High-Performance Scientific Computing

INFO 0939, Fall 2024

http://people.montefiore.ulg.ac.be/geuzaine/INFO0939/

Based in part on material from Victor Eijkhout's SSC 335/394 course at the Texas Advanced Computing Center

Introduction

Mathematics & Science

- In science, we use mathematics to understand physical systems.

- Different fields of science explore different 'domains' of the universe, and have their own sets of equations, encapsulated in theories.

- Determining the theories and governing equations requires observation or experimentation, and testing hypotheses.

THE GRAND CHALLENGE EQUATIONS

$$B_i A_l = E_i A_l + \rho_i \sum_j B_j A_j F_{ji} \qquad \nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \qquad \vec{F} = m\,\vec{a} + \frac{dm}{dt}\,\vec{v}$$

$$dU = \left(\frac{\partial U}{\partial S}\right)_V dS + \left(\frac{\partial U}{\partial V}\right)_S dV \qquad \nabla \cdot \vec{D} = \rho \qquad Z = \sum_j g_j\, e^{-E_j/kT}$$

$$F_j = \sum_{k=0}^{N-1} f_k e^{2\pi ijk/N} \qquad \nabla^2 u = \frac{\partial u}{\partial t} \qquad \nabla \times \vec{H} = \frac{\partial \vec{D}}{\partial t} + \vec{J}$$

$$p_{n+1} = r\, p_n (1 - p_n) \qquad \nabla \cdot \vec{B} = 0 \qquad P(t) = \frac{\sum_i W_i B_i(t) P_i}{\sum_i W_i B_i(t)}$$

$$-\frac{h^2}{8\pi^2 m}\nabla^2 \Psi(r,t) + V\,\Psi(r,t) = -\frac{h}{2\pi i}\frac{\partial \Psi(r,t)}{\partial t} \qquad -\nabla^2 u + \lambda u = f$$

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla)\vec{u} = -\frac{1}{\rho}\nabla p + \gamma \nabla^2 \vec{u} + \frac{1}{\rho}\vec{F} \qquad \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = f$$

• NEWTON'S EQUATIONS • SCHROEDINGER EQUATION (TIME DEPENDENT) • NAVIER-STOKES EQUATION •
• POISSON EQUATION • HEAT EQUATION • HELMHOLTZ EQUATION • DISCRETE FOURIER TRANSFORM •
• MAXWELL'S EQUATIONS • PARTITION FUNCTION • POPULATION DYNAMICS •
• COMBINED 1ST AND 2ND LAWS OF THERMODYNAMICS • RADIOSITY • RATIONAL B-SPLINE •

[Courtesy of San Diego Supercomputer Center]

Scientific Computing

Why should we care about scientific computing?

- Computational research has emerged to complement experimental methods in basic research, design, optimization, and discovery in all facets of engineering and science

- In certain cases, computational simulations are the only possible approach to analyze a problem:
  - Experiments may be cost prohibitive (eg. *flight testing a 1,000 fuselage/wing-body configurations for a modern fighter aircraft*)
  - Experiments may be impossible (eg. *interaction effects between the International Space Station and Shuttle during docking*)

- Simulation capabilities rely heavily on the underlying compute power (e.g. amount of memory, total compute processors, and processor performance)
  - Fostered the introduction and development of *super-computers* starting in the 1960's
  - Large-scale compute power is tracked around the world via the *Top500 List* (more on that later)
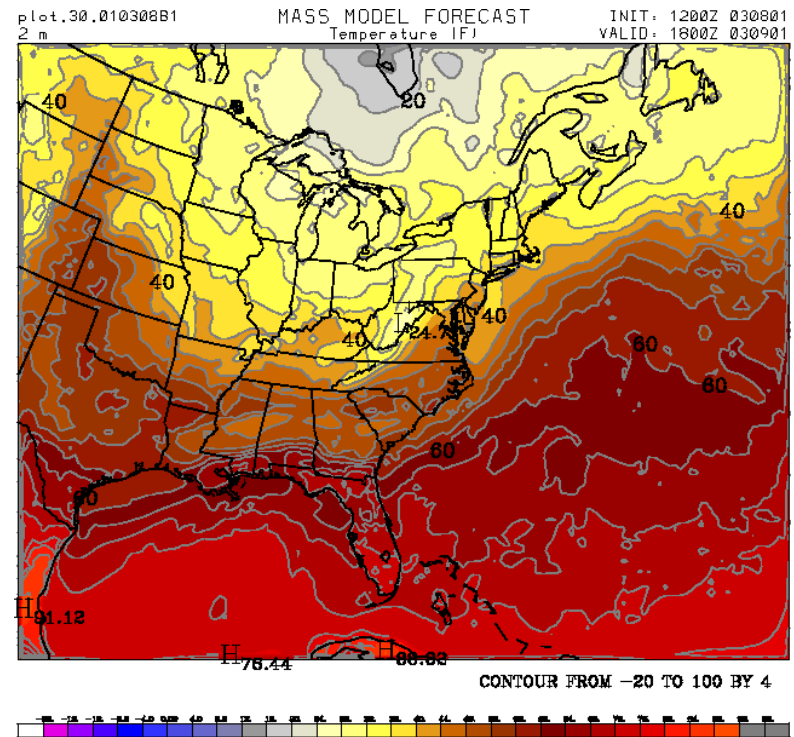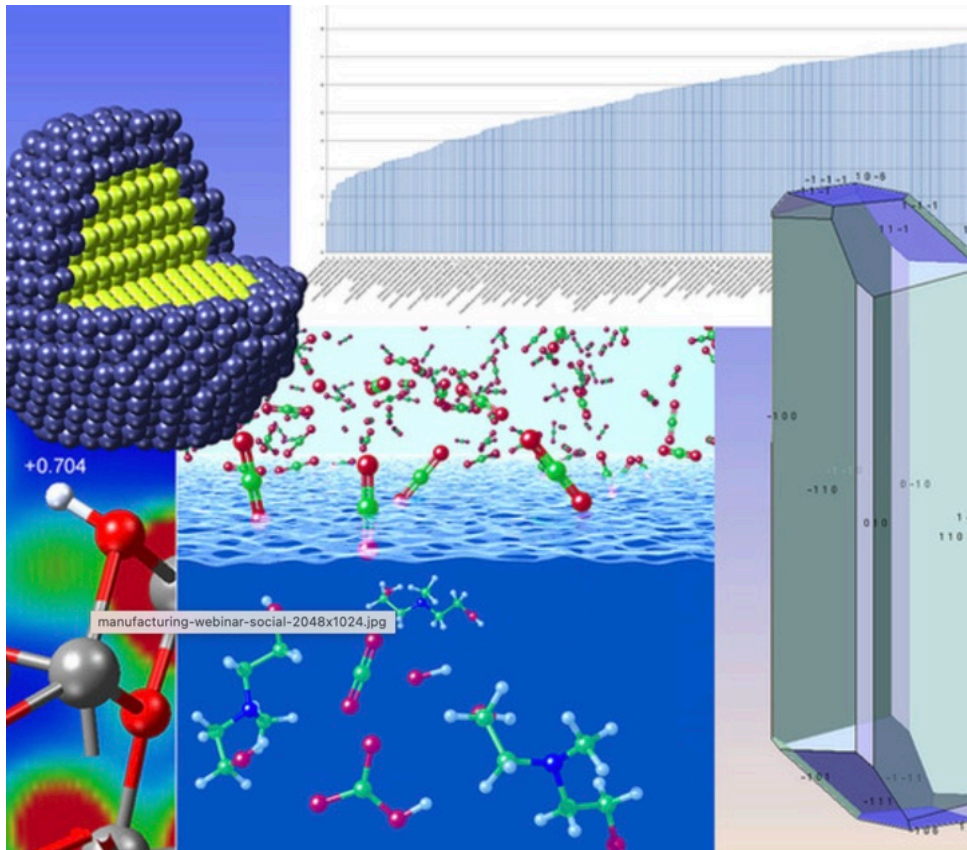
Scientific Computing: a definition

"The efficient computation of constructive methods in applied mathematics"

- Applied math: getting results out of application areas
- Numerical analysis: results need to be correctly and efficiently computable
- Computing: the algorithms need to be implemented on modern hardware

Examples of Scientific Computing
(*it really is everywhere*)

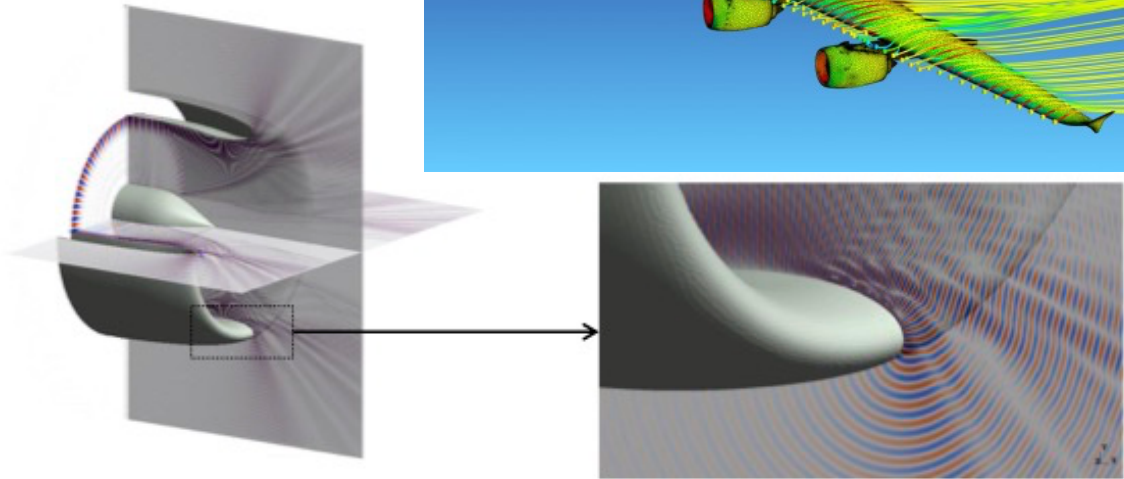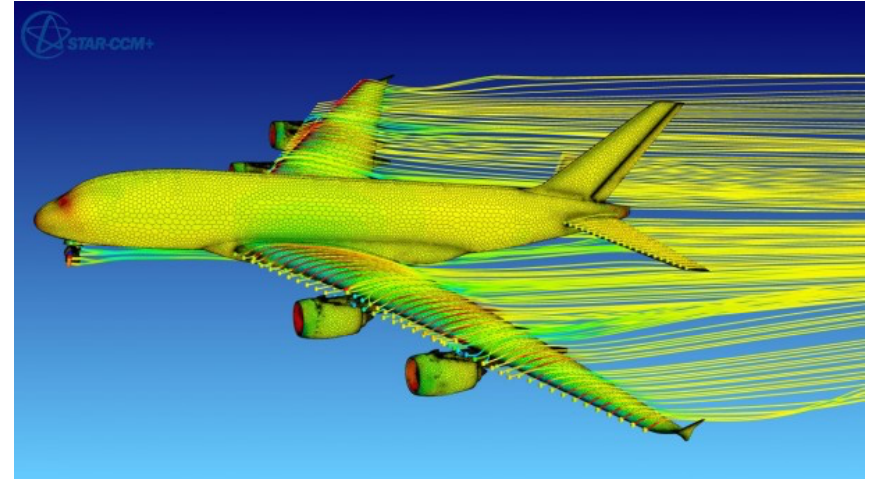Material Science

Weather Forecasting

Examples of Scientific Computing
(*it really is everywhere*)

Aerospace

Streamlines for workstation ventilation
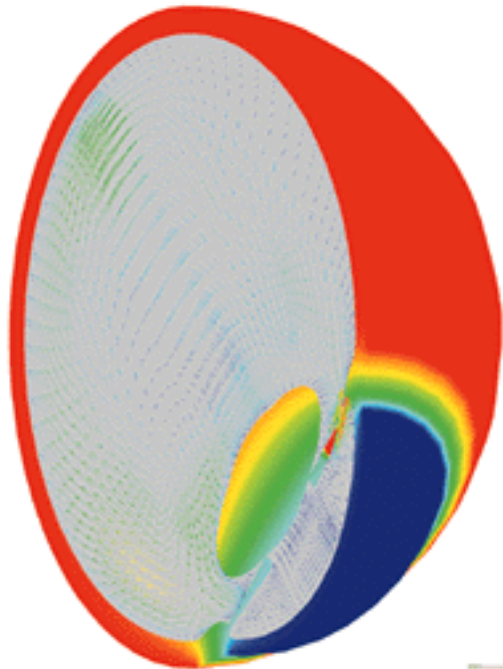
Heating, ventilation, and air conditioning
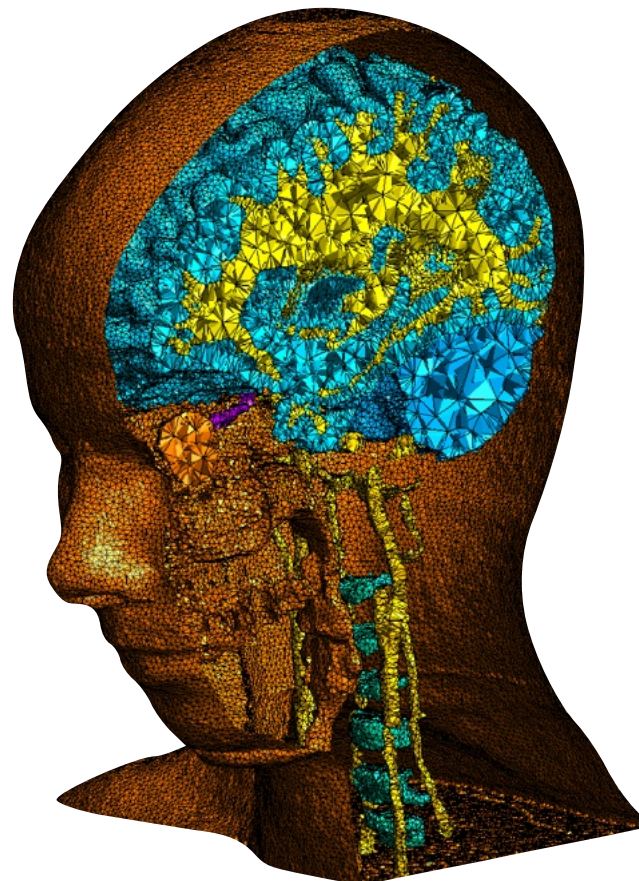
Automotive

8
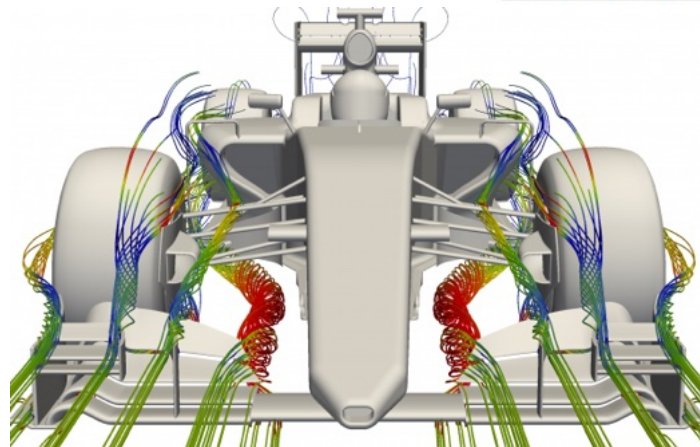
Examples of Scientific Computing
(*it really is everywhere*)

Temperature and natural convection currents in the eye following laser heating.

Biomedical engineering

Fields induced in human body close to power lines

Electric Field [V/m]
5e-05   0.000479   0.00459

Electric Potential [V]
-0.000151   2.31e-05   0.000197

Examples of Scientific Computing
(*it really is everywhere*)

Potentiel électrique (V)

Champ électrique (V/m)

Ligne 220 kV
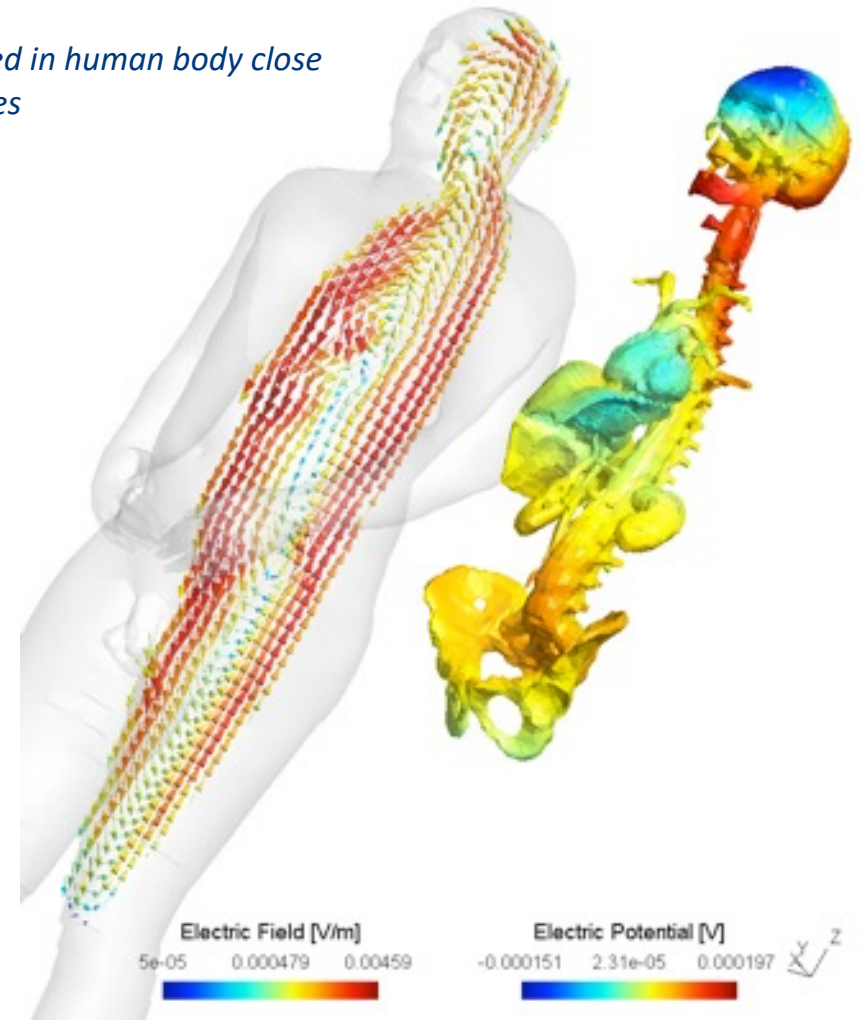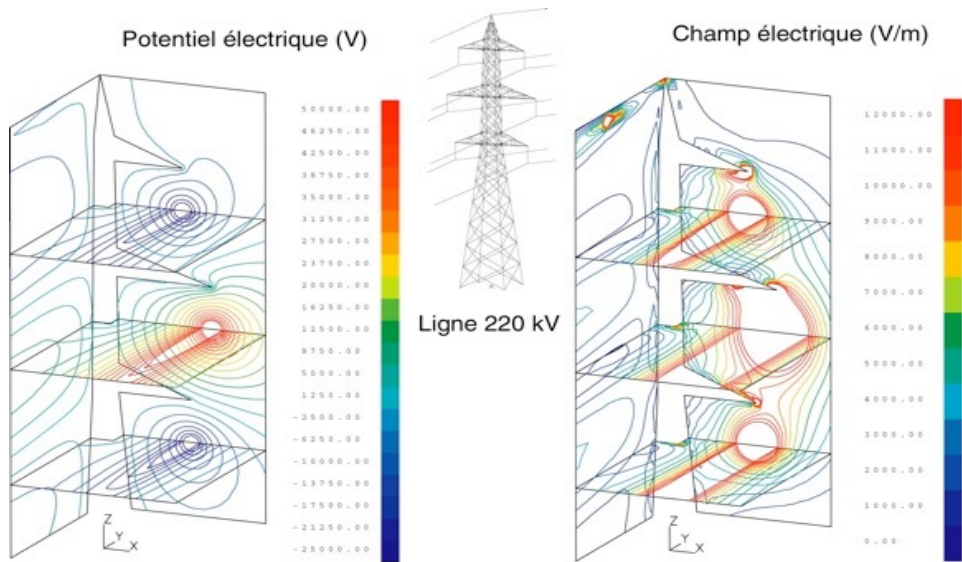
Electrical Engineering
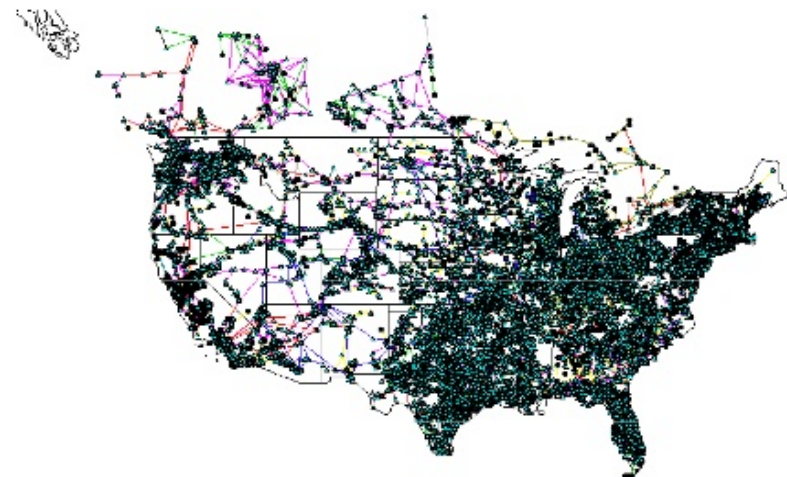
The New York Times
Thursday, September 4, 2008

Report on Blackout Is Said To Describe Failure to React

By MATTHEW L. WALD
Published: November 12, 2003

A report on the Aug. 14 blackout identifies specific lapses by various parties, including FirstEnergy's failure to react properly to the loss of a transmission line, people who have seen drafts of it say.

A working group of experts from eight states and Canada will meet in private on Wednesday to evaluate the report, people involved in the

10

Examples of Scientific Computing
(*it really is everywhere*)

Fluorescent proteins for medical diagnostics

Astronomy and planet habitability

From the nanoscale...

... to day-to-day living ...

... to the infinitely large

Optimizing traffic - virtual Namur at 9:00am

The Top500 List

- http://www.top500.org
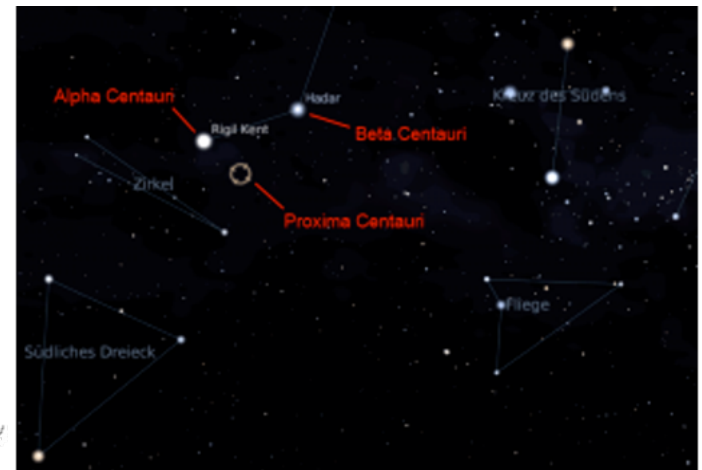
- Owner submitted benchmark performance since 1993

  - based on a dense linear system solve

  - http://www.netlib.org/benchmark/hpl/

Operating system Family - Systems Share

Linux 500 (100.00%)
N/A 0 (0%)
Mixed 0 (0%)
Unix 0 (0%)
BSD Based 0 (0%)
Windows 0 (0%)
Mac OS 0 (0%)

Jun 01, 2024

Linux	500	N/A	0	Mixed	0	Unix	0
BSD Based	0	Windows	0	Mac OS	0		
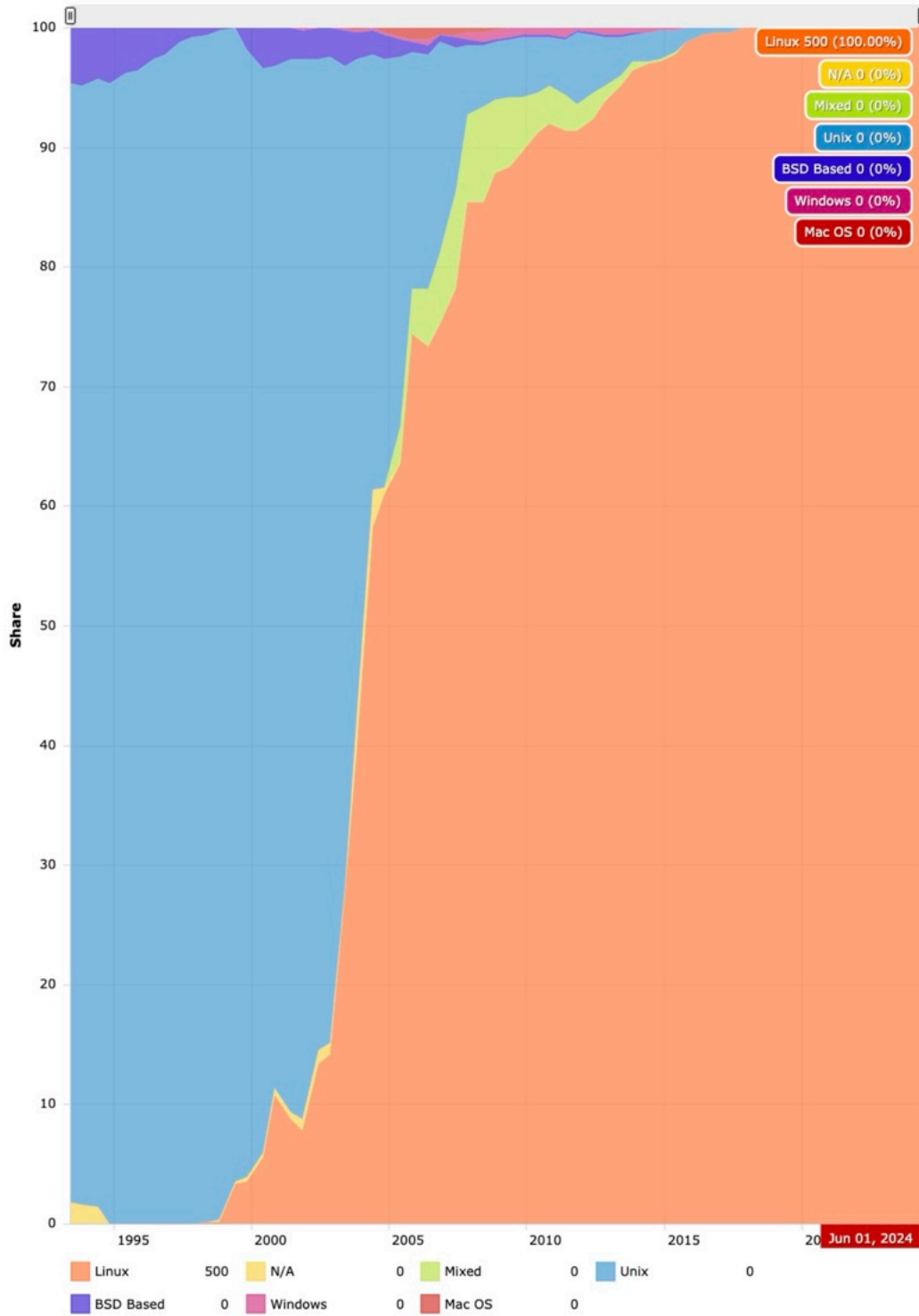
Architecture - Systems Share

MPP 70 (12.37%)
Single Processor 0 (0%)
SIMD 0 (0%)
SMP 0 (0%)
Constellations 0 (0%)
Cluster 496 (87.63%)

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Cluster	496	MPP	70	Single Processor	0	SIMD	0
SMP	0	Constellations	0				
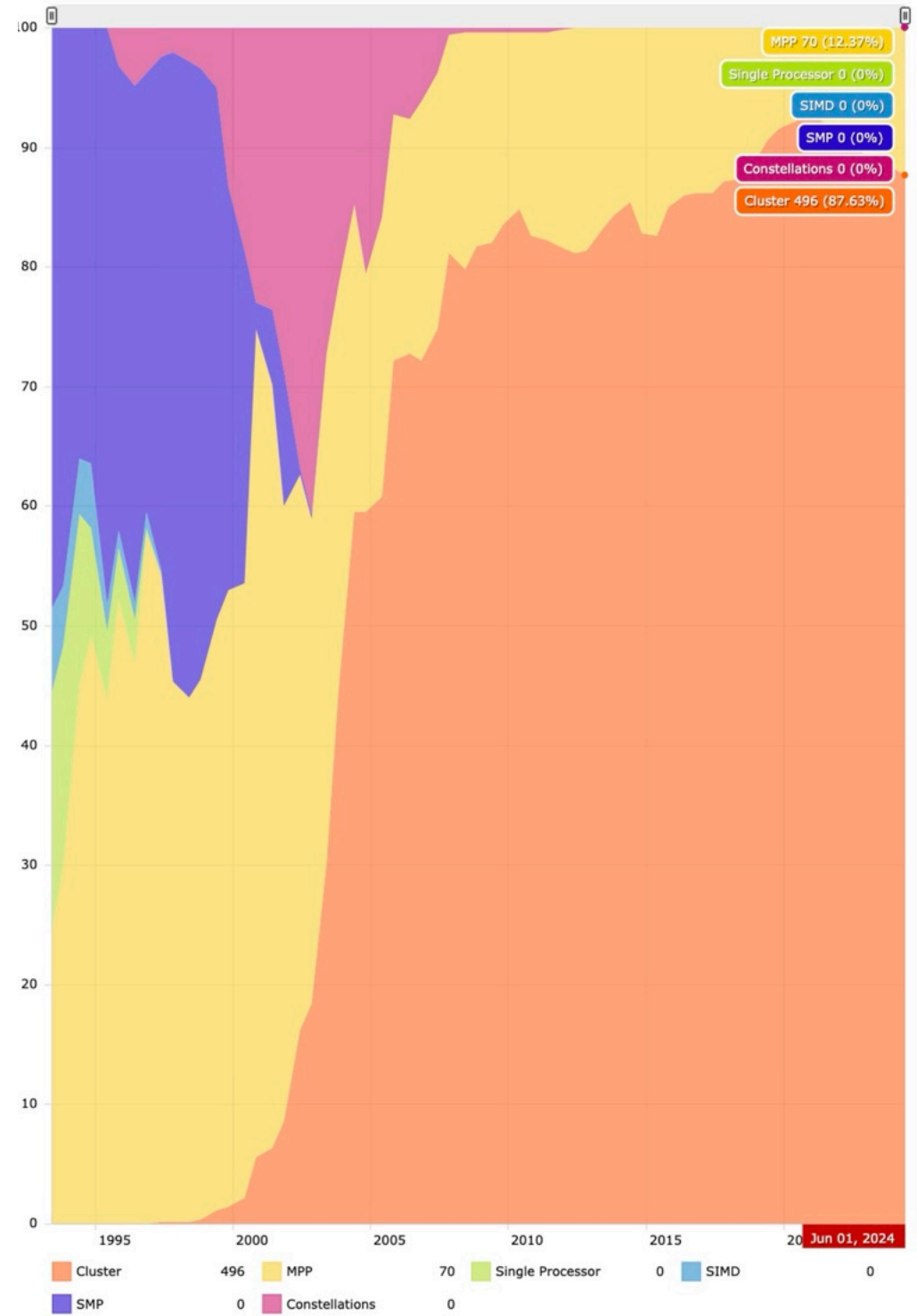
Cores per Socket - Systems Share
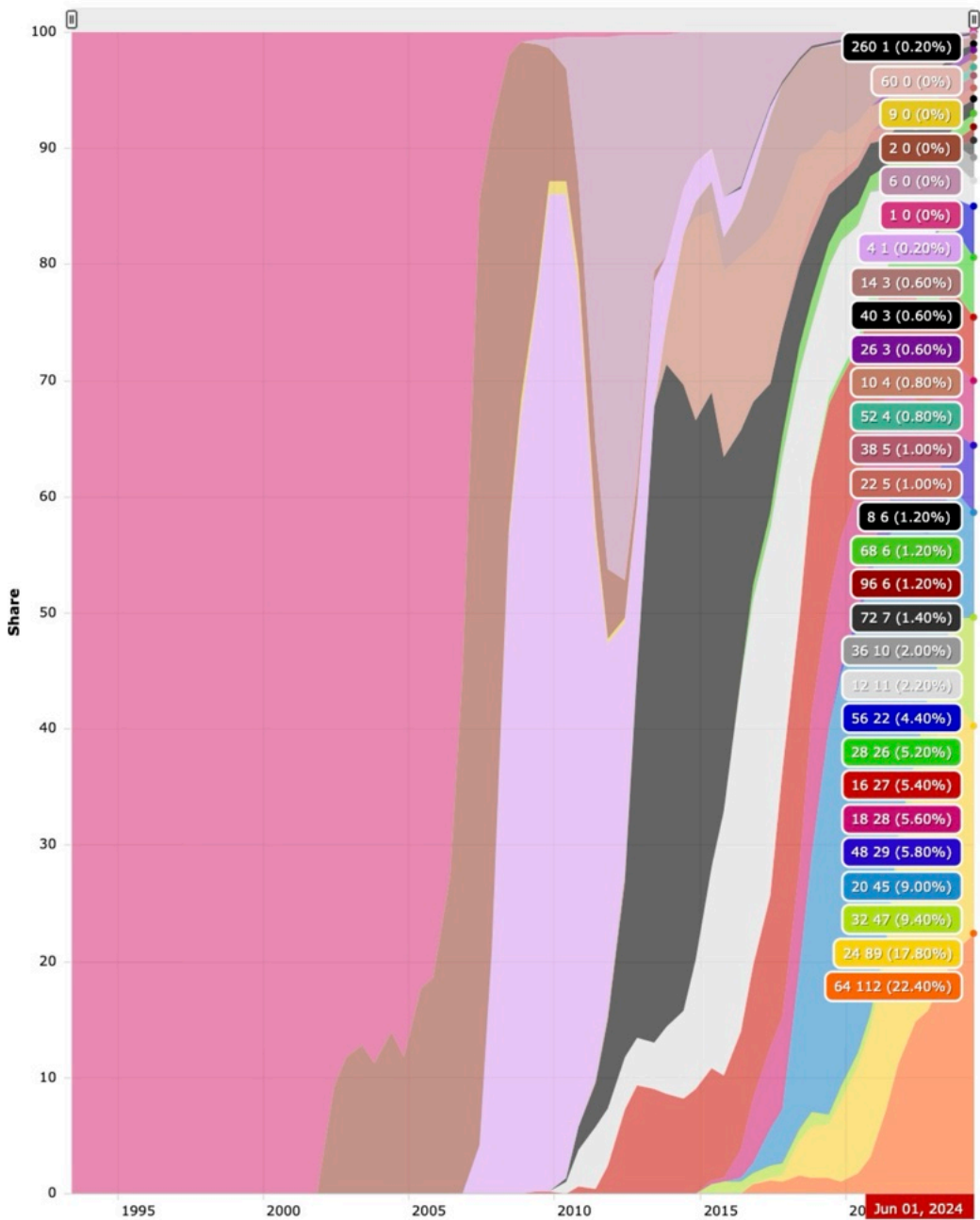
Accelerator/CP Family - Systems Share

Left chart labels (top to bottom):
- 260 1 (0.20%)
- 60 0 (0%)
- 9 0 (0%)
- 2 0 (0%)
- 6 0 (0%)
- 1 0 (0%)
- 4 1 (0.20%)
- 14 3 (0.60%)
- 40 3 (0.60%)
- 26 3 (0.60%)
- 10 4 (0.80%)
- 52 4 (0.80%)
- 38 5 (1.00%)
- 22 5 (1.00%)
- 8 6 (1.20%)
- 68 6 (1.20%)
- 96 6 (1.20%)
- 72 7 (1.40%)
- 36 10 (2.00%)
- 12 11 (2.20%)
- 56 22 (4.40%)
- 28 26 (5.20%)
- 16 27 (5.40%)
- 18 28 (5.60%)
- 48 29 (5.80%)
- 20 45 (9.00%)
- 32 47 (9.40%)
- 24 89 (17.80%)
- 64 112 (22.40%)

Right chart labels (top to bottom):
- Matrix-2000 1 (0.52%)
- IBM Cell 0 (0%)
- ATI Radeon 0 (0%)
- PEZY-SC 0 (0%)
- AMD Vega 0 (0%)
- NVIDIA Fermi 0 (0%)
- Clearspeed 0 (0%)
- None 0 (0%)
- Hybrid 1 (0.52%)
- Intel Xeon Phi 1 (0.52%)
- MN-Core 1 (0.52%)
- N/A 2 (1.03%)
- 19 4 (2.06%)
- NVIDIA Kepler 5 (2.58%)
- NVIDIA Pascal 5 (2.58%)
- 20 7 (3.61%)
- 17 14 (7.22%)
- 18 22 (11.34%)
- NVIDIA Volta 48 (24.74%)
- NVIDIA Ampere 83 (42.78%)

Both charts dated: Jun 01, 2024

Left legend:
64	112	24	89	32	47	20	45	48	29	18	28
16	27	28	26	56	22	12	11	36	10	72	7
96	6	68	6	8	6	22	5	38	5	52	4
10	4	26	3	40	3	14	3	4	1	260	1
60	0	9	0	2	0	6	0	1	0		

Right legend:
NVIDIA Ampere	83	NVIDIA Volta	48	18	22	17	14
20	7	NVIDIA Pascal	5	NVIDIA Kepler	5	19	4
N/A	2	MN-Core	1	Intel Xeon Phi	1	Hybrid	1
Matrix-2000	1	IBM Cell	0	ATI Radeon	0	PEZY-SC	0
AMD Vega	0	NVIDIA Fermi	0	Clearspeed	0	None	0

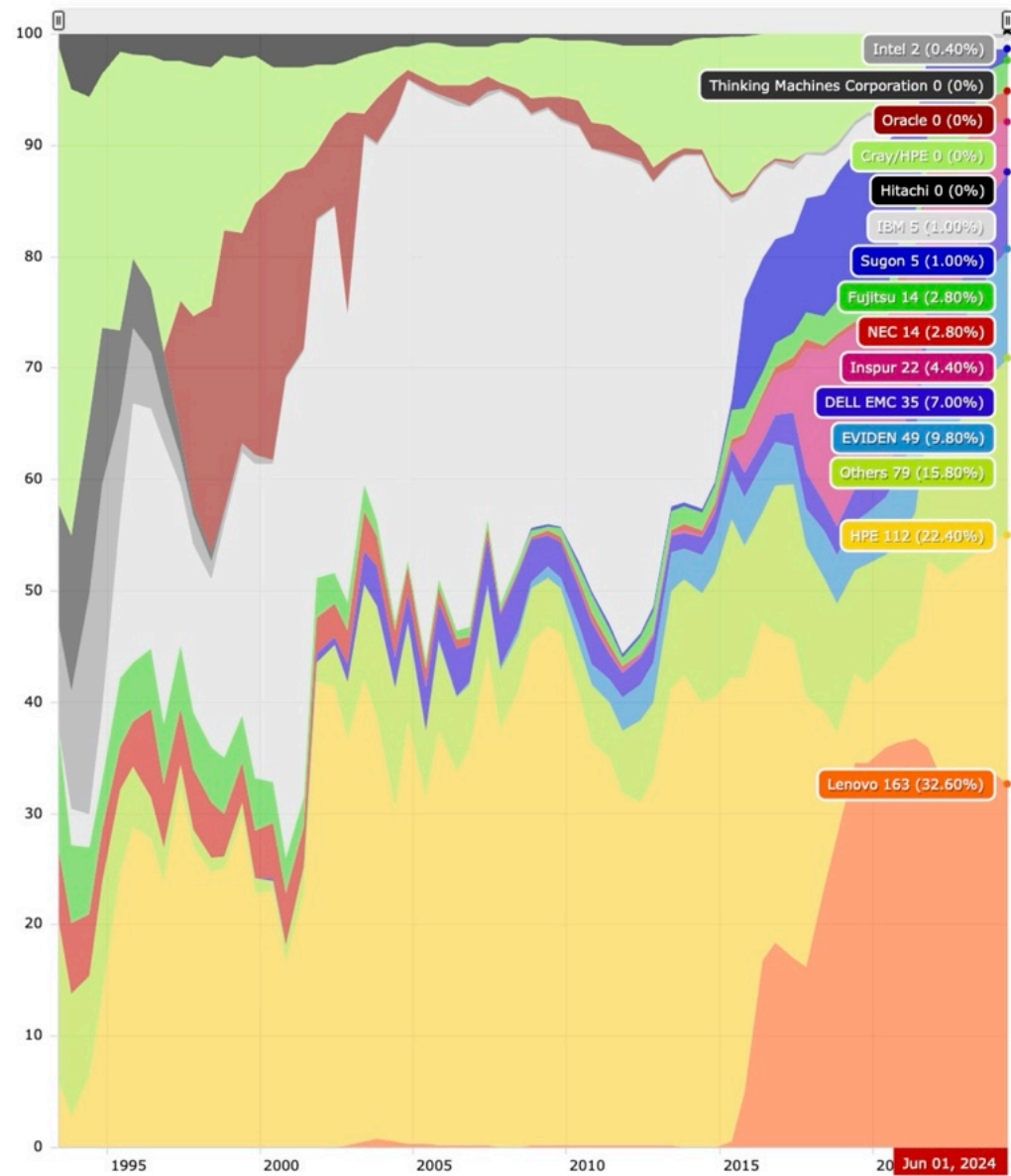## Interconnect Family - Systems Share
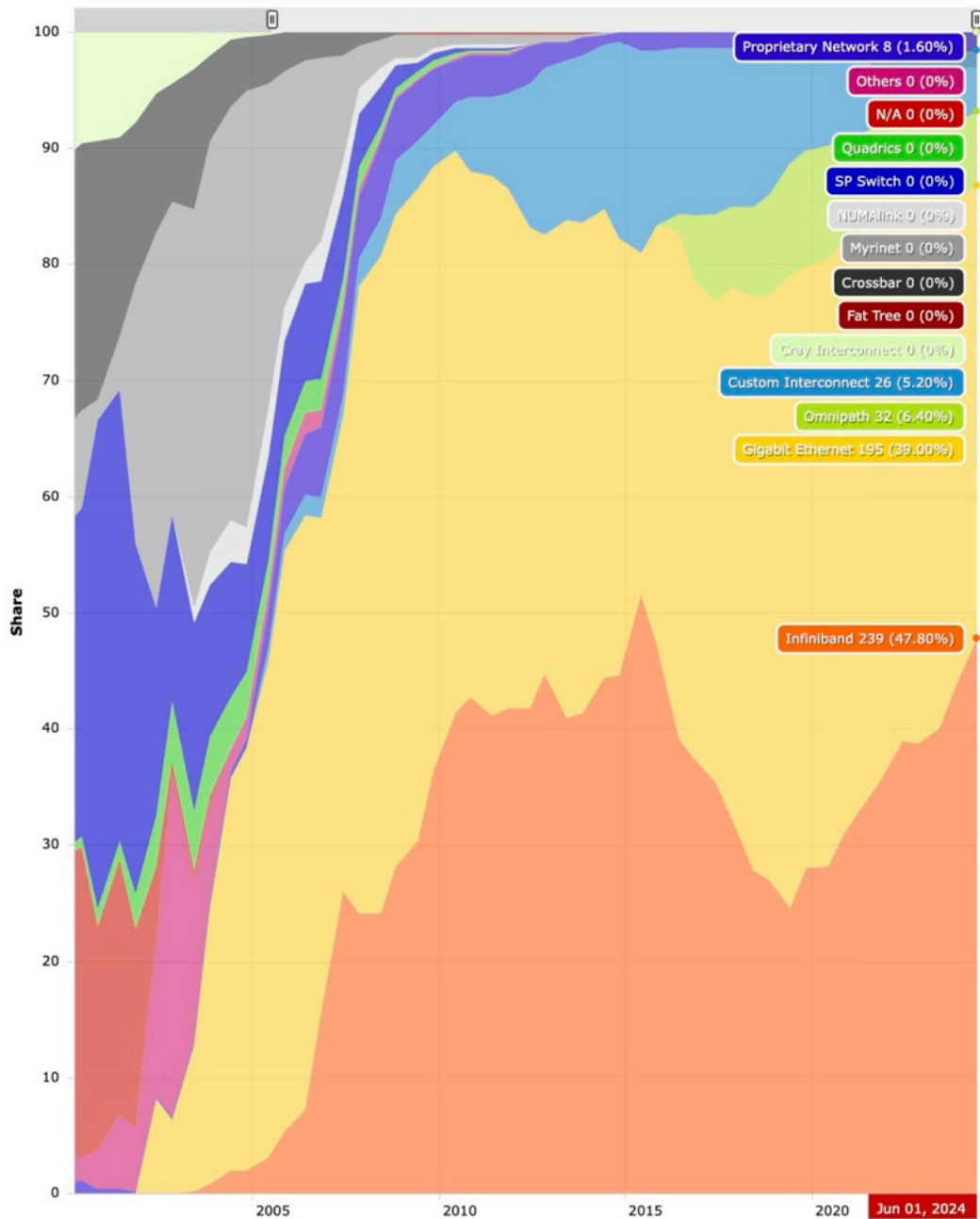
- Infiniband — 239
- Gigabit Ethernet — 195
- Omnipath — 32
- Custom Interconnect — 26
- Proprietary Network — 8
- Others — 0
- N/A — 0
- Quadrics — 0
- SP Switch — 0
- NUMAlink — 0
- Myrinet — 0
- Crossbar — 0
- Fat Tree — 0
- Cray Interconnect — 0

Labels on chart:
- Proprietary Network 8 (1.60%)
- Others 0 (0%)
- N/A 0 (0%)
- Quadrics 0 (0%)
- SP Switch 0 (0%)
- NUMAlink 0 (0%)
- Myrinet 0 (0%)
- Crossbar 0 (0%)
- Fat Tree 0 (0%)
- Cray Interconnect 0 (0%)
- Custom Interconnect 26 (5.20%)
- Omnipath 32 (6.40%)
- Gigabit Ethernet 195 (39.00%)
- Infiniband 239 (47.80%)

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Vendors - Systems Share

- Lenovo — 163
- HPE — 112
- Others — 79
- EVIDEN — 49
- DELL EMC — 35
- Inspur — 22
- NEC — 14
- Fujitsu — 14
- Sugon — 5
- IBM — 5
- Intel — 2
- Thinking Machines Corporation — 0
- Oracle — 0
- Cray/HPE — 0
- Hitachi — 0

Labels on chart:
- Intel 2 (0.40%)
- Thinking Machines Corporation 0 (0%)
- Oracle 0 (0%)
- Cray/HPE 0 (0%)
- Hitachi 0 (0%)
- IBM 5 (1.00%)
- Sugon 5 (1.00%)
- Fujitsu 14 (2.80%)
- NEC 14 (2.80%)
- Inspur 22 (4.40%)
- DELL EMC 35 (7.00%)
- EVIDEN 49 (9.80%)
- Others 79 (15.80%)
- HPE 112 (22.40%)
- Lenovo 163 (32.60%)

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Continents - Systems Share
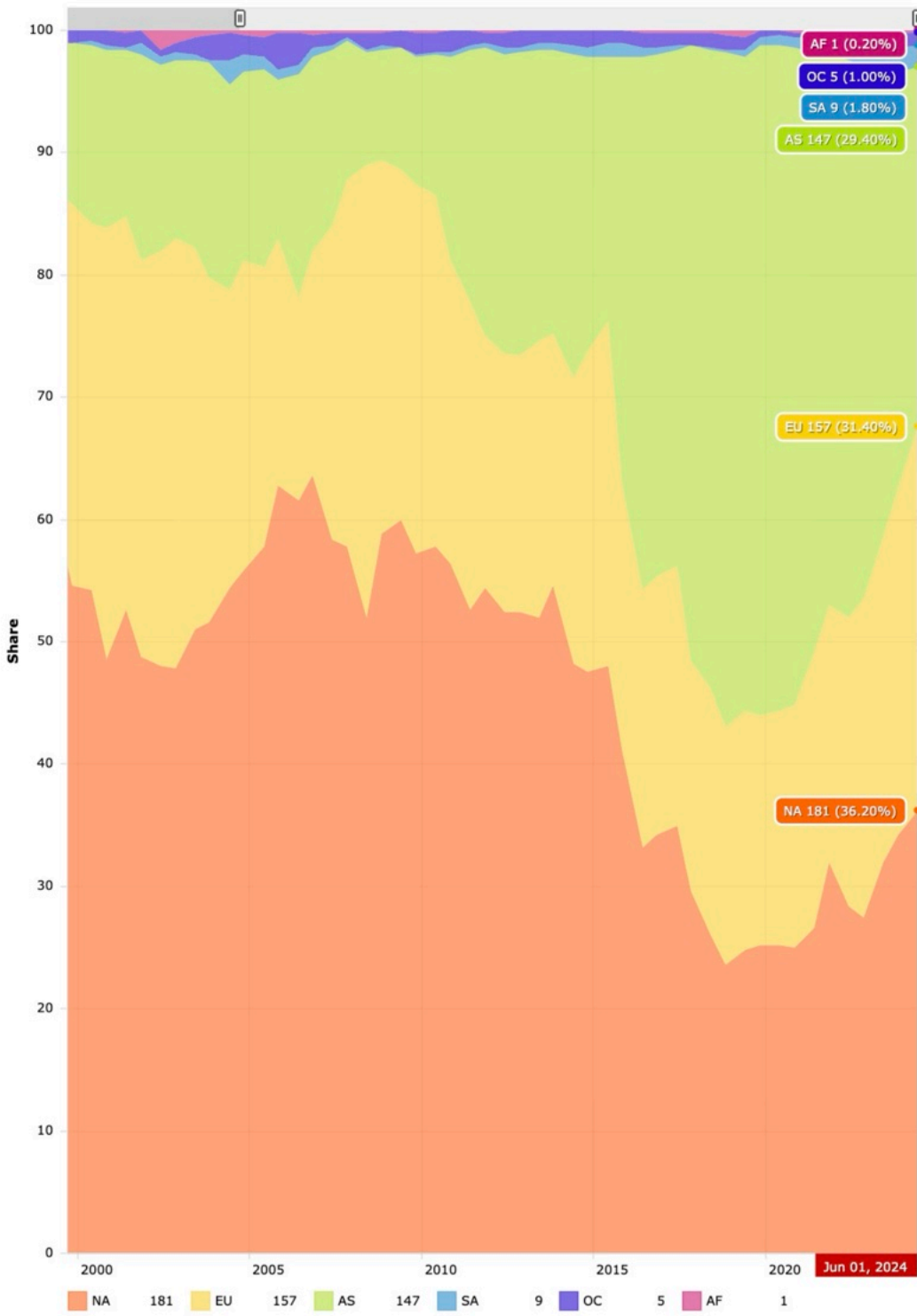
AF 1 (0.20%)
OC 5 (1.00%)
SA 9 (1.80%)
AS 147 (29.40%)
EU 157 (31.40%)
NA 181 (36.20%)

Jun 01, 2024

| NA | 181 | EU | 157 | AS | 147 | SA | 9 | OC | 5 | AF | 1 |

Segments - Systems Share

Others 11 (2.20%)
Classified 0 (0%)
Vendor 21 (4.20%)
Government 28 (5.60%)
Academic 103 (20.60%)
Research 141 (28.20%)
Industry 196 (39.20%)

Jun 01, 2024

| Industry | 196 | Research | 141 | Academic | 103 | Government | 28 |
| Vendor | 21 | Others | 11 | Classified | 0 | | |

HPC and CECI

http://www.ceci-hpc.be
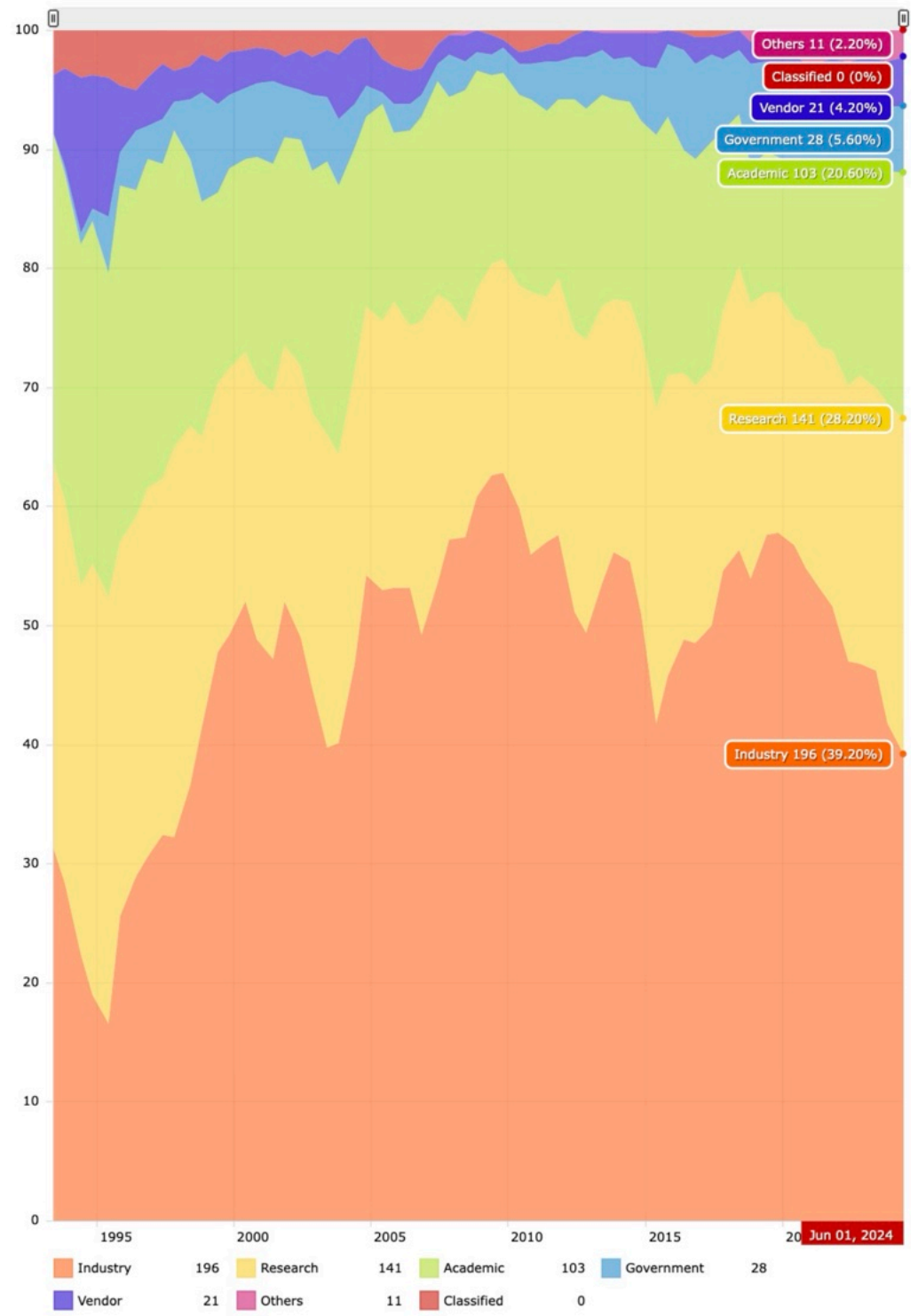
- CECI is the "Consortium des Equipements de Calcul Intensif" in Wallonia/Brussels
  - Once you create an account you can use all the CECI clusters
  - Funded by FNRS
  - UCLouvain, ULB, UNamur, UMons, ULiège
  - Single login for all clusters (more on that later)
- Machines in CECI grid:
  - NIC5 @ ULiège
  - Lemaitre4 @ UCLouvain
  - Hercules2 @ FUNDP
  - Dragon2 @ UMons
  - Soon: Lyra @ ULB

NIC5 System Summary

- 73 compute nodes with two 32-cores AMD Epyc Rome 7542 CPUs at 2.9 GHz and 256 GB or 1TB of RAM

- Infiniband HDR interconnect

- 520 TB BeeGFS parallel filesystem

- The cluster is especially designed for massively parallel jobs (MPI) with many communications and/or a lot of parallel disk I/O, 2 days max.

- SSH to nic5.segi.ulg.ac.be with the appropriate login and id_rsa.ceci file (more on that later).
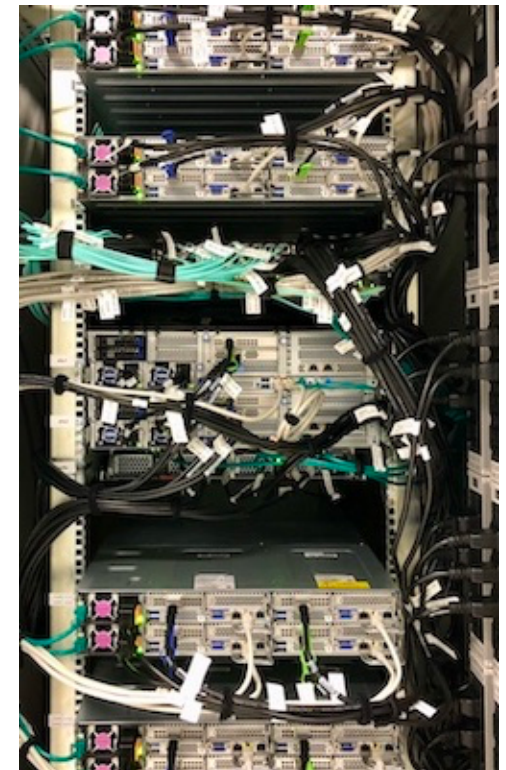
External Power and Cooling
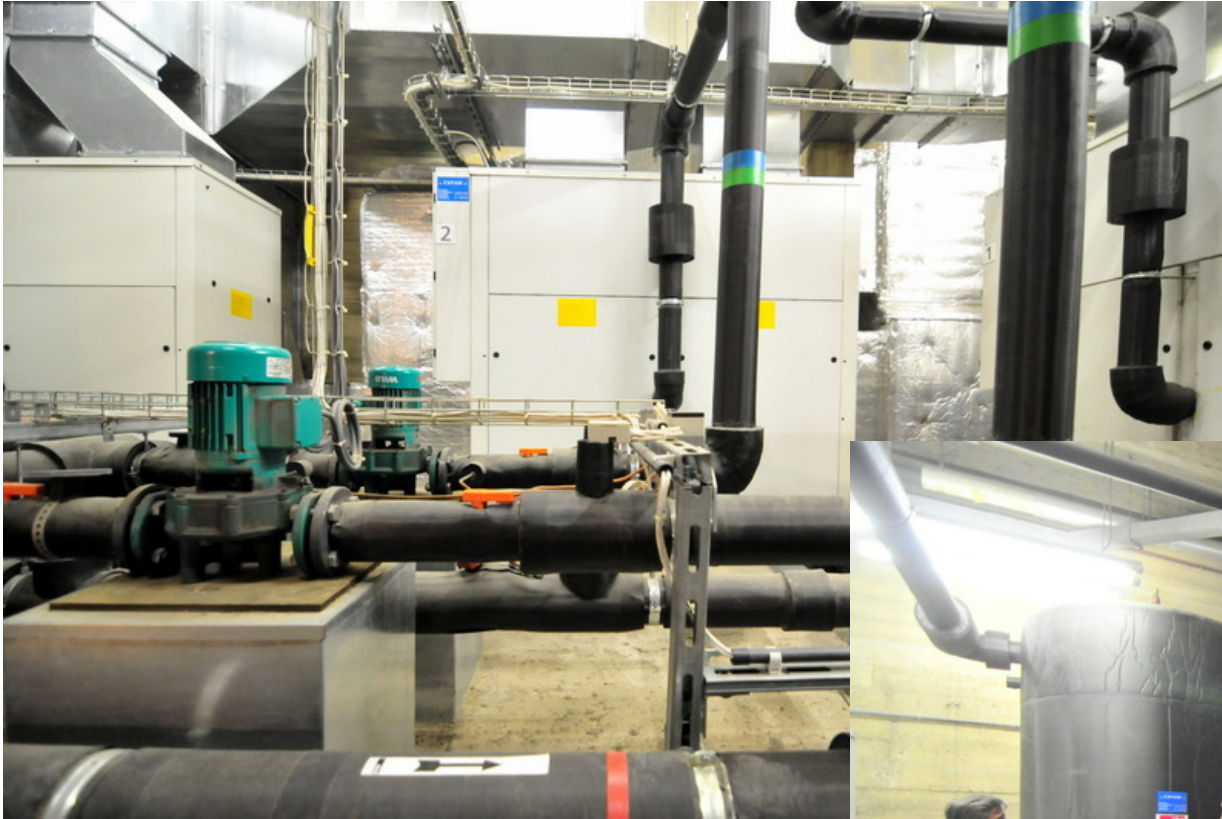
Class Goals/Topics

- Remember that definition "The efficient computation of constructive methods in applied mathematics"
  - Theory: numerical algorithms, (parallel) computation, and how to combine them
  - Practice: the tools of scientific computing, and in particular UNIX exposure (shells/command line, environment, compilers, profilers, debuggers, ...)
- Setup this year:
  - Classes on Tuesday @ 1:45pm, Montefiore R7
  - 1 project ; oral exam during January session

Computer Accounts

- CECI clusters

  - You should create an account now (https://login.ceci-hpc.be)

  - Only SSH access is allowed ; if not on campus, you must use the ULiège VPN:

- Jobs run in a managed environment

  - Login to the login node

  - Submit jobs to the scheduler

  - Wait

  - Collect results

- Production runs on the login node are forbidden

  - Avoid resource intensive tasks

  - Exceptions include compilers, "standard" UNIX commands (ls, mkdir, etc.)

- All required info is available on http://www.ceci-hpc.be

  - Read the FAQ!

CÉCI

Consortium des Équipements de Calcul Intensif

6 clusters, 10k cores, 1 login, 1 home directory

About

CÉCI is the 'Consortium des Équipements de Calcul Intensif'; a consortium of high-performance computing centers of UCLouvain, ULB, ULiège, UMons, and UNamur. The CÉCI is supported by the F.R.S-FNRS and the Walloon Region. Read more.

Videos of the training sessions

The training sessions Youtube channel is now ready.

Do not hesitate to have a look at the videos of the training sessions.

Latest News

MONDAY, 25 JANUARY 2021

LUMI Training - Practical course on the CUDA to HIP porting

CSC and the *LUMI User Support Team* organize their first training day that will focus on porting CUDA applications to HIP. This training aims to help the users to port their code to LUMI, the European pre-exascale supercomputer, that will achieve its high computing power thanks to a large number of nodes with AMD GPUs. This event will take place on **February 26**.

This session will provide an extensive dive into the Hipify tools, many examples and a hands-on session. If you're developing your code with CUDA and wish to harness the computing power of LUMI in the future this training is a fantastic opportunity.

You can find further details and the registration form here.

Quick links

- Connecting from a Windows computer
- Connecting from a UNIX/Linux or MacOS computer
- Slurm tutorial and quick start
- Slurm Frequently Asked Questions
- Tier-1 Zenobe quickstart
- Submission Script Generation Wizard

WEDNESDAY, 13 JANUARY 2021

NIC5 installed at ULiège

The new NIC5 HPC cluster is now available. It features 70 nodes with two 32 cores AMD EPYC Rome 7542 cpus at 2.9 GHz and 256 GB of RAM, 3 nodes with 1 TB of RAM, 520 TB of fast BeeGFS /scratch and a 100 Gbps Infiniband HDR interconnect (blocking factor 1,2:1),