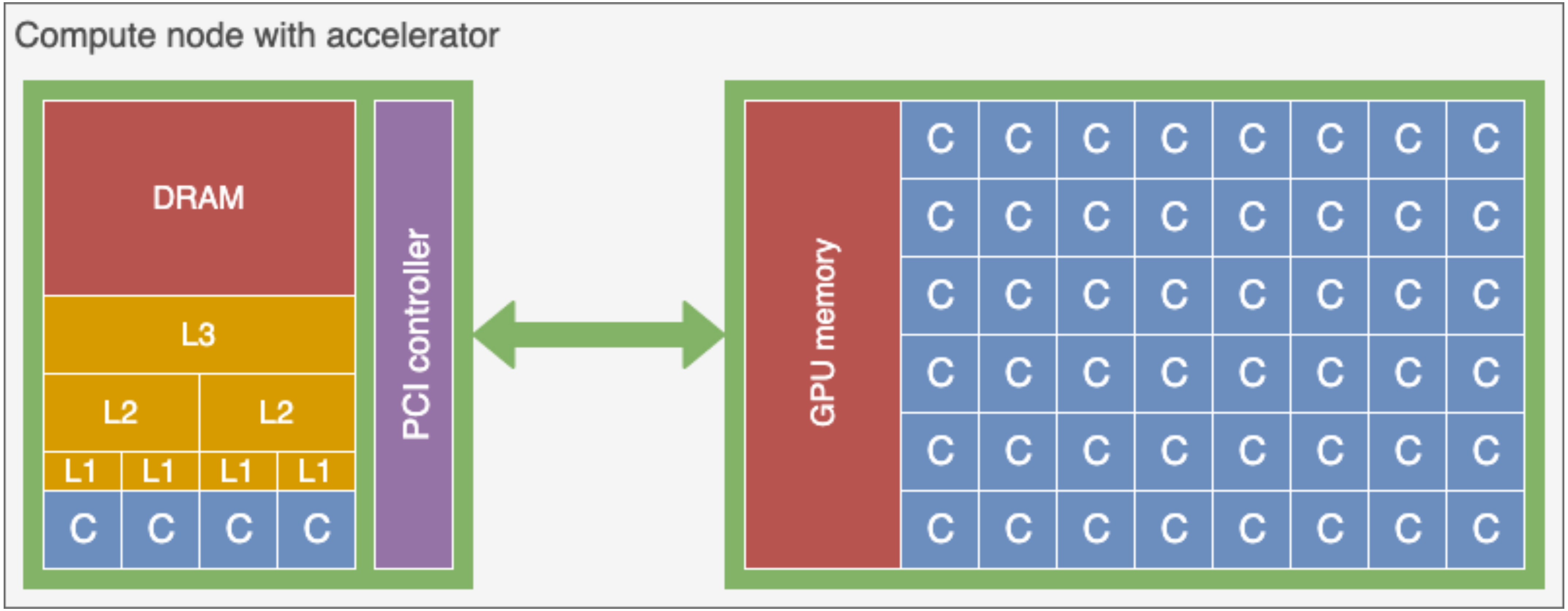
Performance can only grow through node-level parallelism!

Beyond multicores

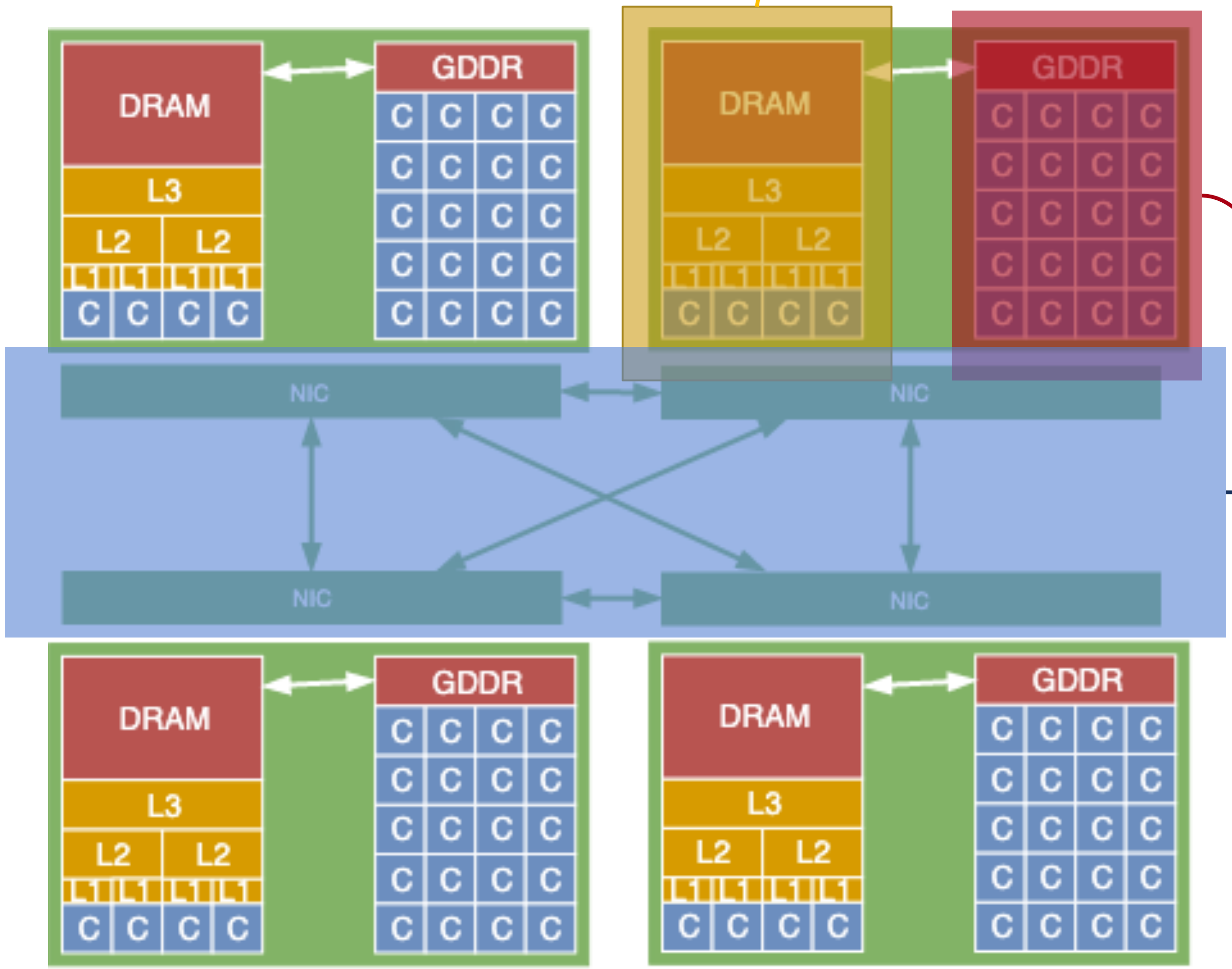
- Multicores have limitations
  - Fat cores (branch prediction, out-of-order execution, large caches)
    - Optimized for latency and multiprocessing
  - Still high frequencies
  - Still high power consumption
  - But programming is easy; matches better our brain’s serial way of thinking

- 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

- HPE Cray XC40/XC50 system
  - Top500: #23 in the world, #6 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

Alps (Piz Daint successor)

- HPE Cray EX
- Phase 1
  - 1024x AMD EPYC 7742 (Zen2 – Rome)
  - HPE Cray Slingshot 11
  - HPL performance: **3.09 Pflop/s** – #174 in Top500
- Phase 2 (ongoing)
- Phase 3 (full scale out planned in 2023)
  - Hybrid system with Arm-Based NVIDIA Grace CPUs + NVIDIA GPUs

Energy efficiency of accelerators and specialized processors

Rank	Top500 rank	System	Rmax (Pflop/s)	Power (kW)	Efficiency (Gflops/W)
1	29	**Frontier TDS –** HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE DOE/SC/Oak Ridge National Laboratory	19.2	309	62.684
2	1	**Frontier** – HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE DOE/SC/Oak Ridge National Laboratory	1’102	21’100	52.227
3	3	**LUMI** – HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE EuroHPC/CSC Finland	151.90	2’942	51.629

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