High-Performance Scientific Computing

INFO 0939, Fall 2025

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

$$B_i A_i = E_i A_i + \rho_i \sum_j B_j A_j F_{ji}$$

$$\nabla \times \vec{E} = - \frac{\partial \vec{B}}{\partial t}$$

$$\vec{F} = m \vec{a} + \frac{dm}{dt} \vec{v}$$

$$dU = \left(\frac{\partial U}{\partial S}\right)_V dS + \left(\frac{\partial U}{\partial V}\right)_S dV$$

$$\nabla \bullet \vec{D} = \rho$$

$$Z = \sum_j g_j e^{-E_j/kT}$$

$$F_j = \sum_{k=0}^{N-1} f_k e^{2\pi i j k/N}$$

$$\nabla^2 u = \frac{\partial u}{\partial t}$$

$$\nabla \times \vec{H} = \frac{\partial \vec{D}}{\partial t} + \vec{J}$$

$$P(t) = \frac{\sum_i W_i B_i(t) P_i}{\sum_i W_i B_i(t)}$$

$$\nabla \bullet \vec{B} = 0$$

$$p_{n+1} = r p_n (1 - p_n)$$

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

$$-\nabla^2 u + \lambda u = f$$

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u} \bullet \nabla) \vec{u} = - \frac{1}{\rho} \nabla p + \gamma \nabla^2 \vec{u} + \frac{1}{\rho} \vec{F}$$

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = f$$

• 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

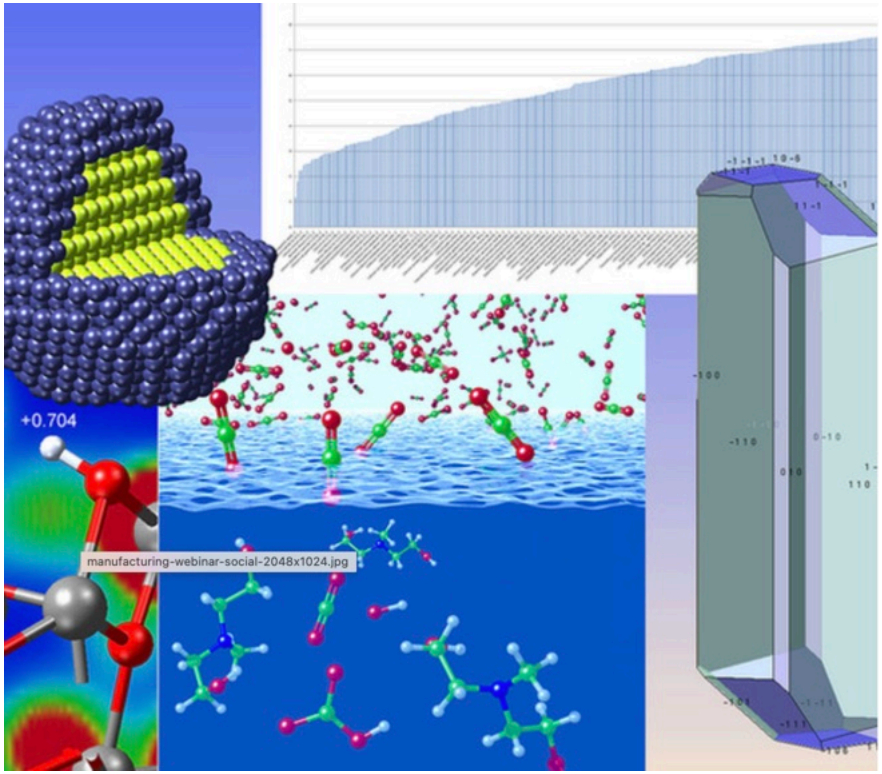
"The efficient computation of constructive methods in applied mathematics"

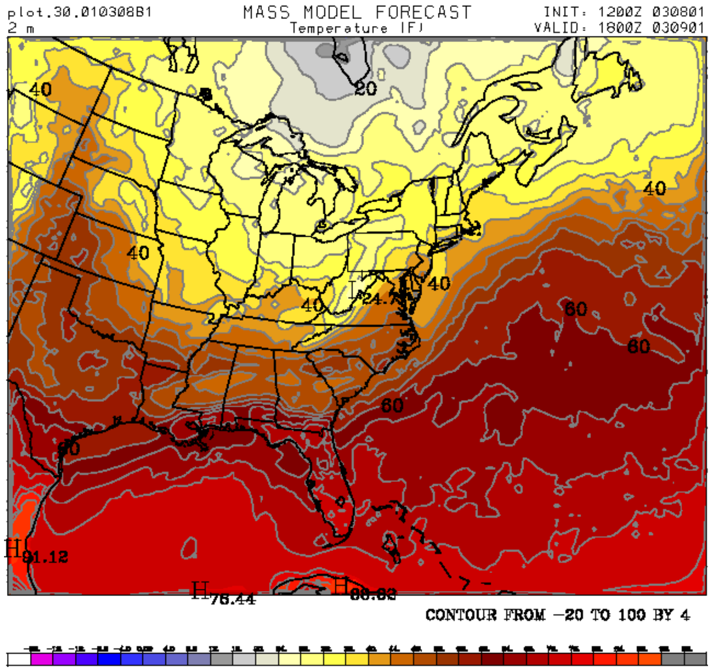
- Applied math: getting results out of application areas
- Numerical analysis: results need to be correctly and efficiently computable
- Computing: the algorithms need to be implemented on modern hardware

Examples of Scientific Computing

(*it really is everywhere*)

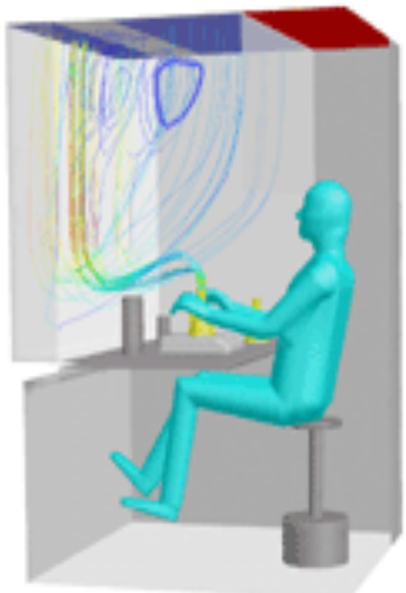
Material Science





Weather Forecasting

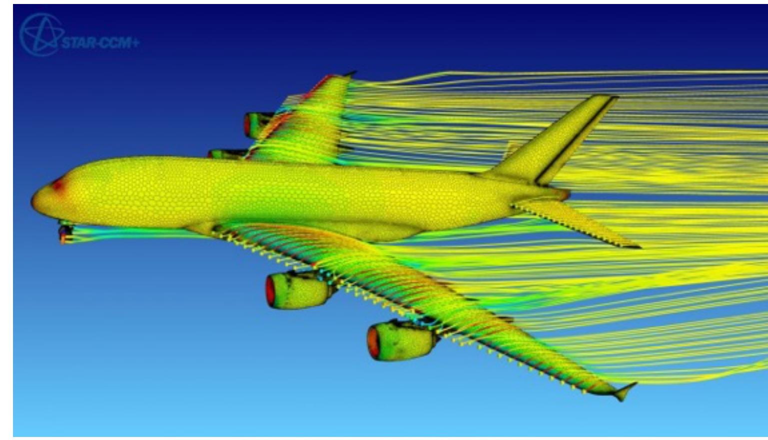
Examples of Scientific Computing
(*it really is everywhere*)

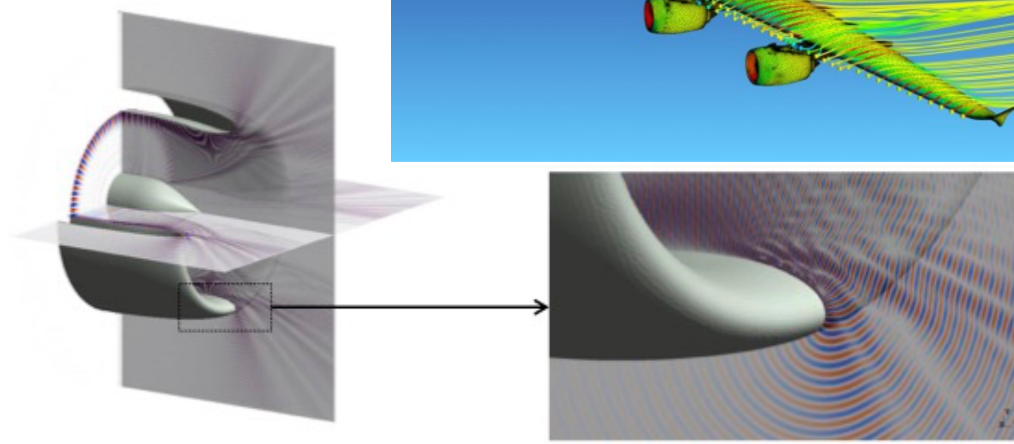


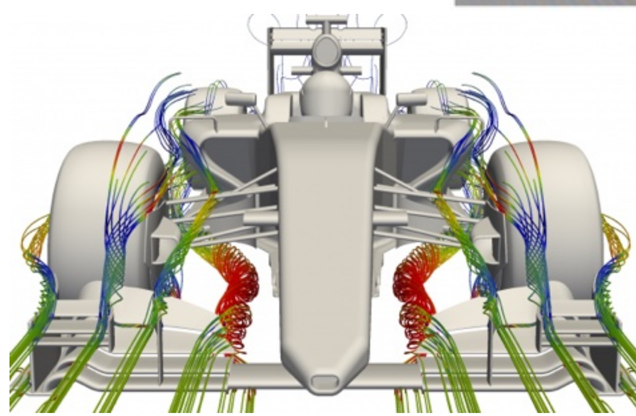
Streamlines for workstation ventilation

Heating, ventilation, and air conditioning

Aerospace





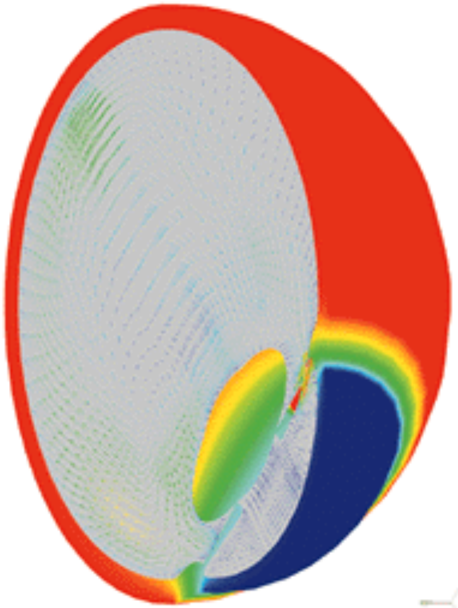


Automotive

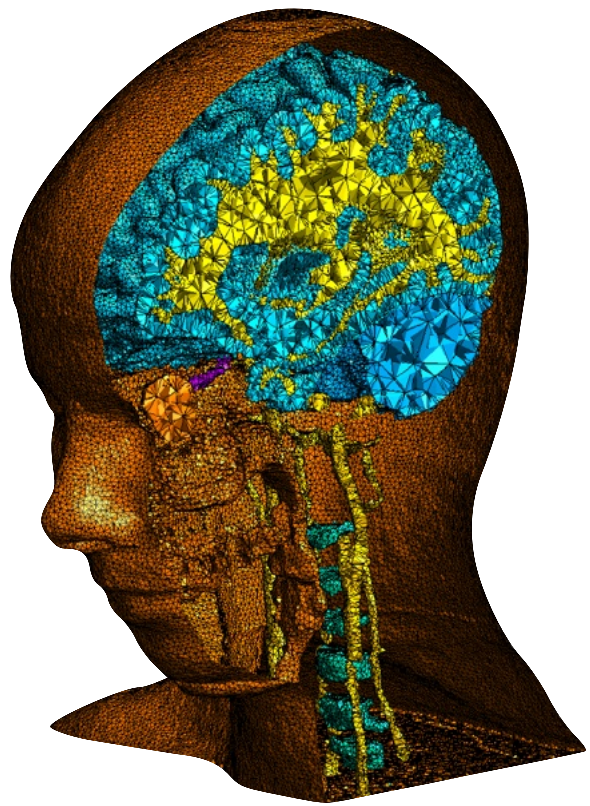
Examples of Scientific Computing

(*it really is everywhere*)

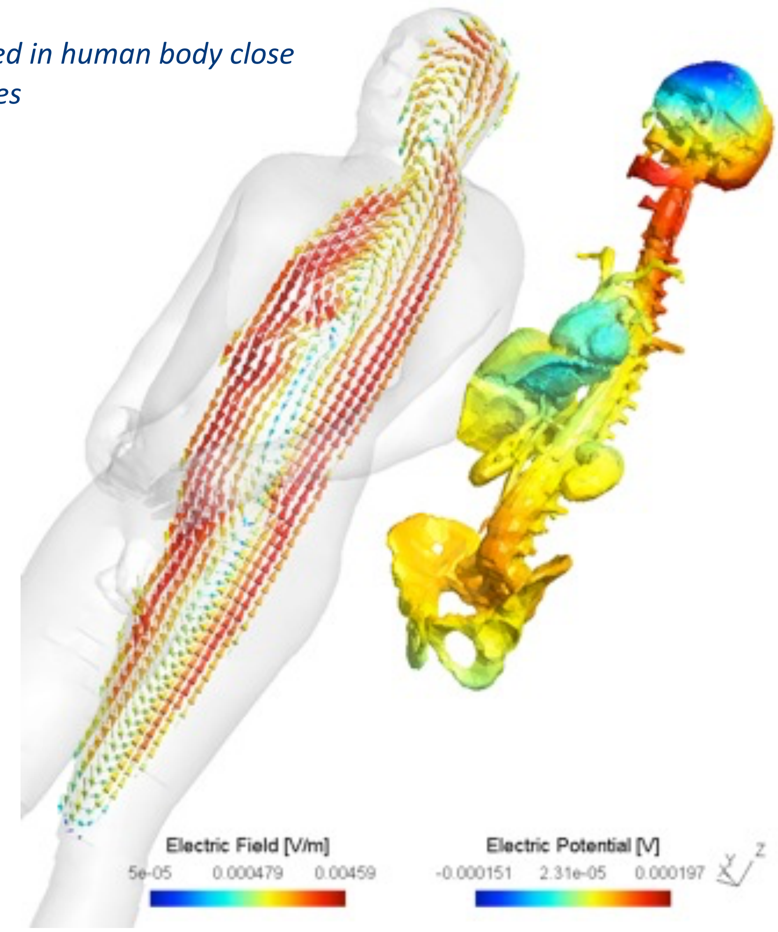
Biomedical engineering



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

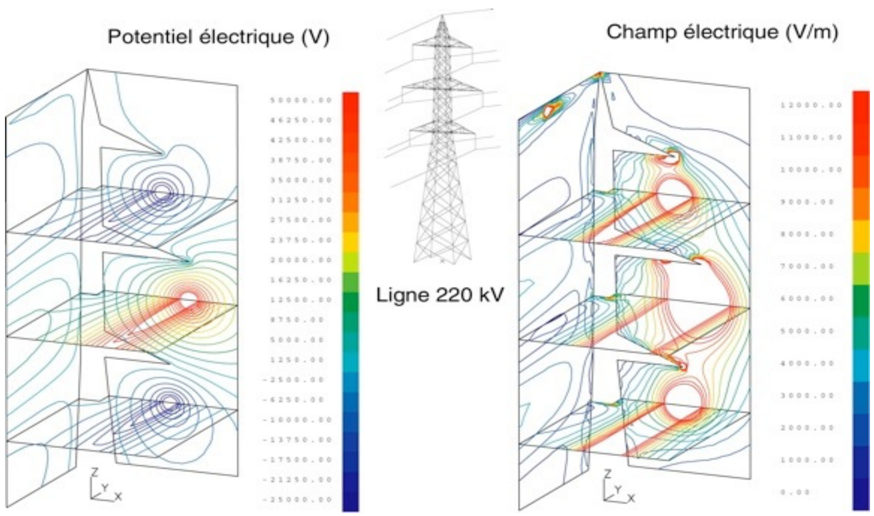


Fields induced in human body close to power lines

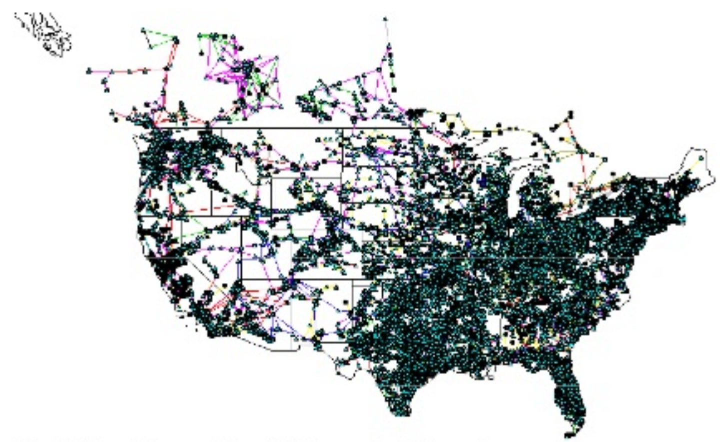


Examples of Scientific Computing

(*it really is everywhere*)



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

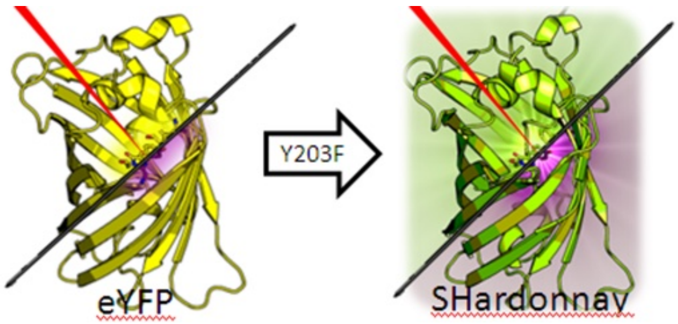
A report on the Aug. 14 blackout identifies specific lapses by various parties, including FirstEnergy's failure to react properly to the loss of a transmission line, people who have seen drafts of it say.

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

E-MAIL
PRINT
SINGLE-PAGE
REPRINTS
SAVE
SHARE

Examples of Scientific Computing

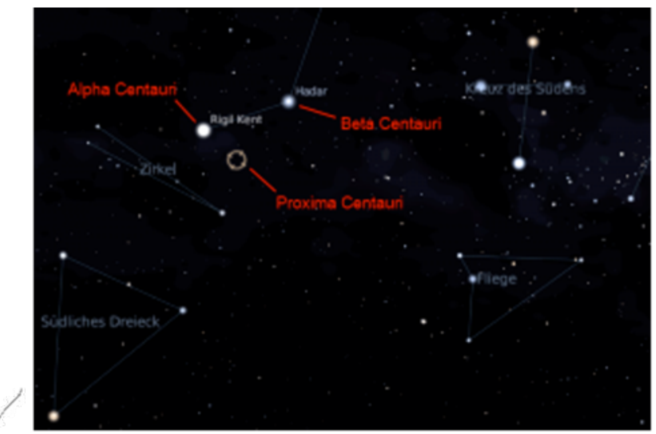
(it really is everywhere)



Fluorescent proteins for medical diagnostics

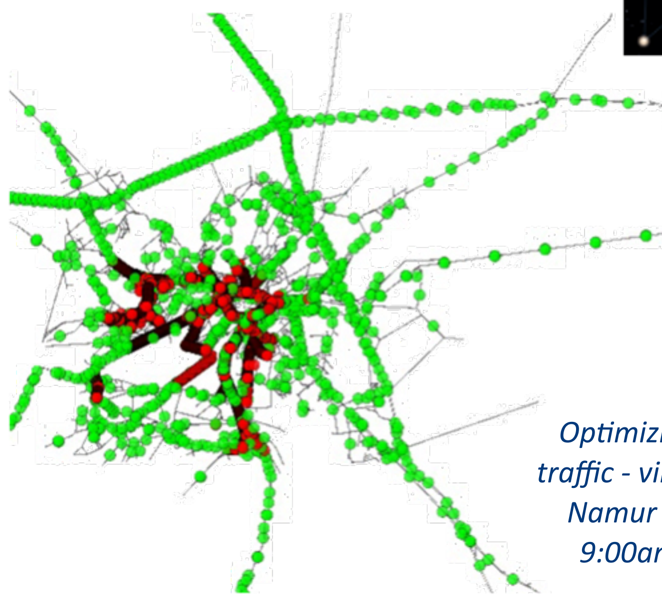
From the nanoscale...

Astronomy and planet habitability



... to the infinitely large

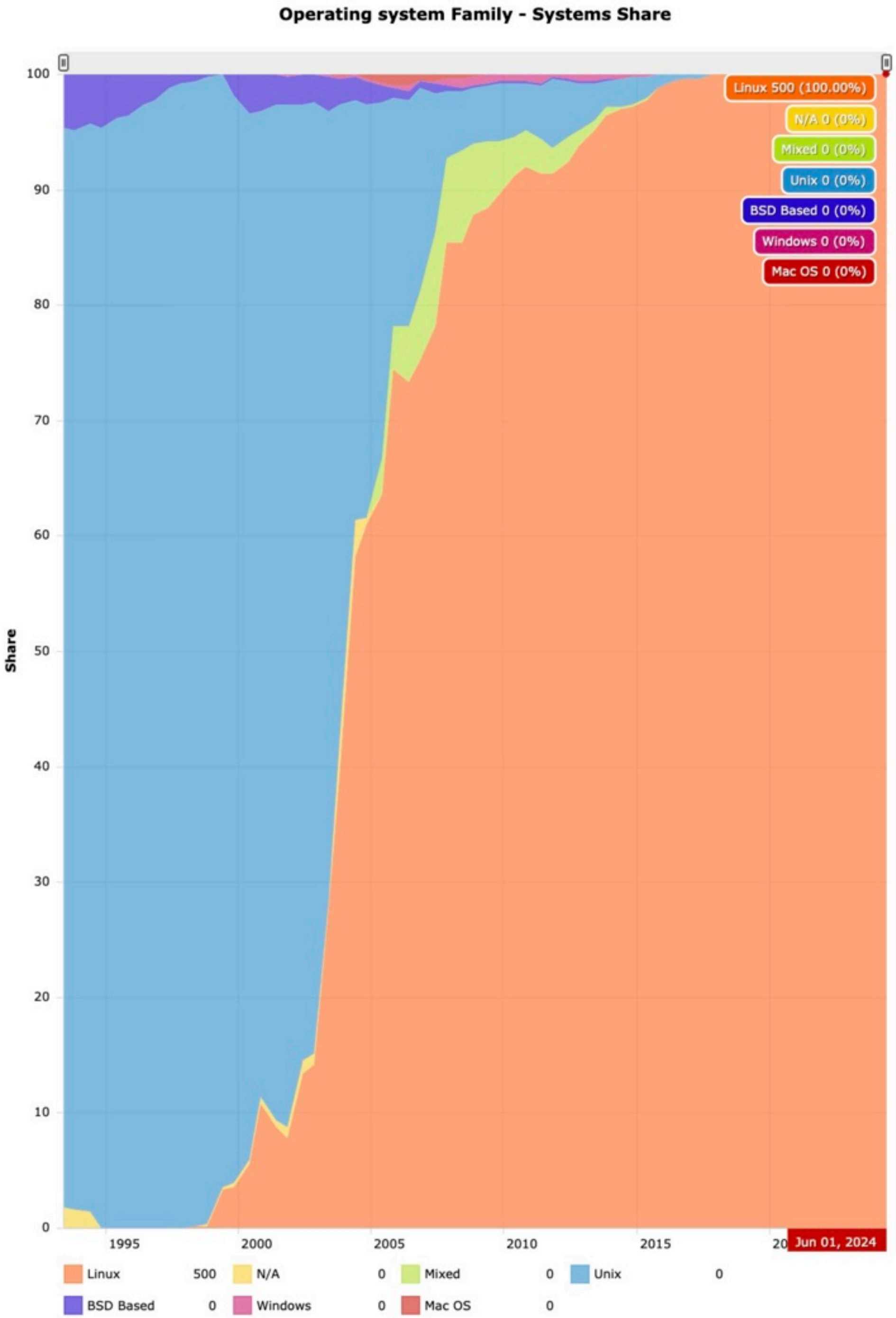
... to day-to-day living ...



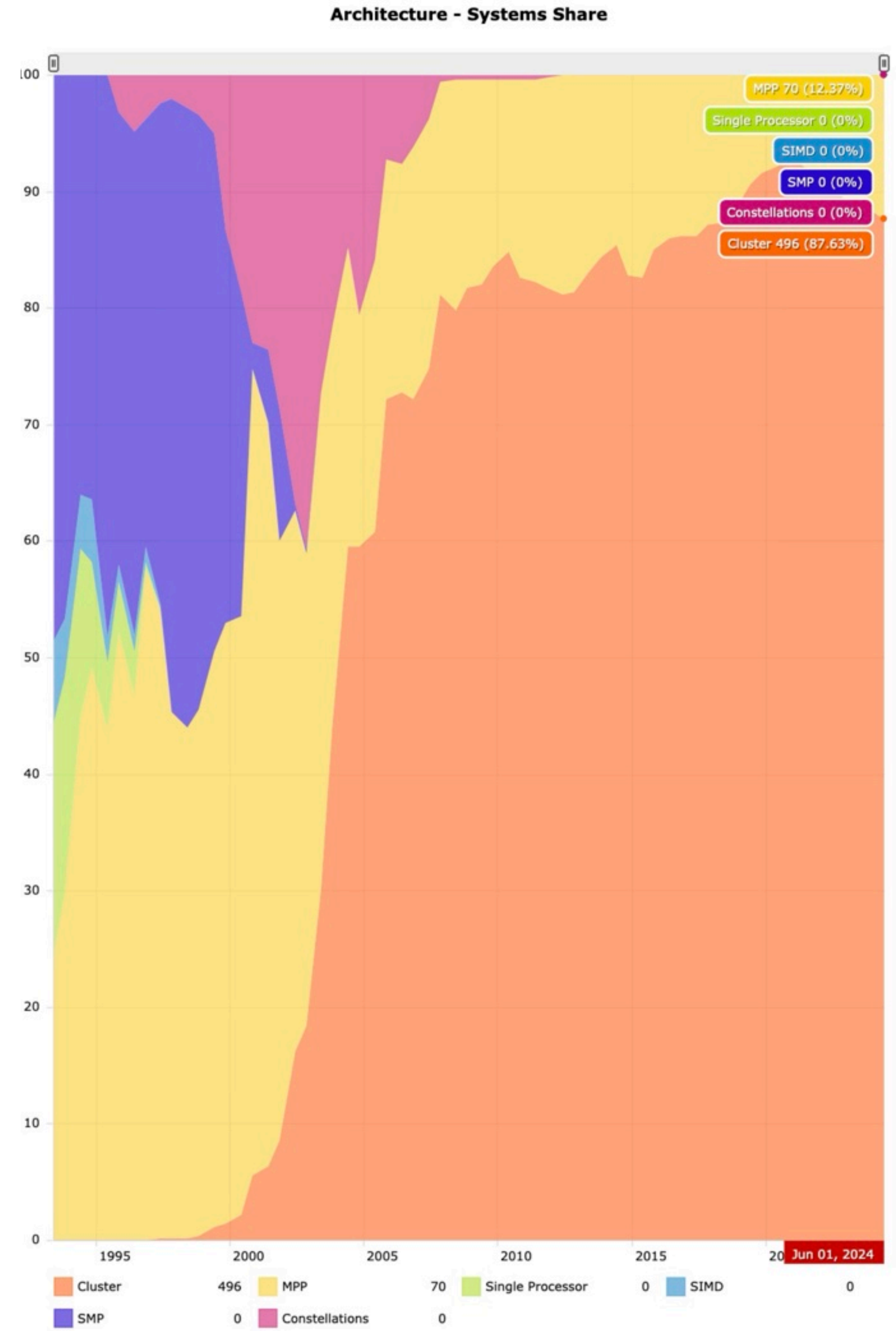
Optimizing traffic - virtual Namur at 9:00am

The Top500 List

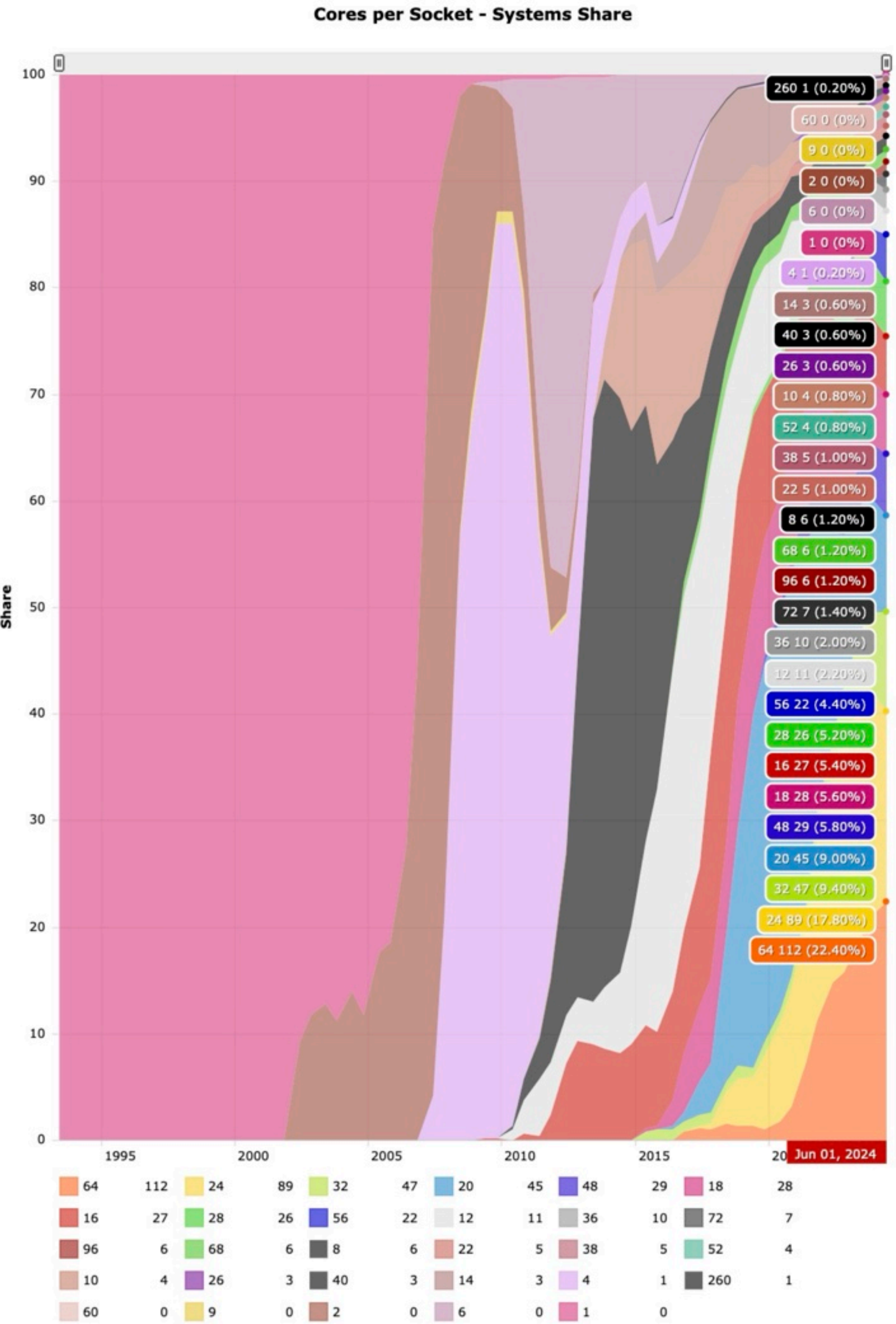
- http://www.top500.org
- Owner submitted benchmark performance since 1993
  - based on a dense linear system solve
  - http://www.netlib.org/benchmark/hpl/



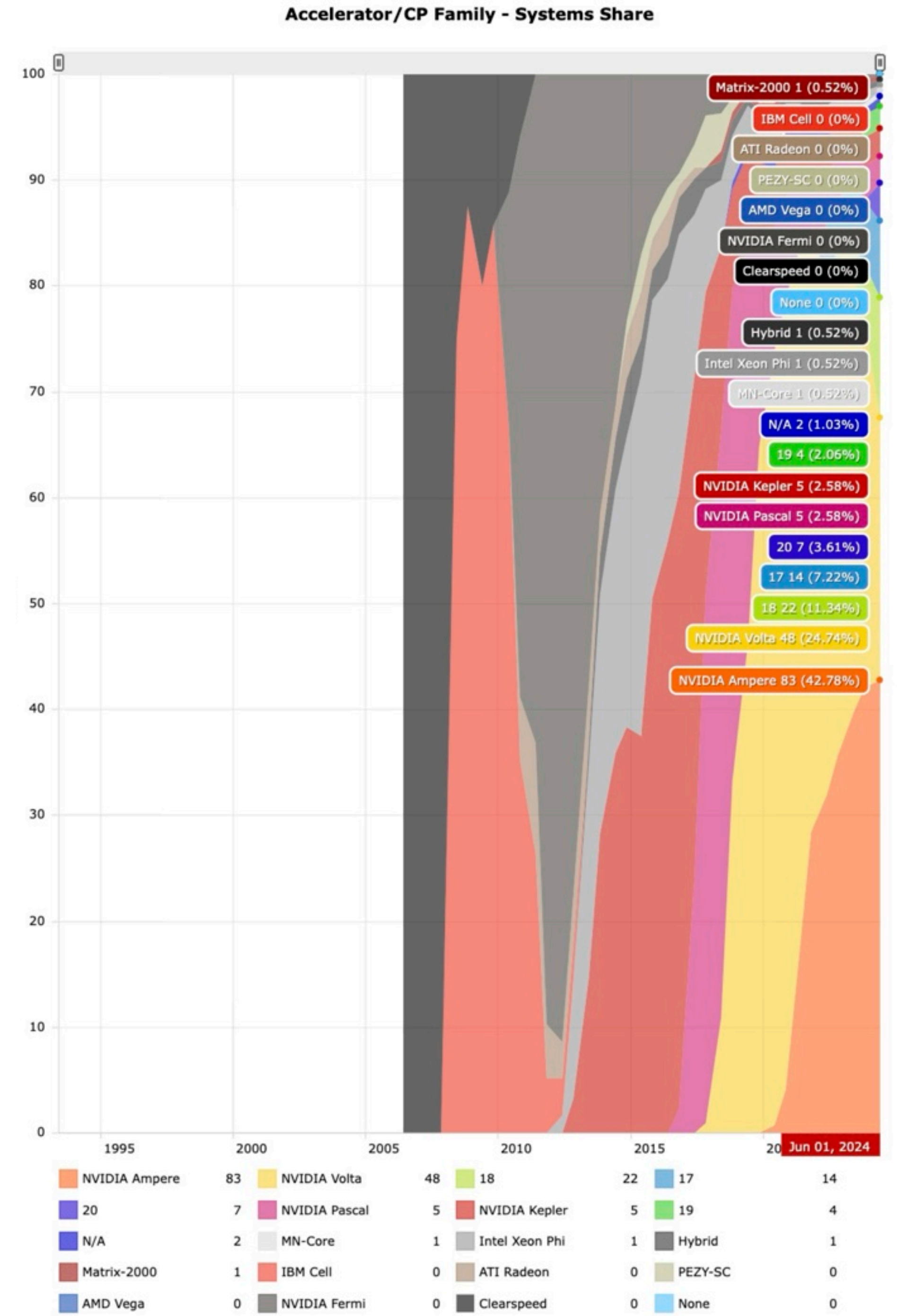
Operating system Family - Systems Share
Share
Linux 500 (100.00%)
N/A 0 (0%)
Mixed 0 (0%)
Unix 0 (0%)
BSD Based 0 (0%)
Windows 0 (0%)
Mac OS 0 (0%)
Jun 01, 2024
Linux 500
N/A 0
Mixed 0
Unix 0
BSD Based 0
Windows 0
Mac OS 0



Architecture - Systems Share
MPP 70 (12.37%)
Single Processor 0 (0%)
SIMD 0 (0%)
SMP 0 (0%)
Constellations 0 (0%)
Cluster 496 (87.63%)
Jun 01, 2024
Cluster 496
MPP 70
Single Processor 0
SIMD 0
SMP 0
Constellations 0

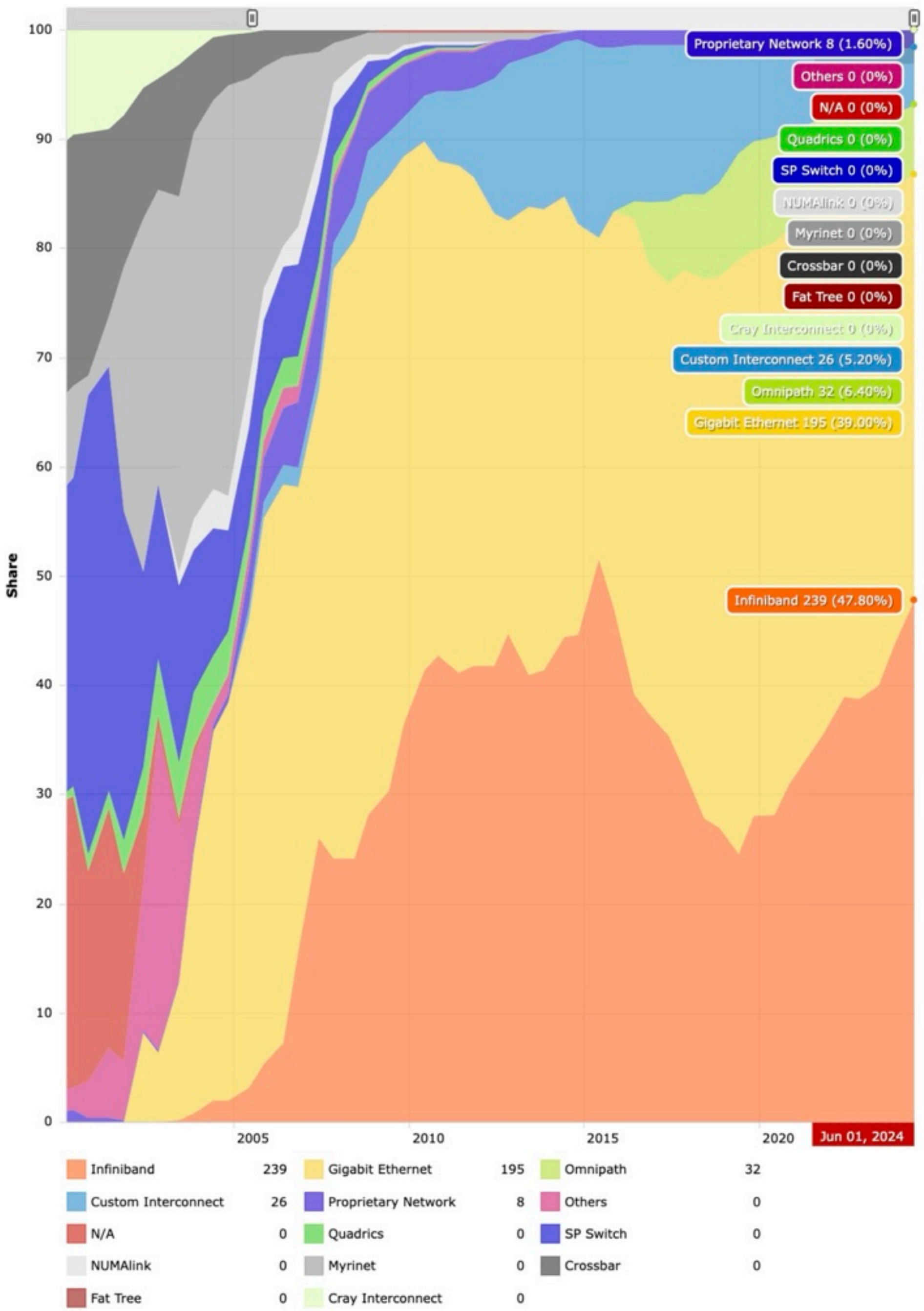


Cores per Socket - Systems Share
Share
Jun 01, 2024
260 1 (0.20%)
60 0 (0%)
9 0 (0%)
2 0 (0%)
6 0 (0%)
1 0 (0%)
4 1 (0.20%)
14 3 (0.60%)
40 3 (0.60%)
26 3 (0.60%)
10 4 (0.80%)
52 4 (0.80%)
38 5 (1.00%)
22 5 (1.00%)
8 6 (1.20%)
68 6 (1.20%)
96 6 (1.20%)
72 7 (1.40%)
36 10 (2.00%)
12 11 (2.20%)
56 22 (4.40%)
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%)
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

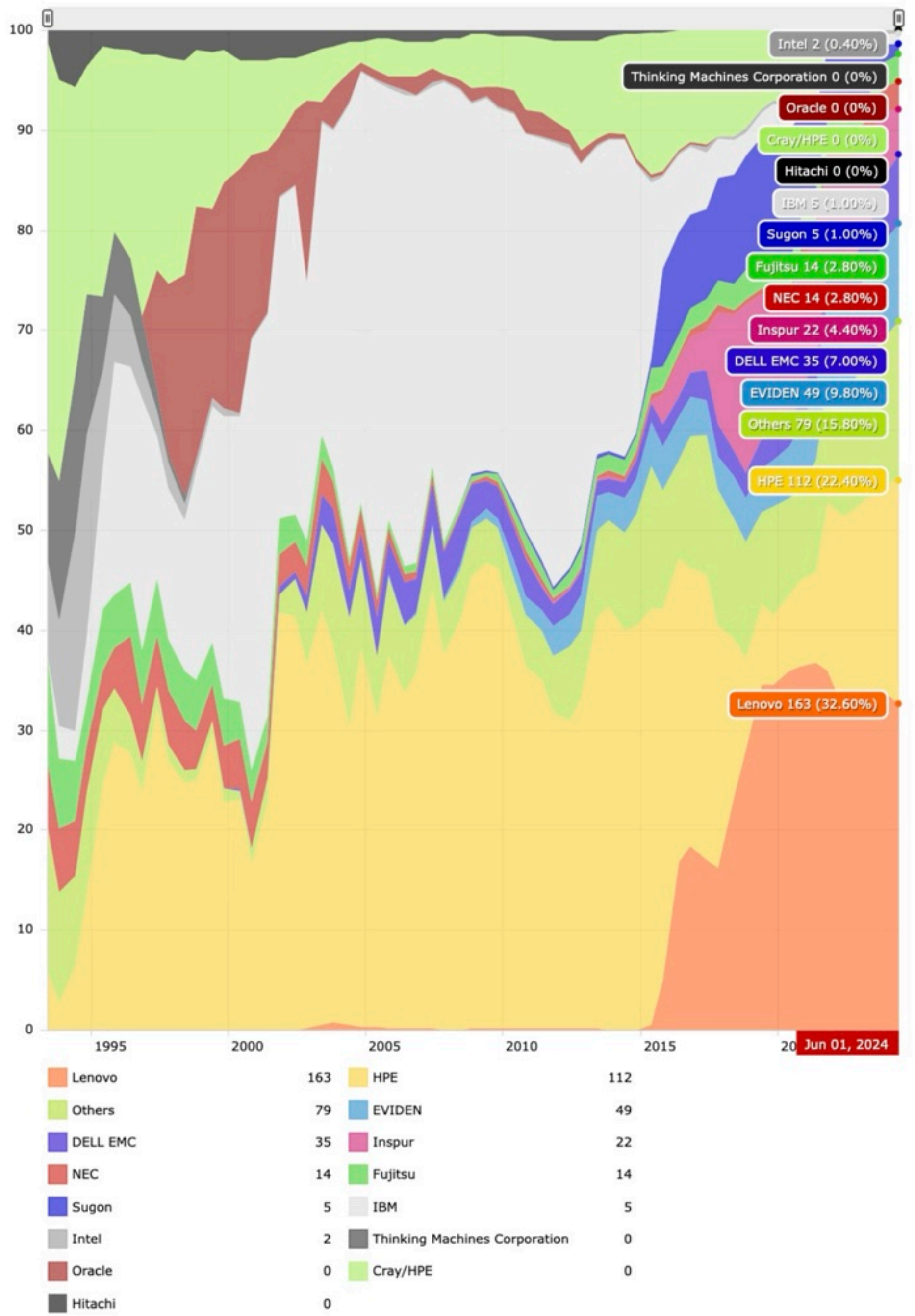


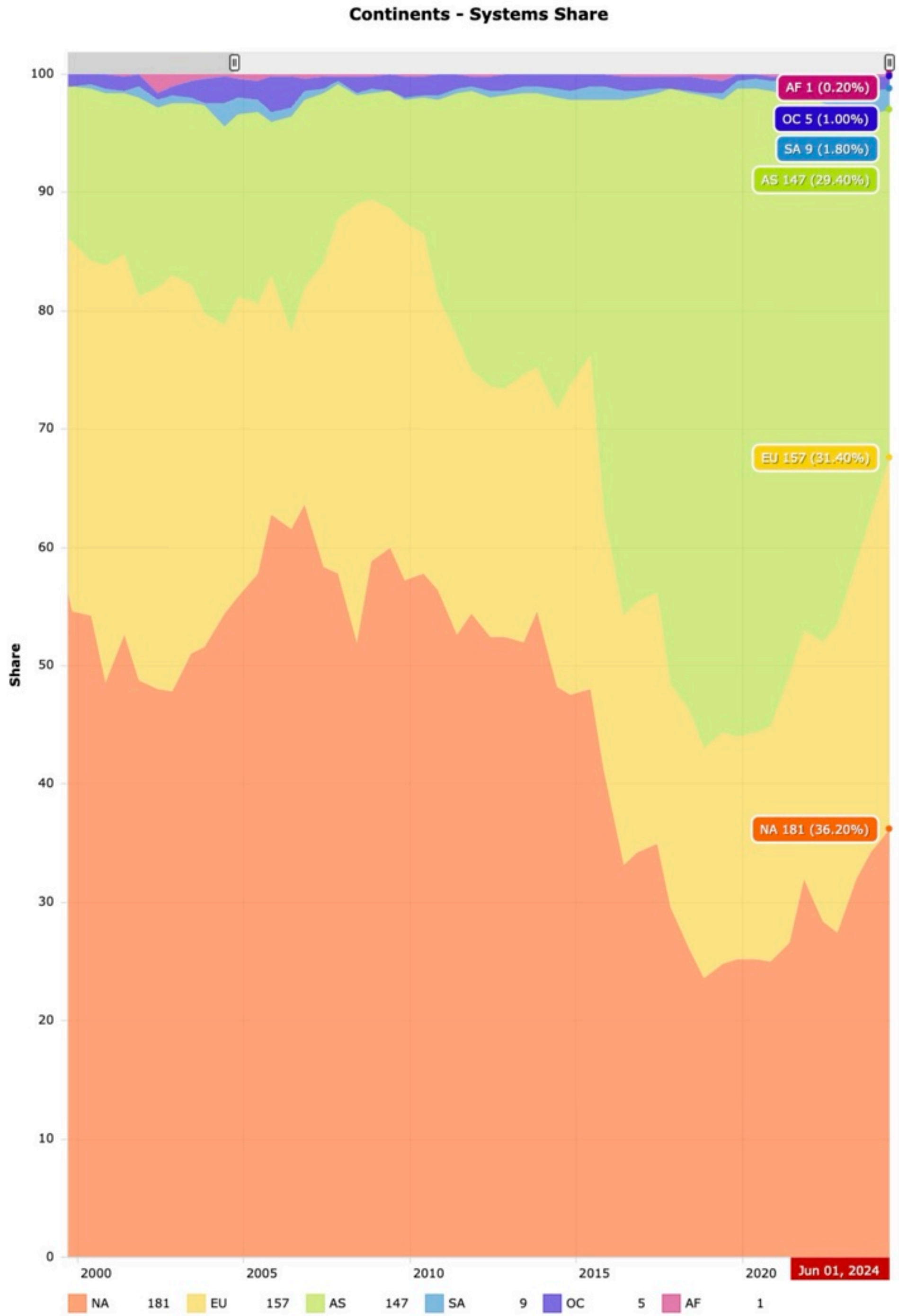
Accelerator/CP Family - Systems Share
Jun 01, 2024
Matrix-2000 1 (0.52%)
IBM Cell 0 (0%)
ATI Radeon 0 (0%)
PEZY-SC 0 (0%)
AMD Vega 0 (0%)
NVIDIA Fermi 0 (0%)
Clearspeed 0 (0%)
None 0 (0%)
Hybrid 1 (0.52%)
Intel Xeon Phi 1 (0.52%)
MN-Core 1 (0.52%)
N/A 2 (1.03%)
19 4 (2.06%)
NVIDIA Kepler 5 (2.58%)
NVIDIA 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%)
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

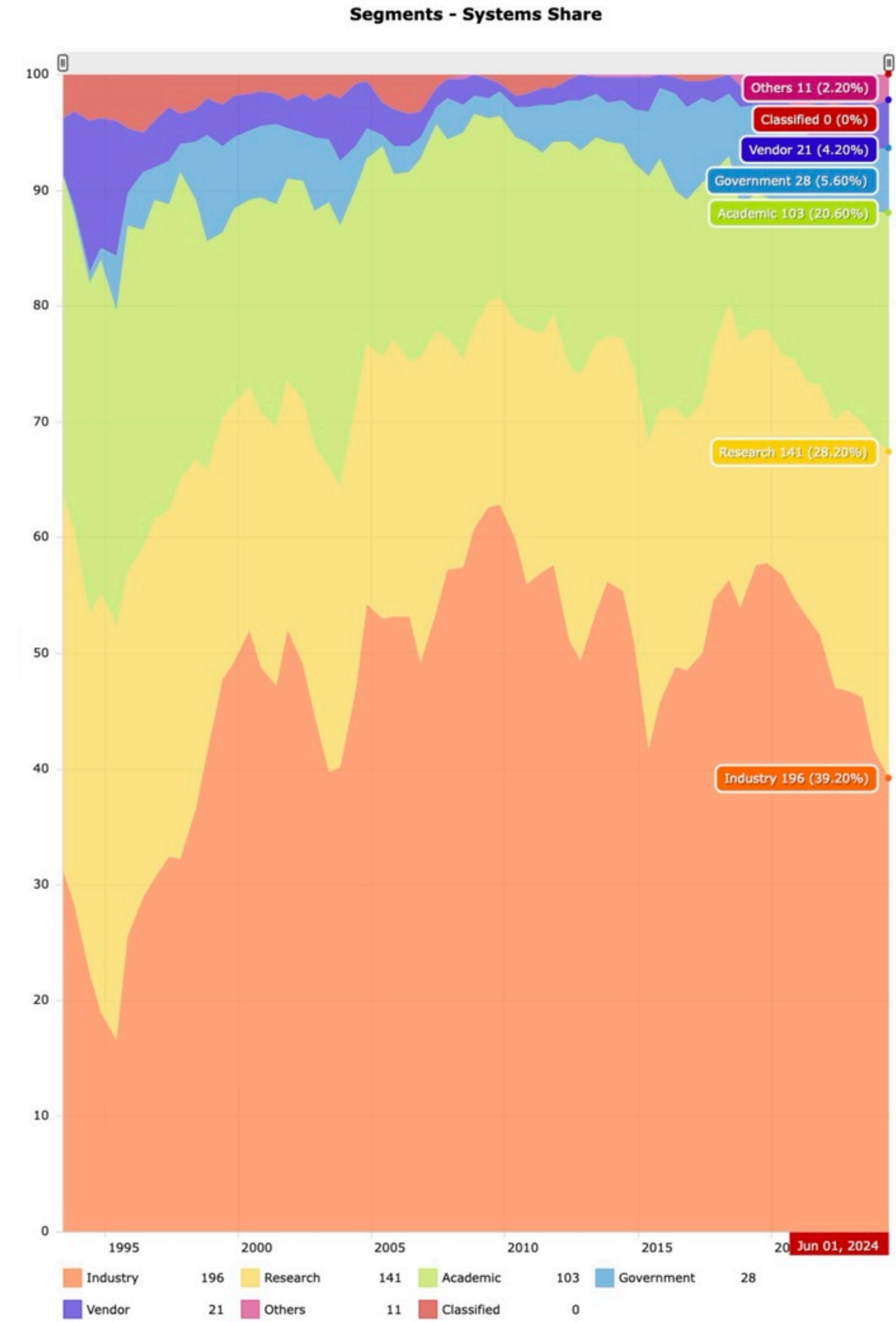
Interconnect Family - Systems Share



Vendors - Systems Share




Continents - Systems Share
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

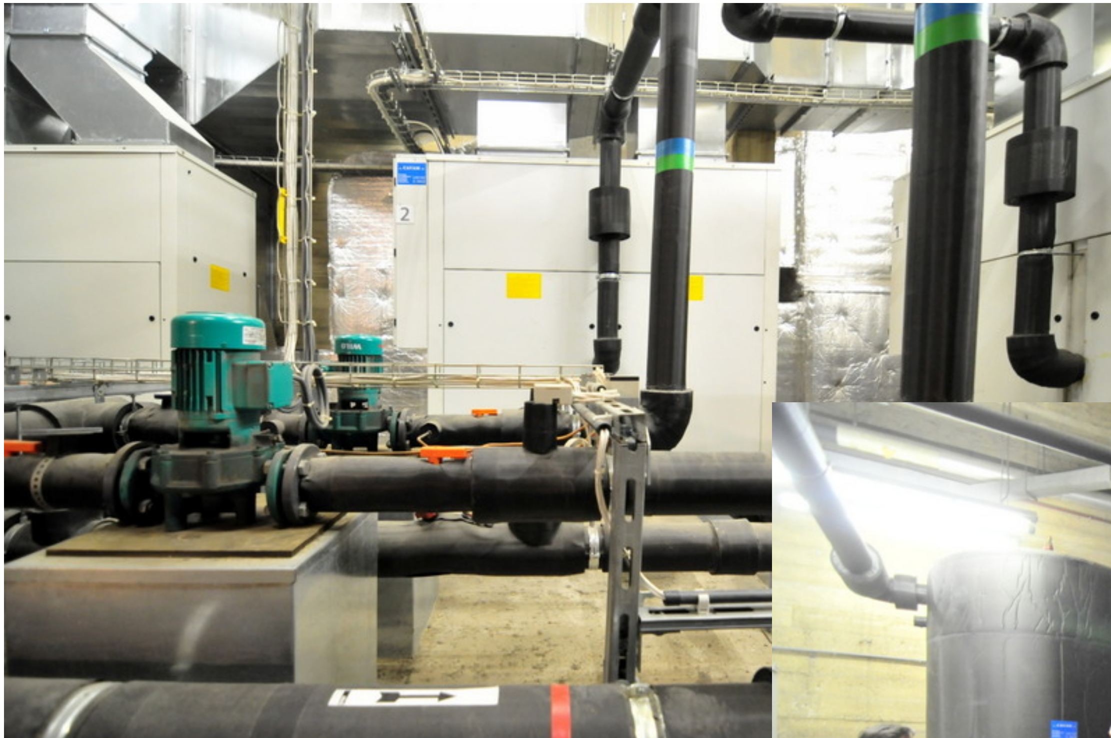
http://www.ceci-hpc.be

- 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
  - 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!

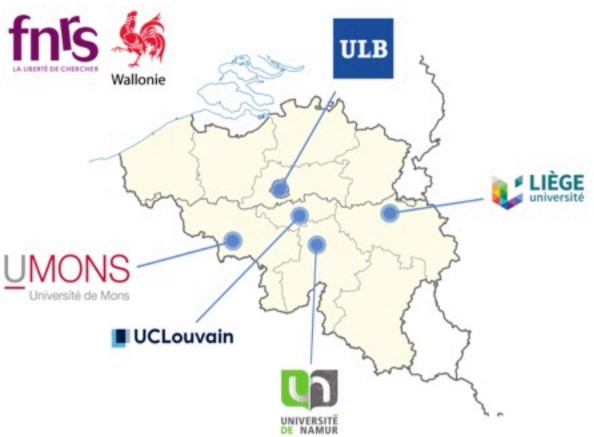
CÉCI Clusters News Training FAQ Documentation Status Support Contact Create/Manage Account

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.



Quick links

Latest News

TUESDAY, 06 MAY 2025

New LYRA cluster joining the CECI infrastructure!

The LYRA GPU/HTC cluster is now part of our HPC platform!

- 40 virtual nodes, each fitted with an NVIDIA RTX 6000 (48 GB)
- 32 CPU cores per node (24 for CPU-only workflows)

For a minimal submission example, see the updated documentation.

MONDAY, 03 FEBRUARY 2025

14th CÉCI Users Meeting at ULiège on April 25

ULiège will host the 14th CÉCI Users Meeting on April 25, 2025, featuring talks on HPC in scientific research and the future of CÉCI infrastructures. The event offers a great opportunity for researchers to connect with CÉCI sysadmins and board. Program and registration

SUNDAY, 01 SEPTEMBER 2024

Pieter Heremans is the new CÉCI logisticien

We are happy to announce the hire of a new CECI logisticien: Pieter Heremans. Welcome Pieter!