

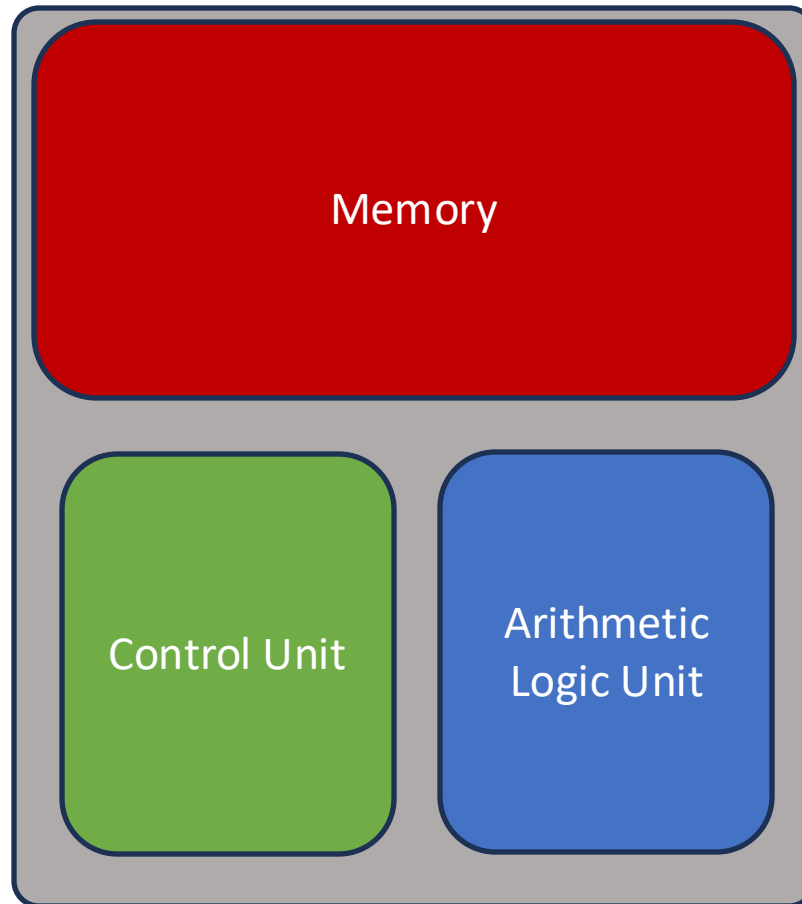
Energy Efficient Computing

Benjamin Czaja
HPC Advisor SURF
May 2025

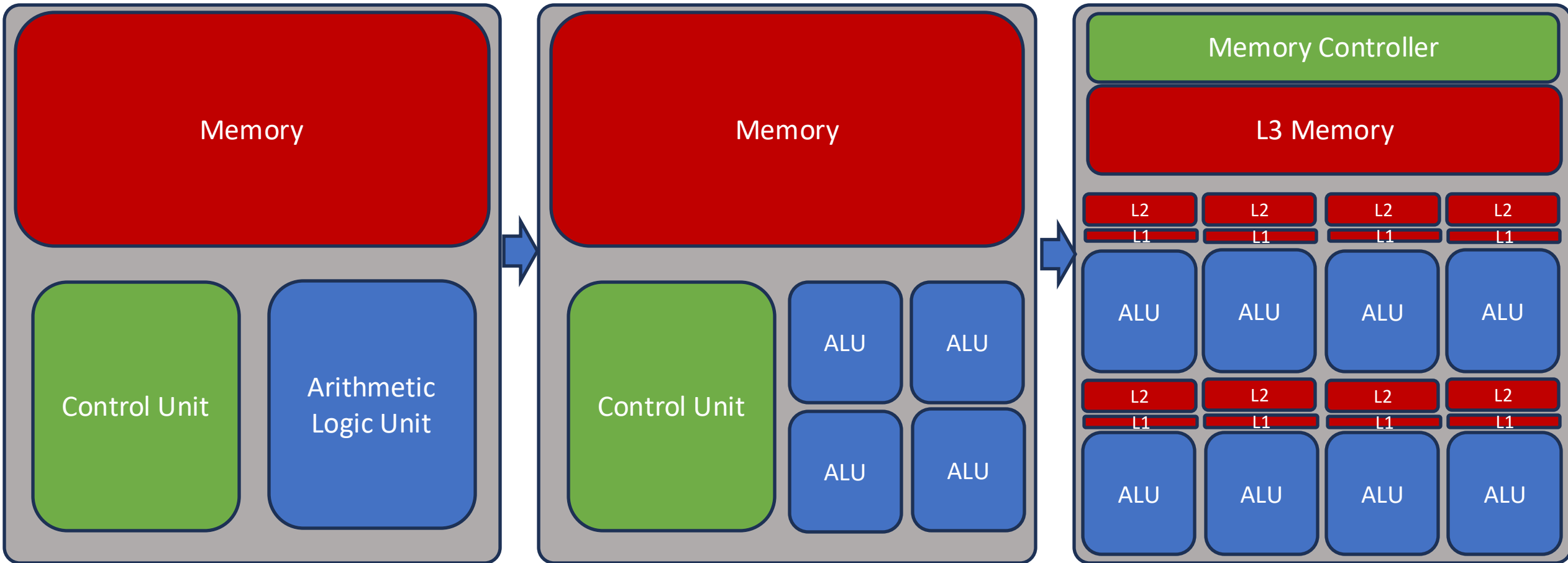
- We are becoming more energy efficient
- We are using more energy



Single “core” Processor/CPU

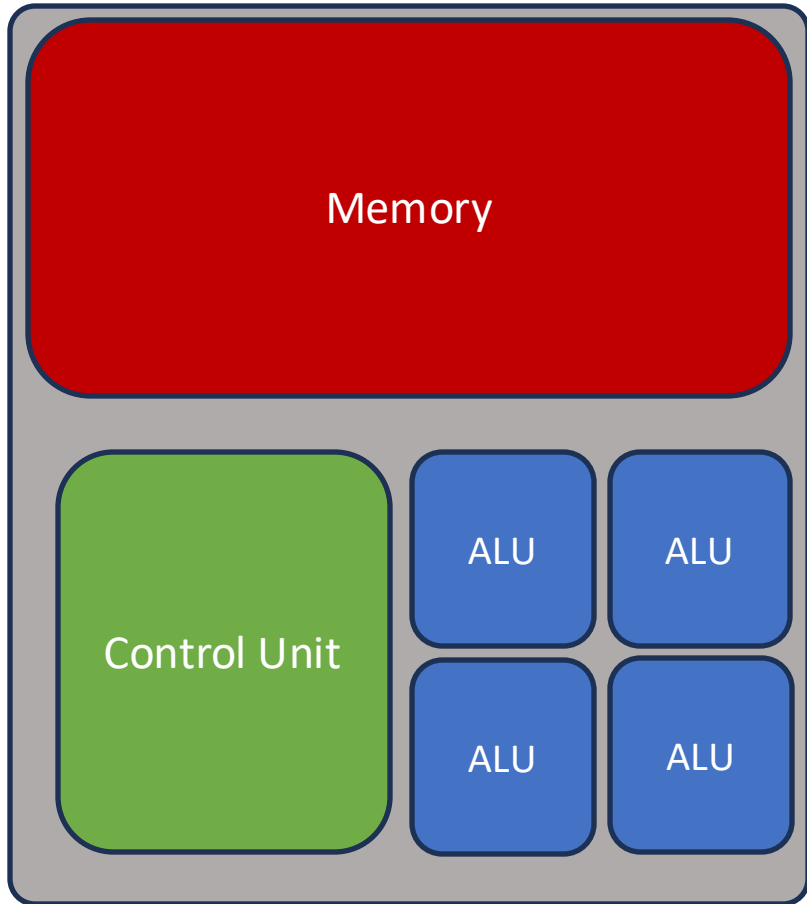


Single-core CPU to Multi-core CPU



Multi-core

4 cores



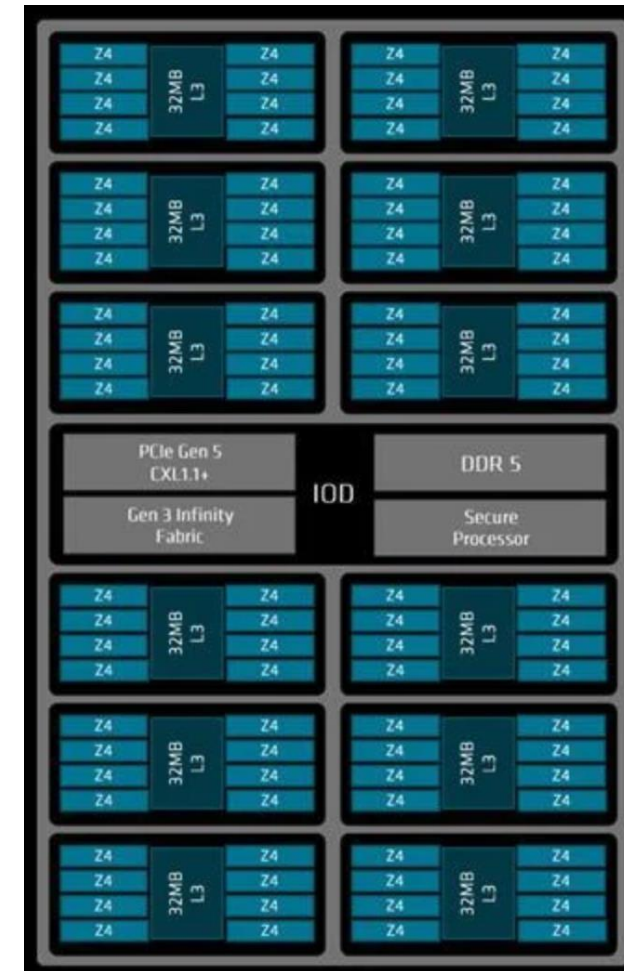
AMD Rome (Zen2)

64 cores

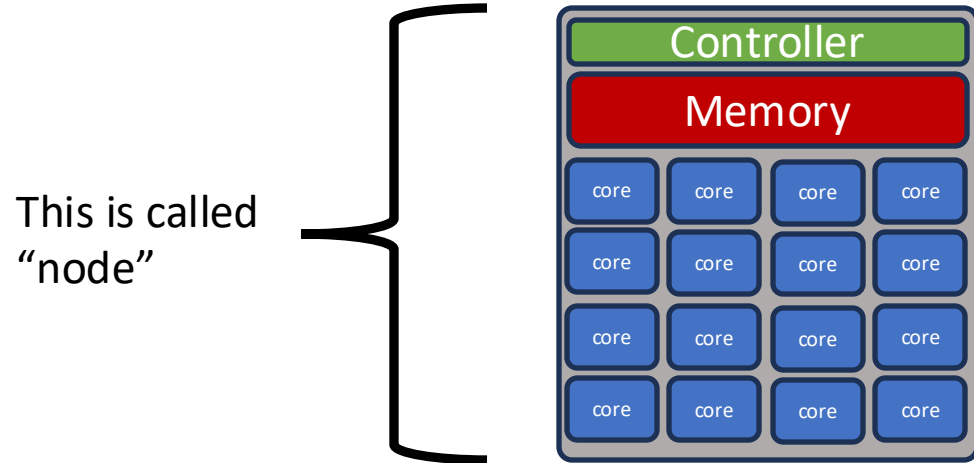


AMD Genoa (Zen4)

96 cores

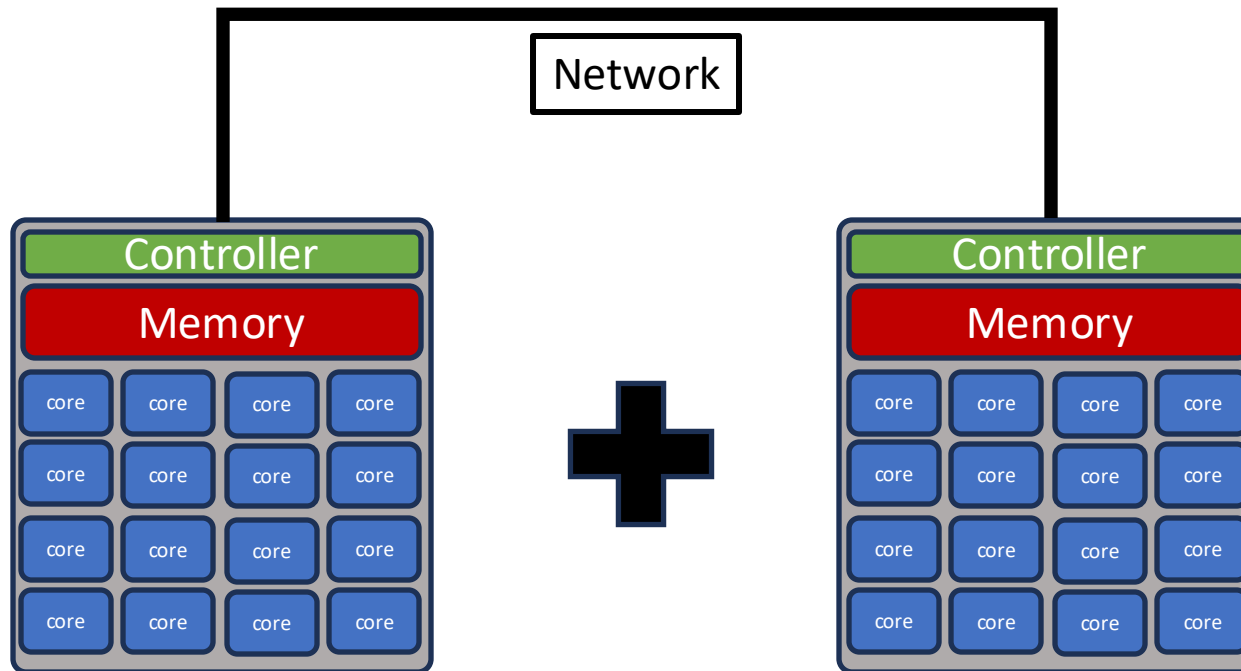


Lets Build a Compute Cluster



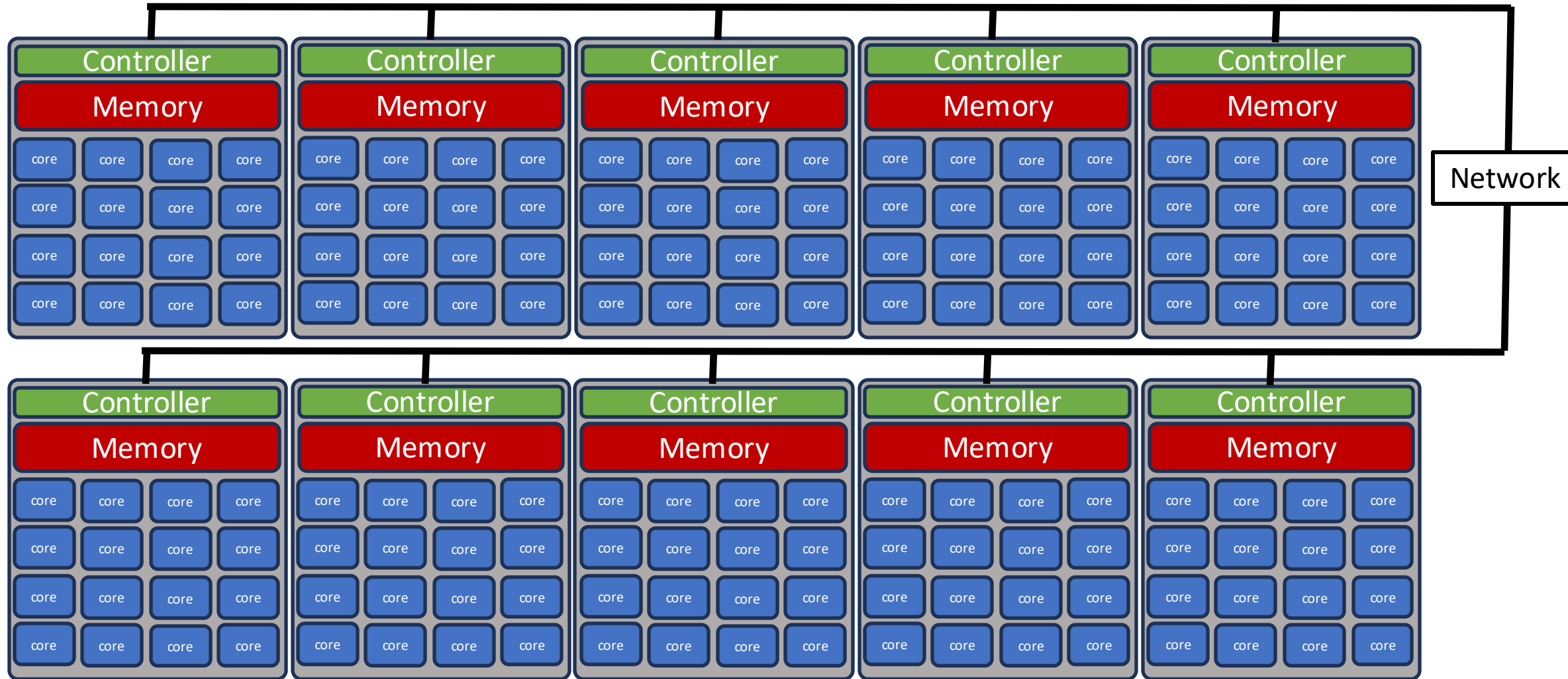
Lets take our theoretical 16 core CPU and connect it to more of the same CPUs

Lets Build a Compute Cluster



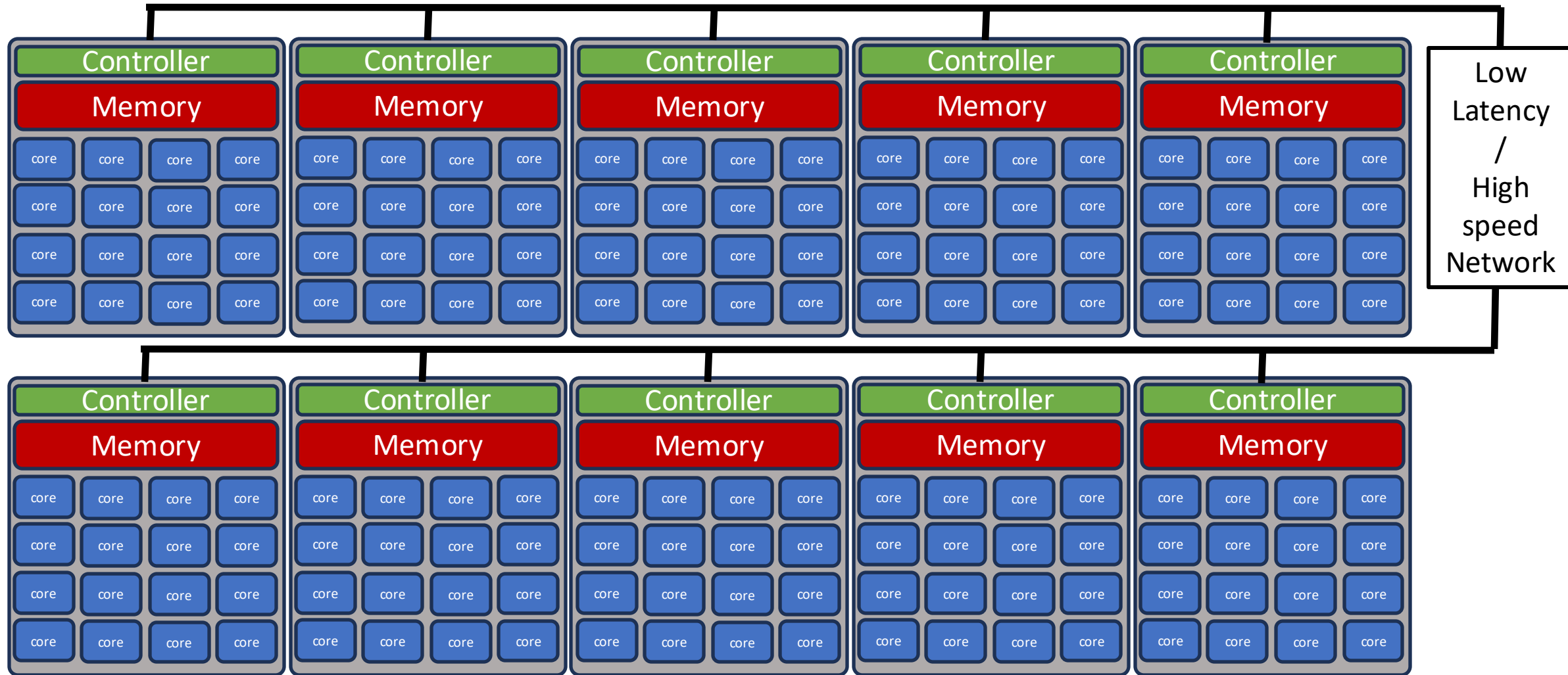
- We now have a 32 core machine!!
- Ok Ben's PowerPoint skills are limited

Lets Build a Compute Cluster



- We now have a 144 core machine!!
- Ok Ben's PowerPoint skills are limited

Lets Build a Supercomputer!!!!



- We now have a 144 core SUPERCOMPUTER!!
- Ok Ben's PowerPoint skills are limited

Snellius - Dutch National supercomputer

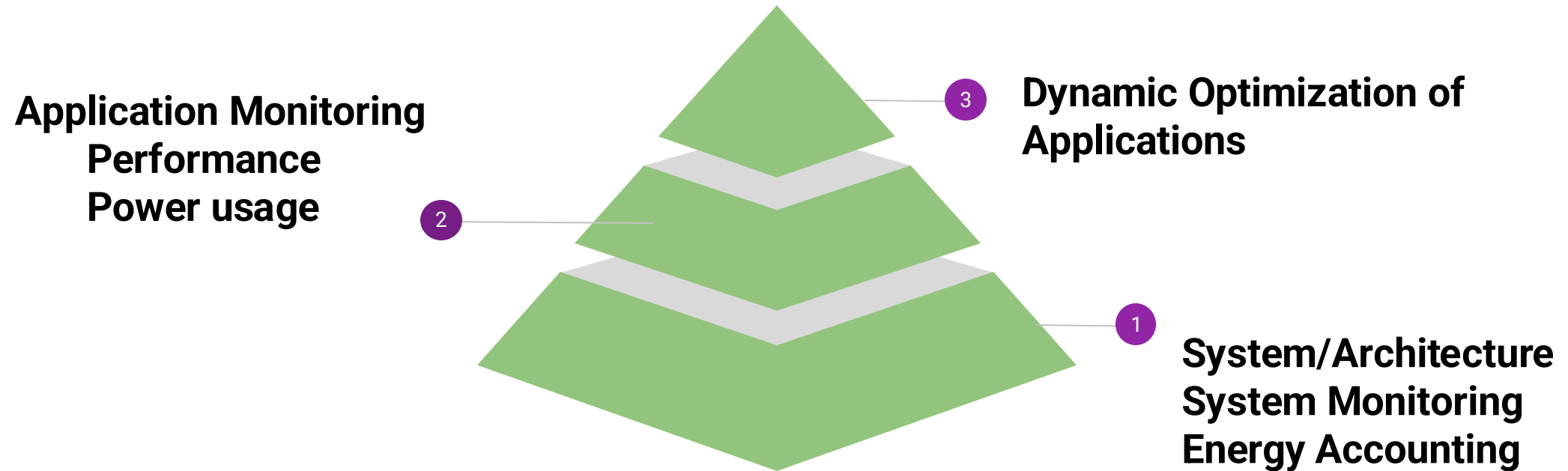
> 240,000 cores

- CPU partitions:
 - 522 thin-rome nodes (256 GiB) (128 cores)
 - 785 thin-geoa nodes (336 GiB) (192 cores)
 - 72 Fat nodes (1 TiB)
 - 4 high memory (2x 8 TiB, 2x 4 TiB)
- GPU partition (4x NVIDIA A100 GPUs):
 - 72 GPU (Intel Xeon Platinum 8360Y (2x) hosts)

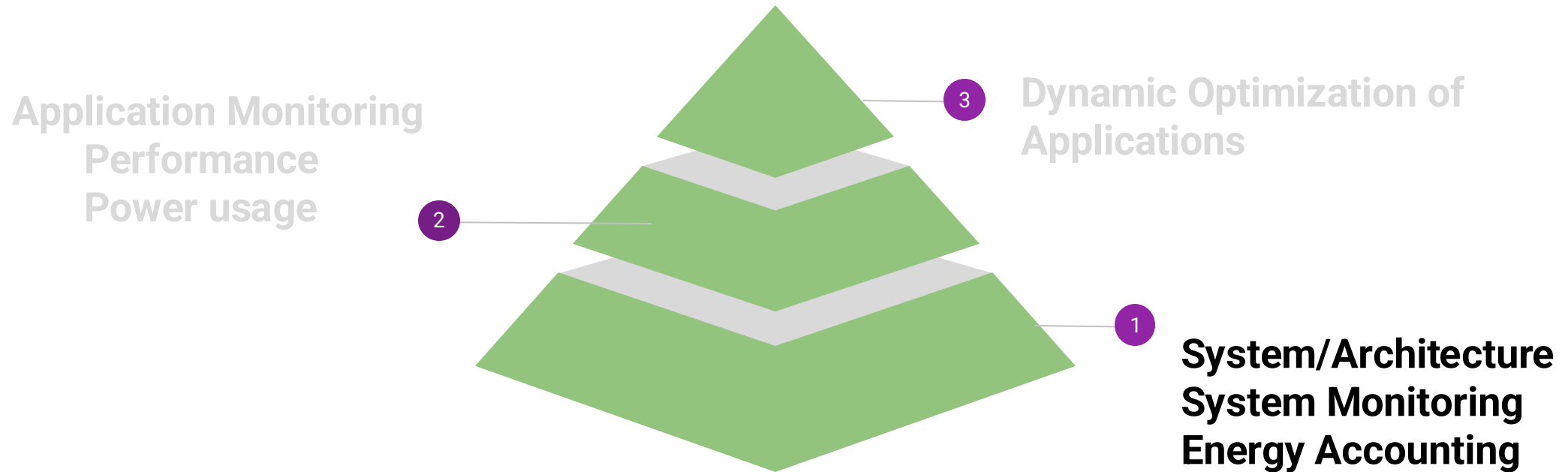
(#374) CPU: LINPACK Rmax (0.5 MW) 2.13 PFlop/s
(#176) GPU: LINPACK Rmax (0.13 MW) 3.6 PFlop/s



Energy-aware focus

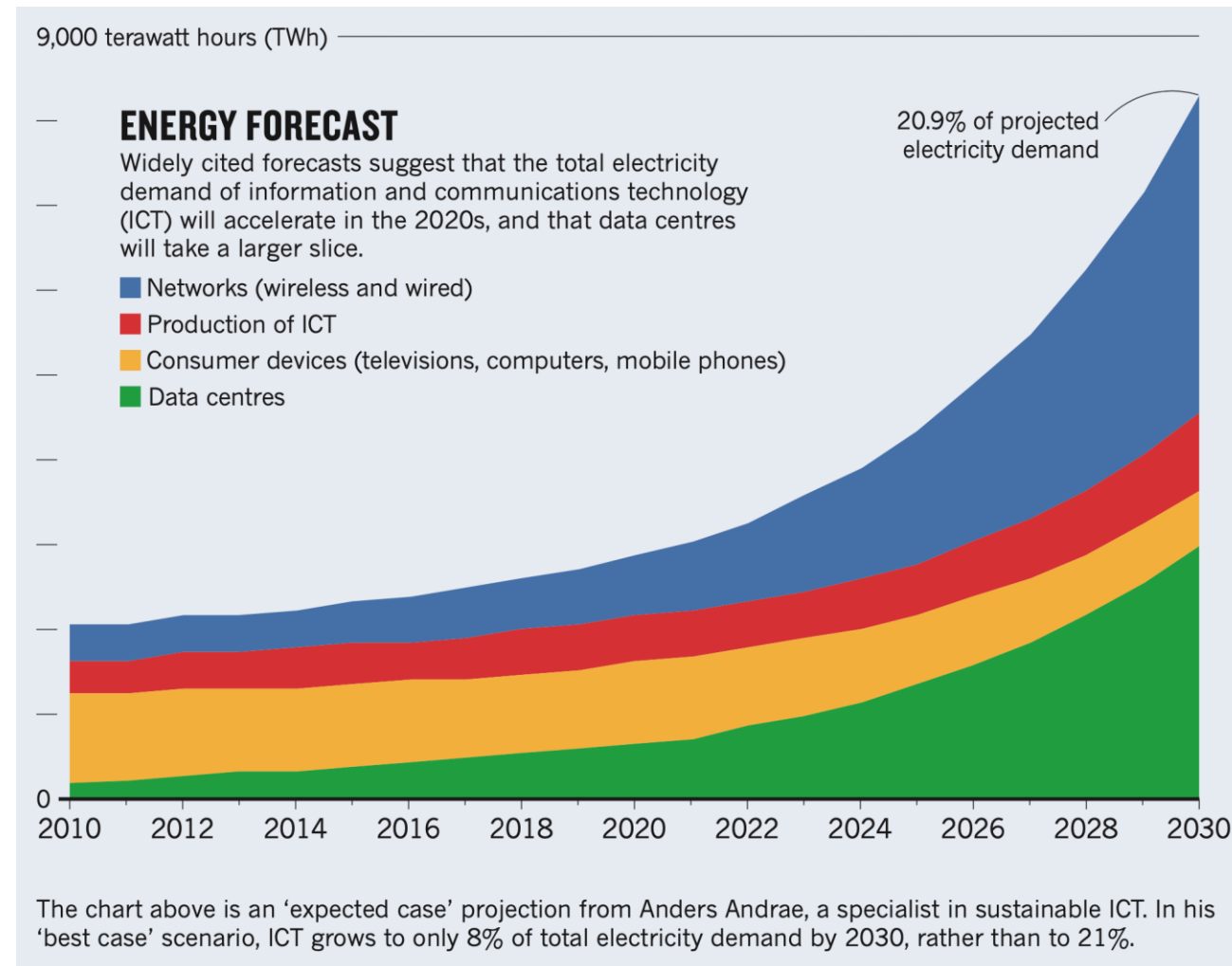


Energy-aware focus



ICT/Data center energy forecast

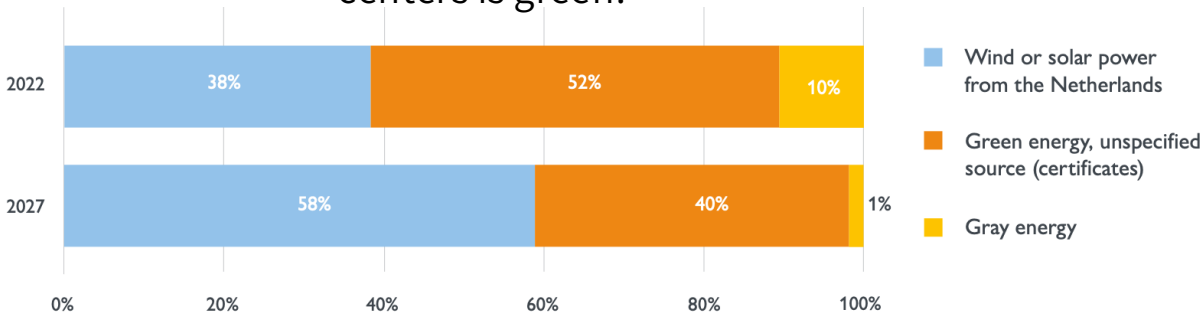
- Data centre energy usage:
 - ~ 200 TWh for data centres in 2018
 - ~ 3000 TWh in 2030
- Dutch Data Center Usage (2019)
 - 1300 MW installed capacity
 - 0.3 % electricity usage of the Netherlands (CBS)
 - 3x as much power than the NS



- Jones, Nicola. "How to stop data centres from gobbling up the world's electricity." *Nature* 561. 7722 (2018): 163-166.
- Andrae, Anders SG, and Tomas Edler. "On global electricity usage of communication technology: trends to 2030." *Challenges* 6.1 (2015): 117-157.
- Bakkeren, Hanno. "Datacenters verbruiken drie keer zoveel stroom als de NS". NRC, 14 May 2019
- State of the Dutch Data Centers, The Dutch Data Center Report, 2022, <https://www.dutchdatacenters.nl/>

ICT/Data center energy forecast

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 - ~ 200 TWh for data centres in 2018
 - ~ 3000 TWh in 2030
- Dutch Data Center Usage (2019)
 - 1300 MW installed capacity
 - 0.3 % electricity usage of the Netherlands (CBS)
 - 3x as much power than the NS
- Dutch Data center energy consumption (2022)
 - 90% of all energy consumed by colocation data centers is green.



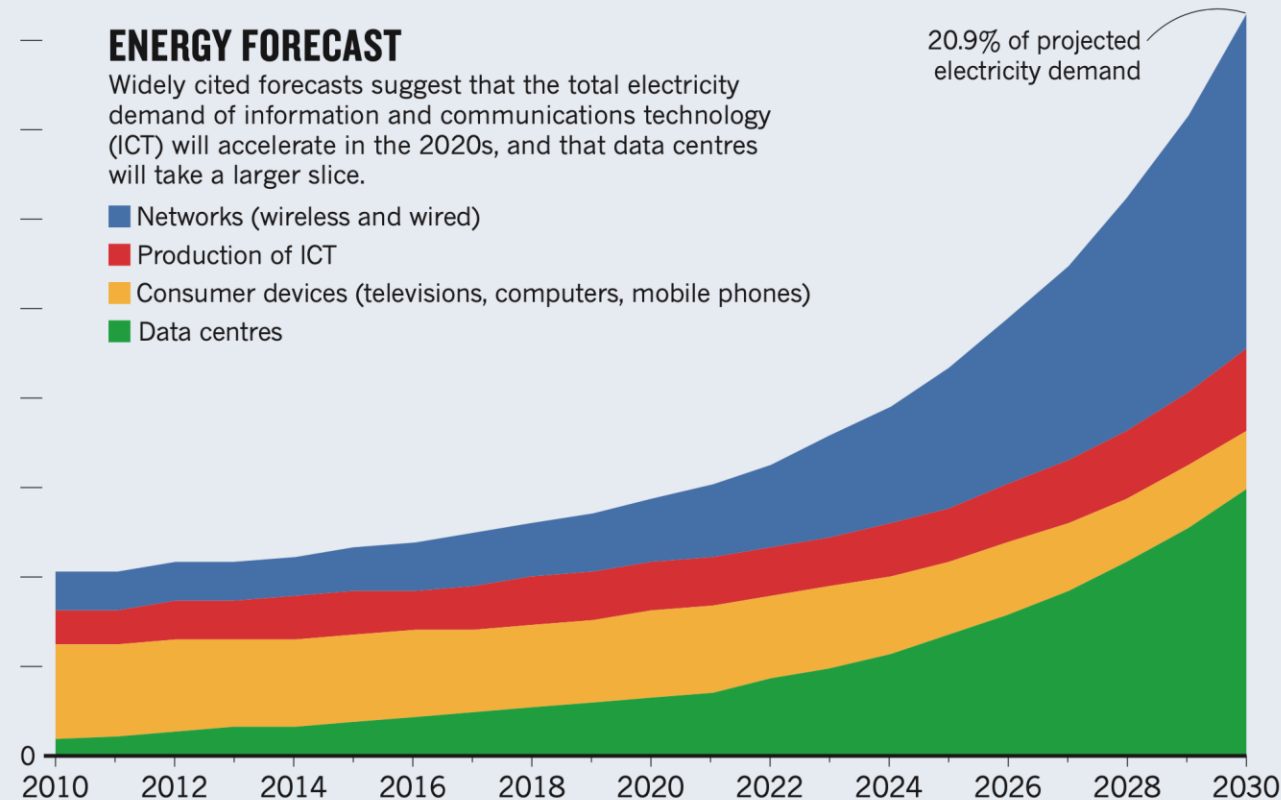
9,000 terawatt hours (TWh)

ENERGY FORECAST

Widely cited forecasts suggest that the total electricity demand of information and communications technology (ICT) will accelerate in the 2020s, and that data centres will take a larger slice.

- Networks (wireless and wired)
- Production of ICT
- Consumer devices (televisions, computers, mobile phones)
- Data centres

20.9% of projected electricity demand



The chart above is an 'expected case' projection from Anders Andrae, a specialist in sustainable ICT. In his 'best case' scenario, ICT grows to only 8% of total electricity demand by 2030, rather than to 21%.

- Jones, Nicola. "How to stop data centres from gobbling up the world's electricity." *Nature* 561. 7722 (2018): 163-166.
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Top 500 (Nov-2024)

1. El Capitan-US (30 MW) 1,742.0 PFlops
2. Frontier-US (24 MW) 1,353.0 PFlop/s
3. Aurora-US (38 MW) 1,012.0 Pflop/s
4. Eagle-US, Microsoft (??) 561 Pflop/s
5. HP6 (8 MW) 477.01 PFlop/s

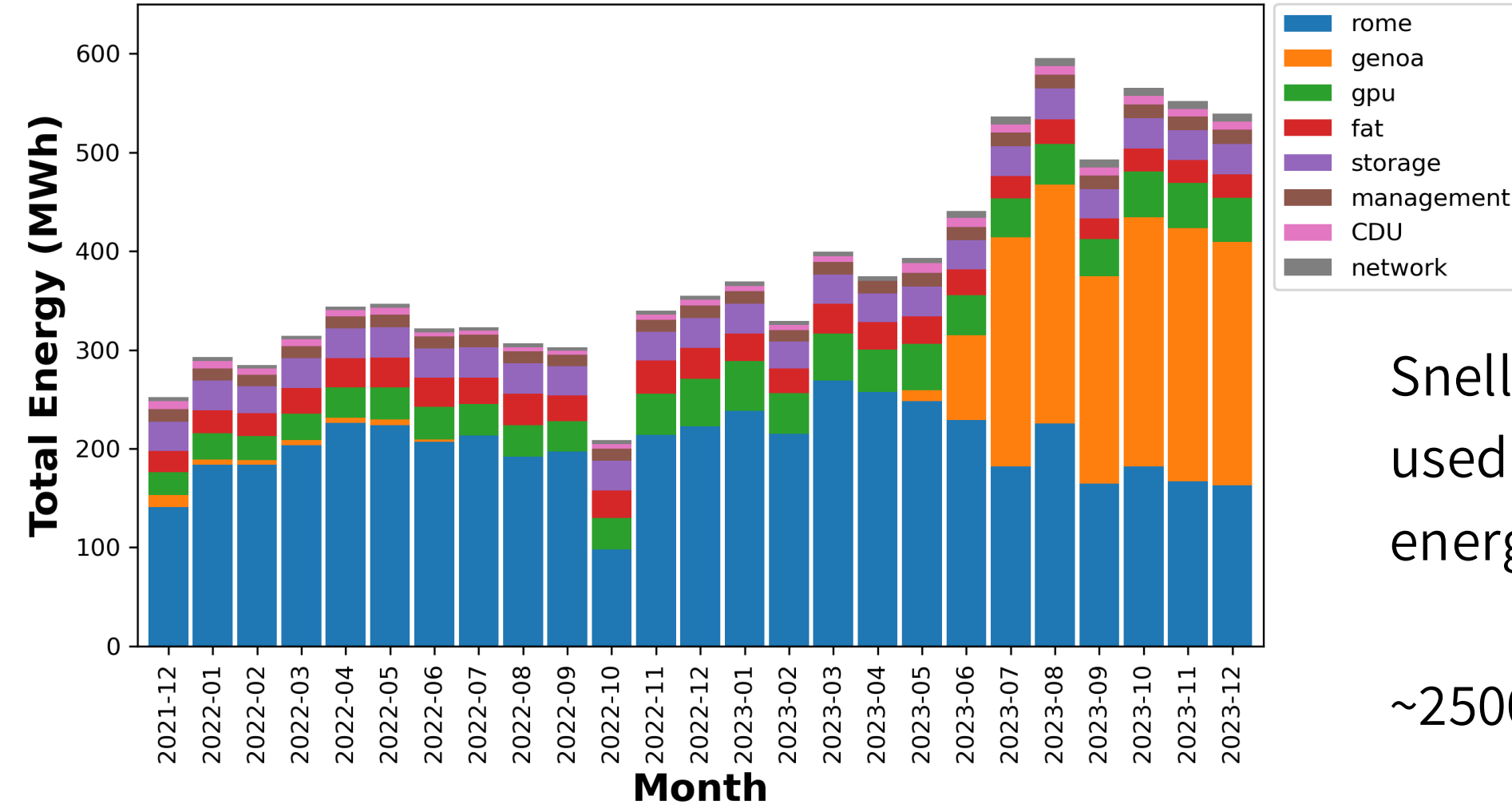
Snellius

(#197) CPU: LINPACK Rmax (0.8 MW) 5.4 PFlop/s

(#94) GPU: LINPACK Rmax (0.3 MW) 13.64 PFlop/s



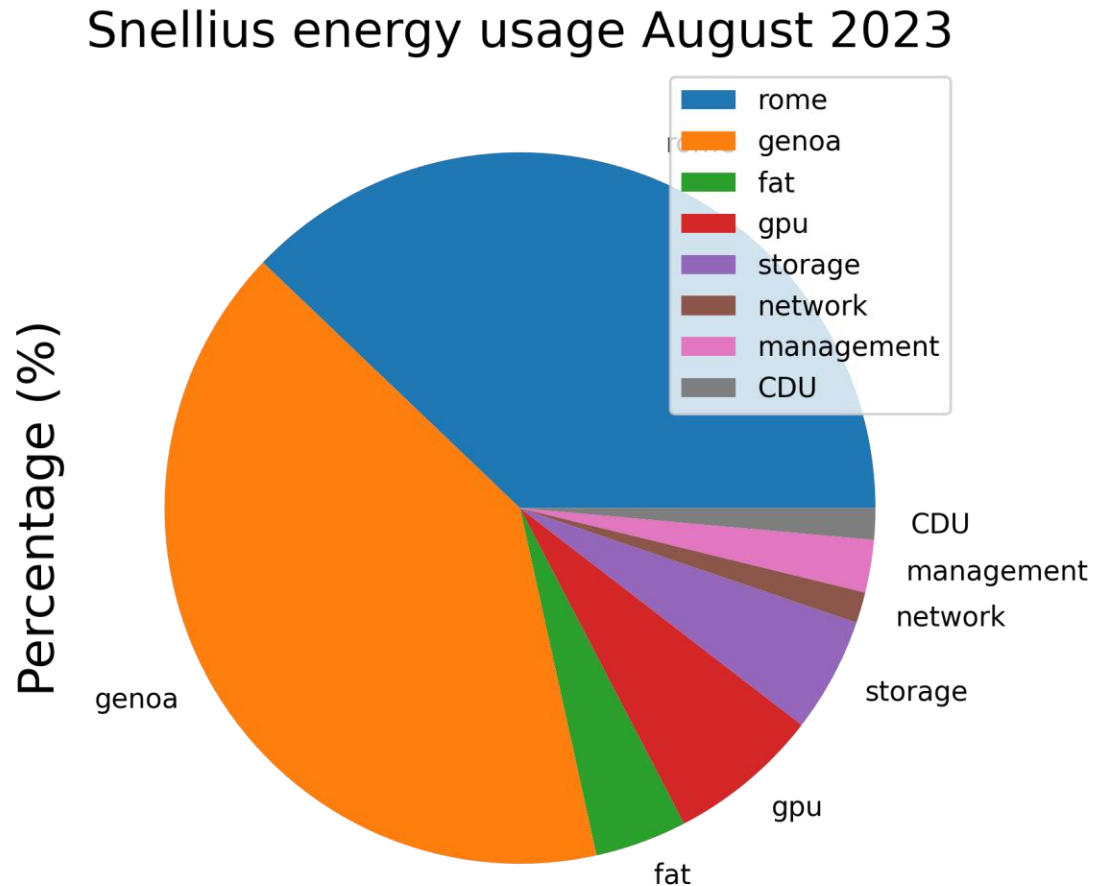
Snellius - Total Energy Usage



Snellius in December used ~ 600MWh of energy.

~2500 house holds worth

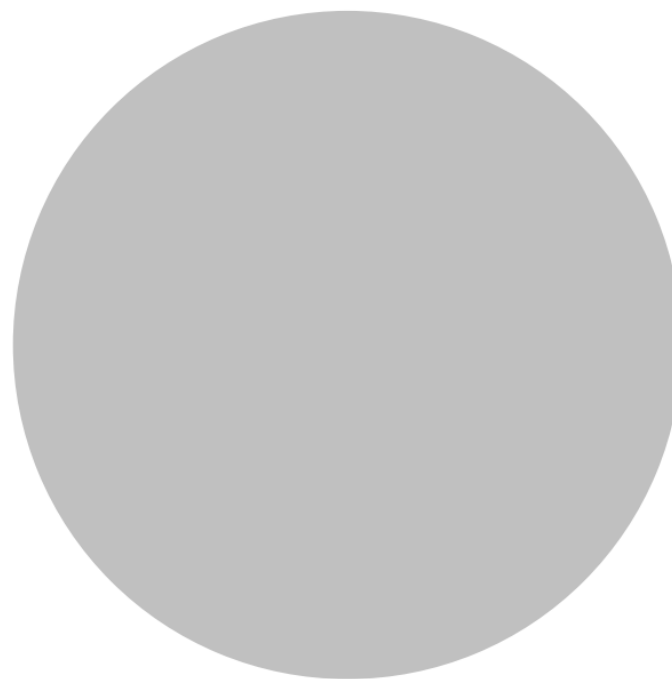
Snellius - Energy usage per partition



- 90% Compute
 - 80% CPU
 - 39% Rome
 - 41% Genoa
 - 7% Gpu
 - 3% Fat
- 10% Other
 - 5.0% Storage
 - 2.4% Management
 - 1.5% Cooling
 - 1.1% Network

Energy Breakdown by users

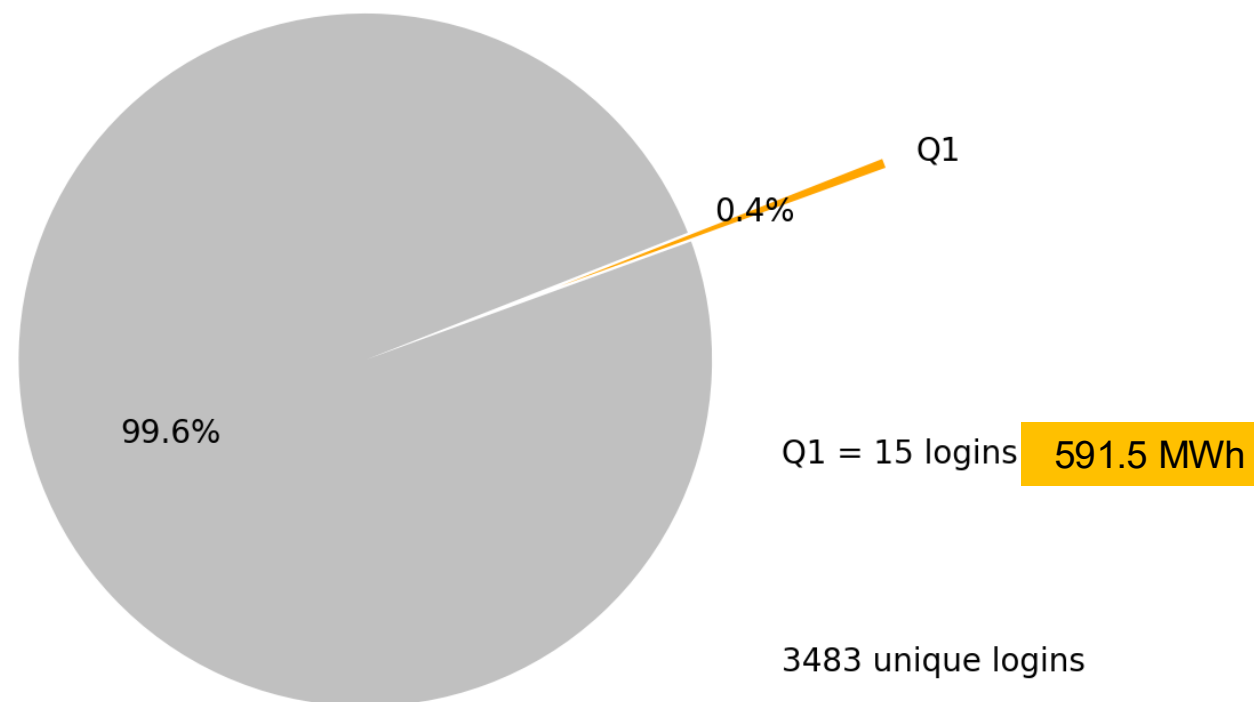
% of logins that use a Quartile (1/4th) of
total Snellius Energy (2023)
~ 2.3 GWh



3483 unique logins

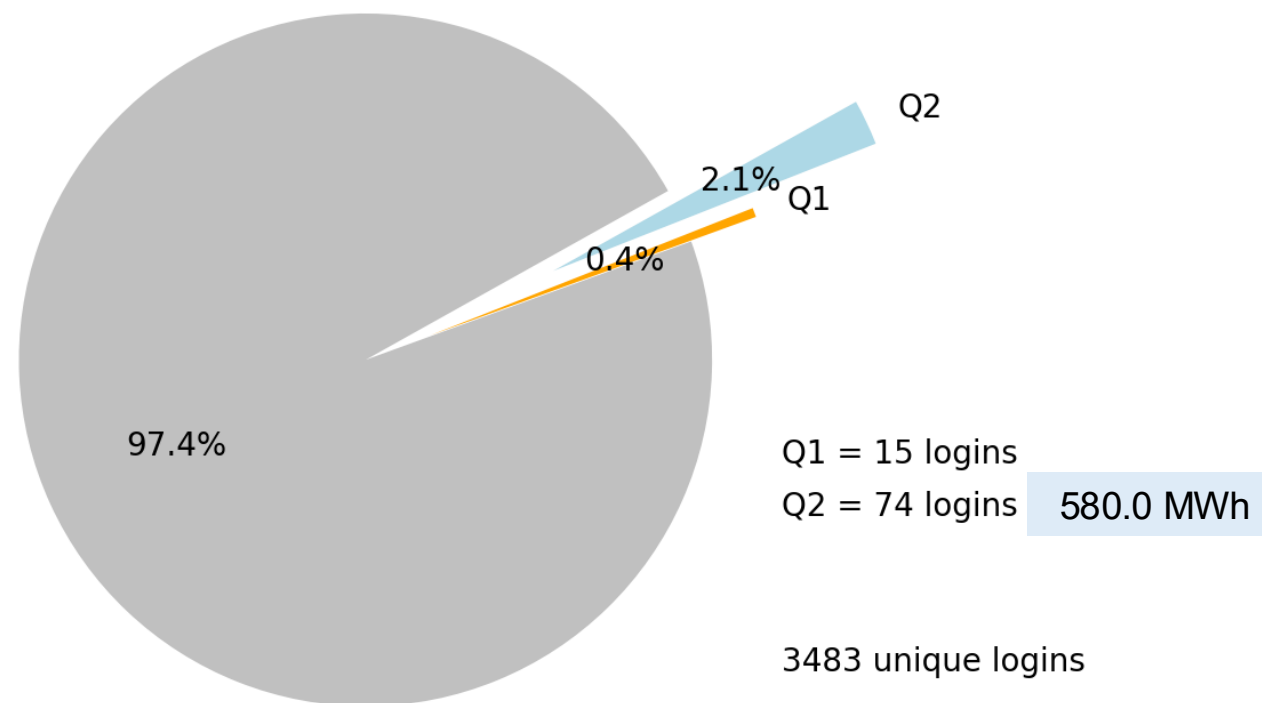
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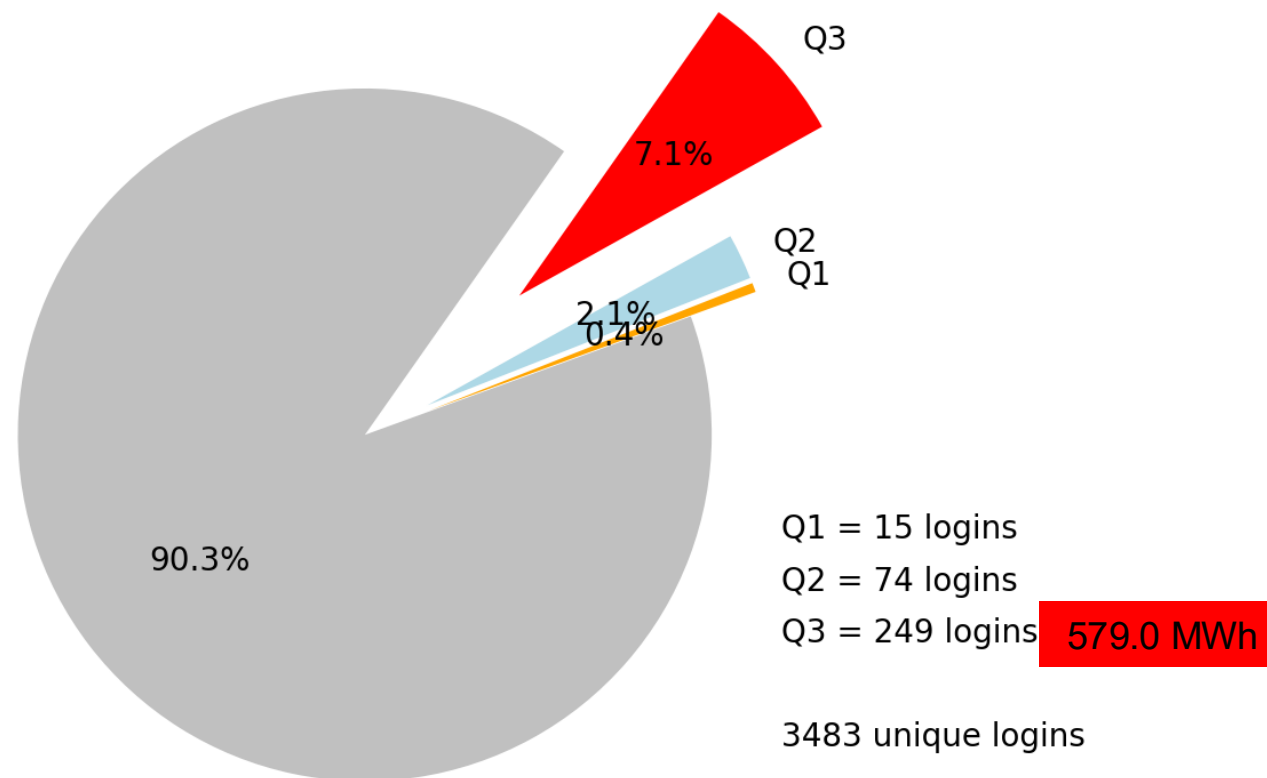
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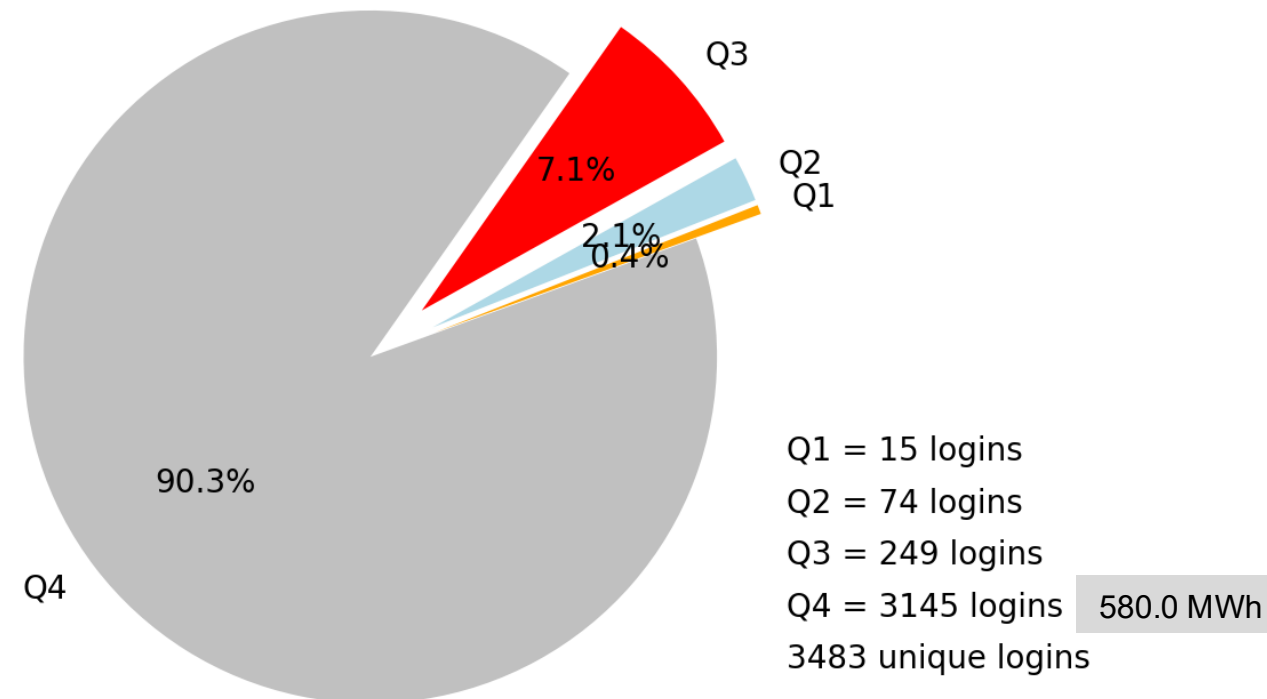
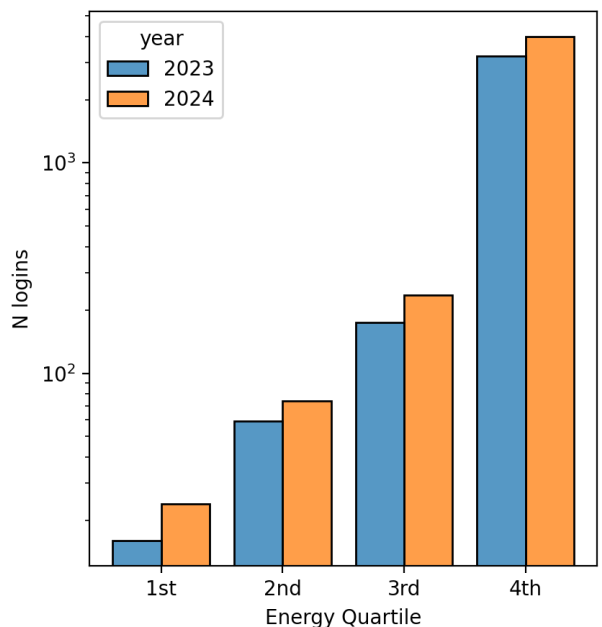
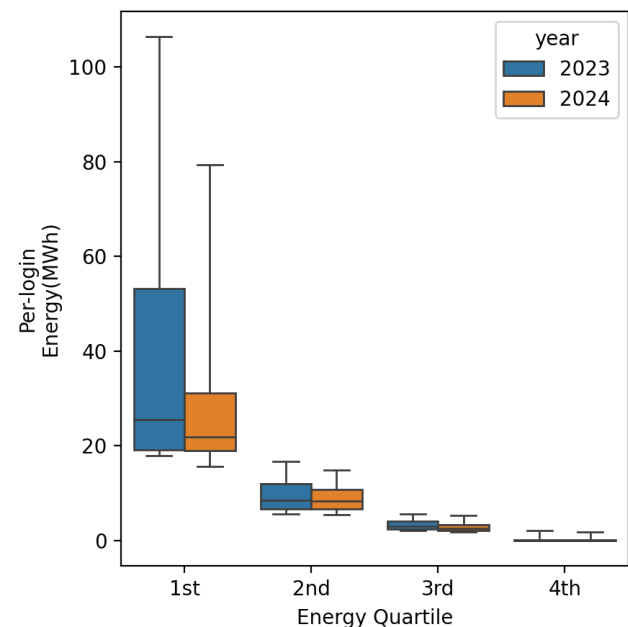
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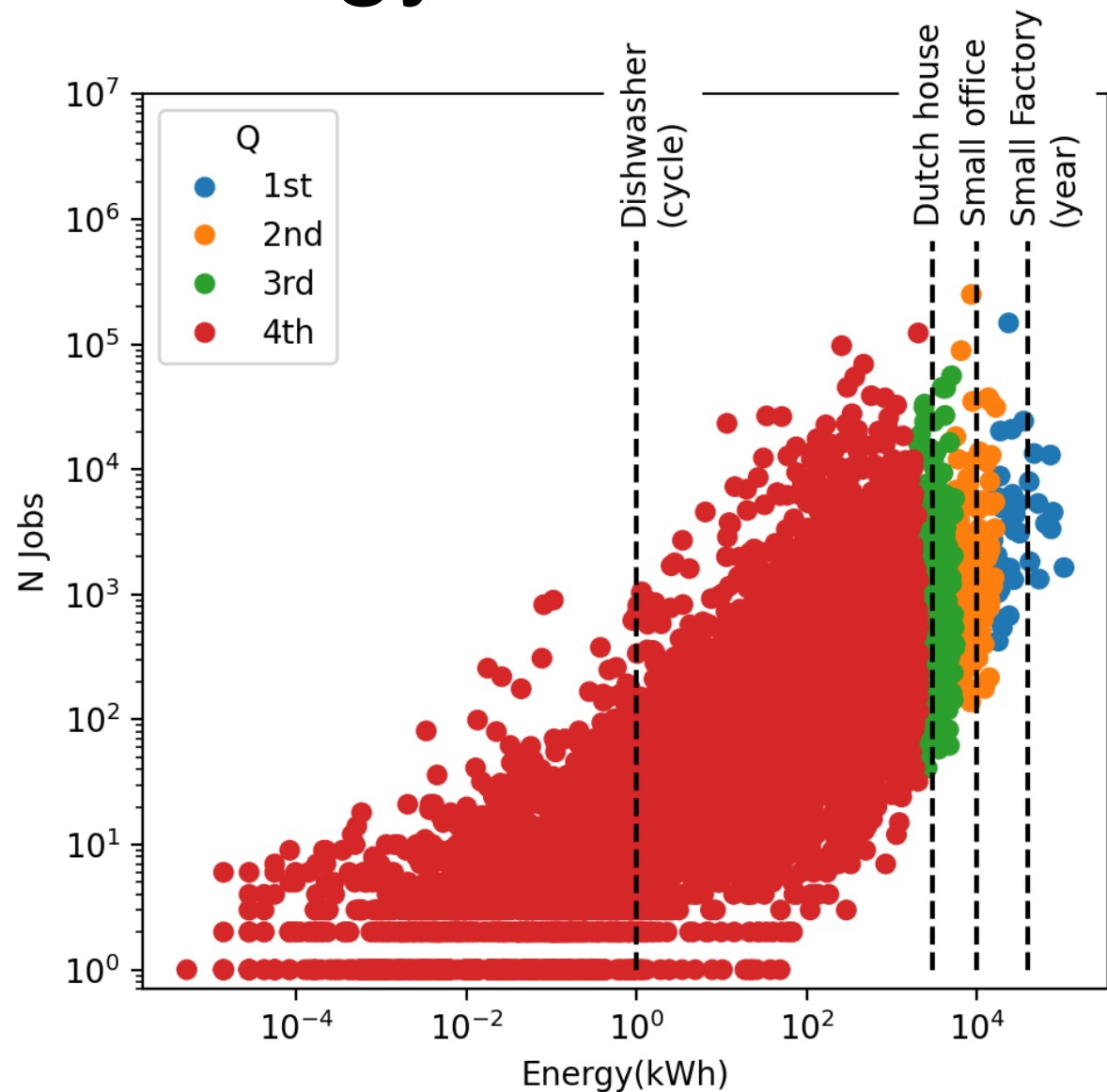


Energy Breakdown by users

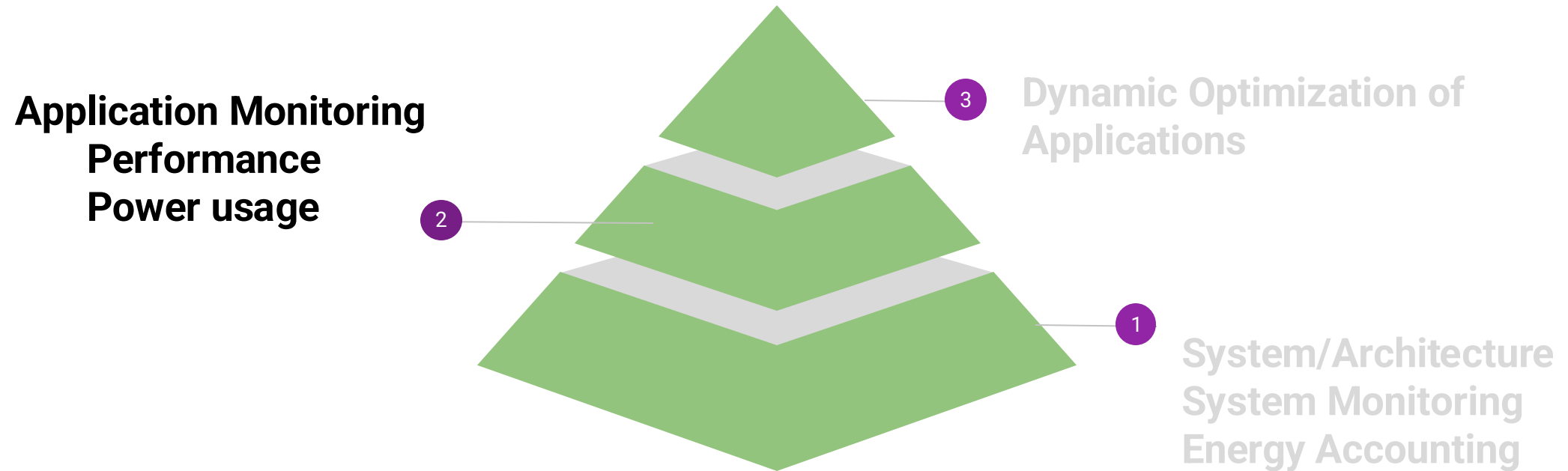
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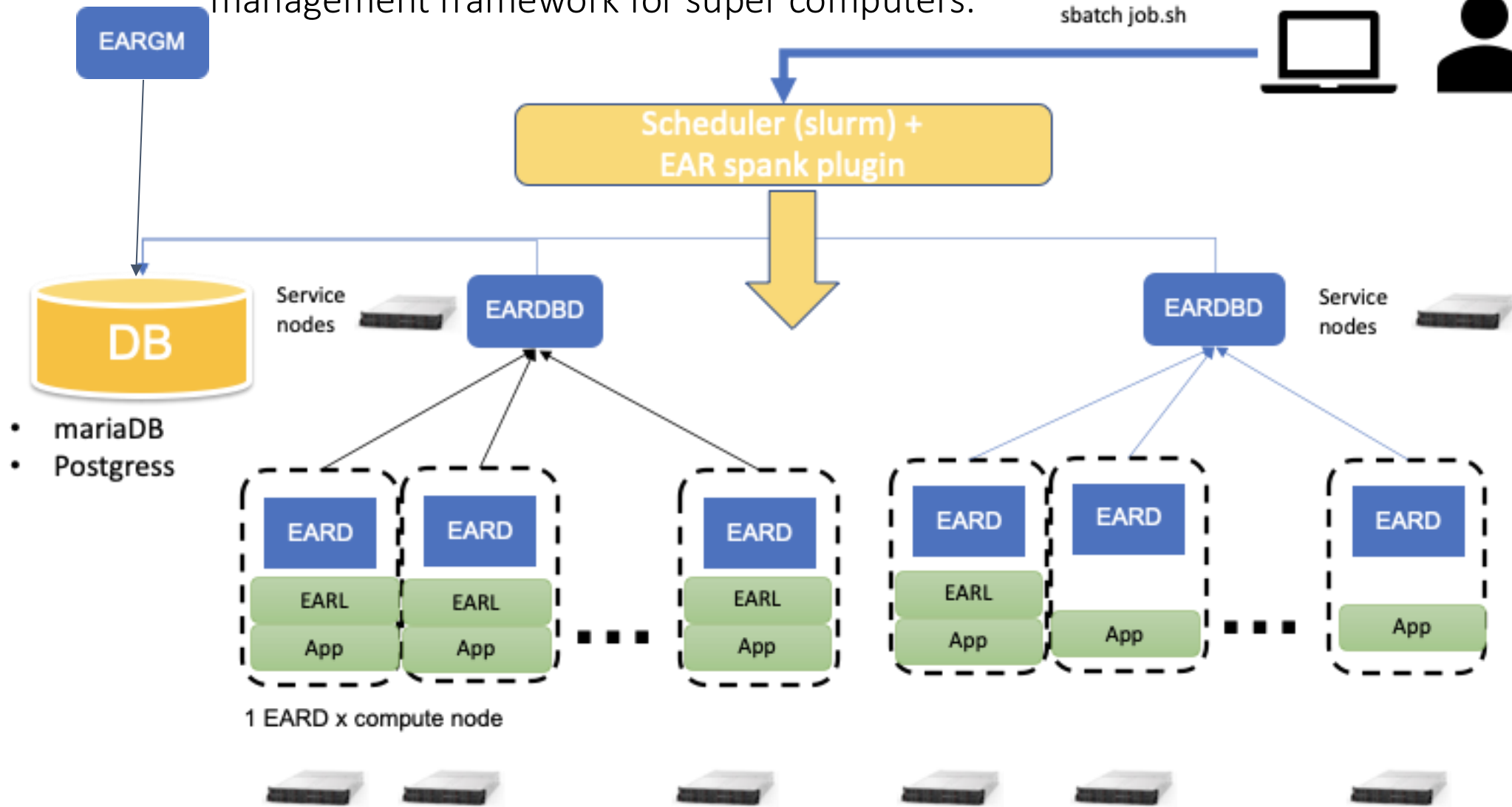


Energy-aware focus



Energy Aware Runtime (EAR)

Energy Aware Runtime (EAR) package provides an energy management framework for super computers.



Energy Aware Runtime (EAR)

Energy Aware Runtime (EAR) package provides an energy management framework for super computers.



- **EAR Node Manager (EARD) “Daemon”**
 - Energy metrics via the RAPL (Running Average Power Limit) function
 - Global energy limits or just offer global cluster monitoring
- **EARL** is a library that is loaded next to the application
 - Offers application metrics monitoring
 - Can select the frequencies based on the application behavior on the fly.
 - Integrated with SLURM on Snellius.
 - Intercepts the MPI symbols through the PMPI interface to provide “traces” of MPI applications.

```
#!/bin/bash

#SBATCH --ntasks=256
#SBATCH --time=24:0:0
#SBATCH -p thin --exclusive

#SBATCH --ear=on
#SBATCH --ear-policy=monitoring

module load 2021
module load foss/2021a
module load CMake/3.20.1-GCCcore-10.3.0
module load VASP6/6.2.1-foss-2021a-CUDA-11.3.1

srun vasp_std
```

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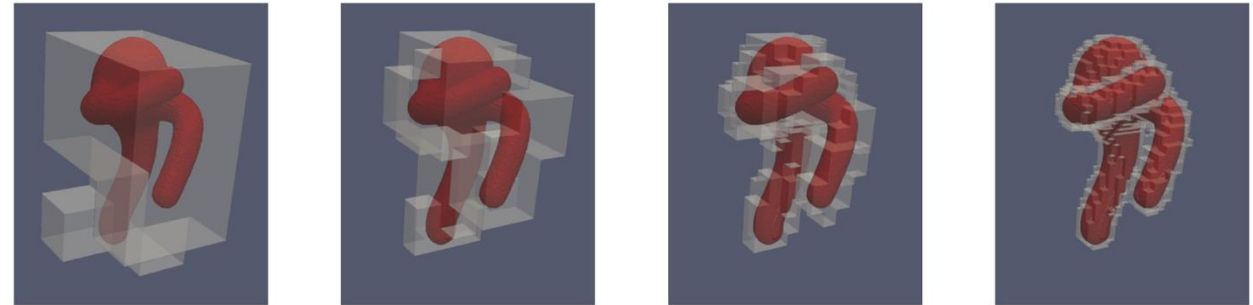
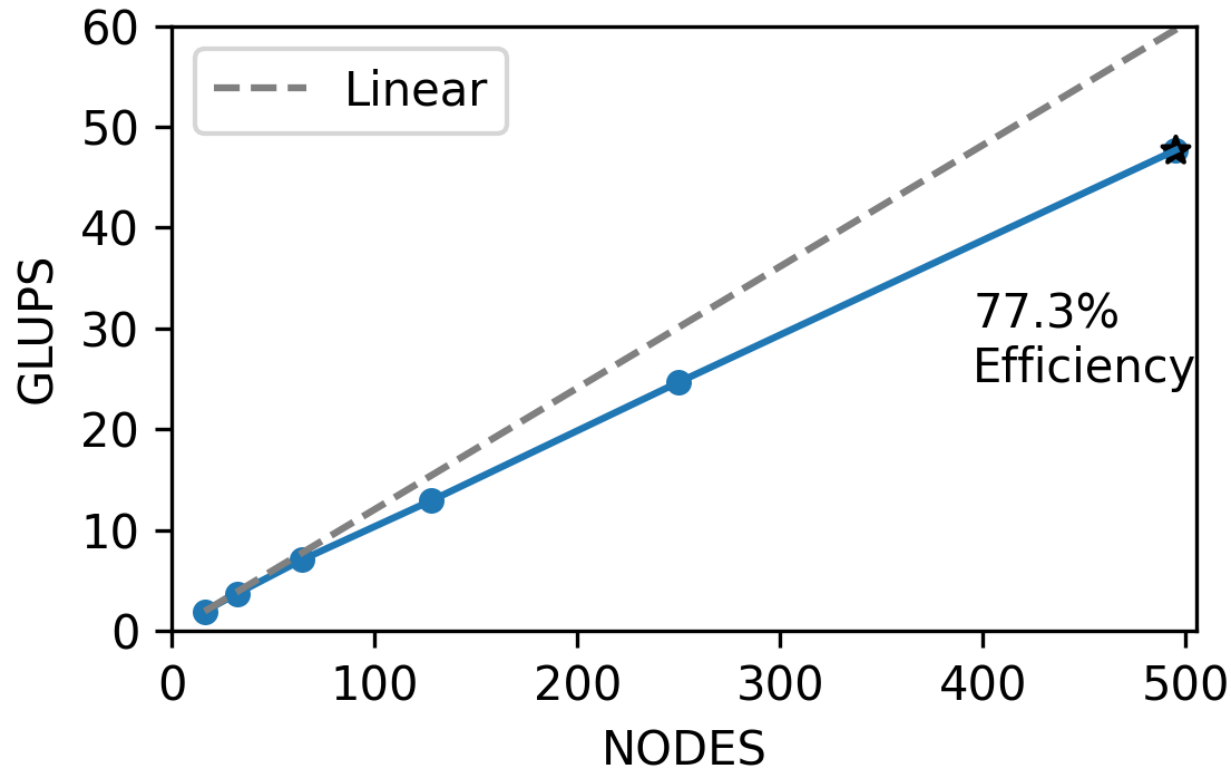
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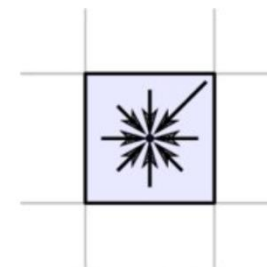
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```

Palabos: Lattice-Boltzmann Solver

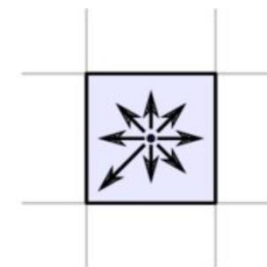
Strong Scaling Benchmark



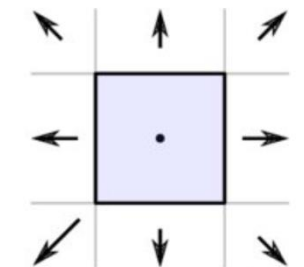
J. Latt, O. Malaspinas, D. Kontaxakis et al. / Computers and Mathematics with Applications 81 (2021) 334–350



initial constellation



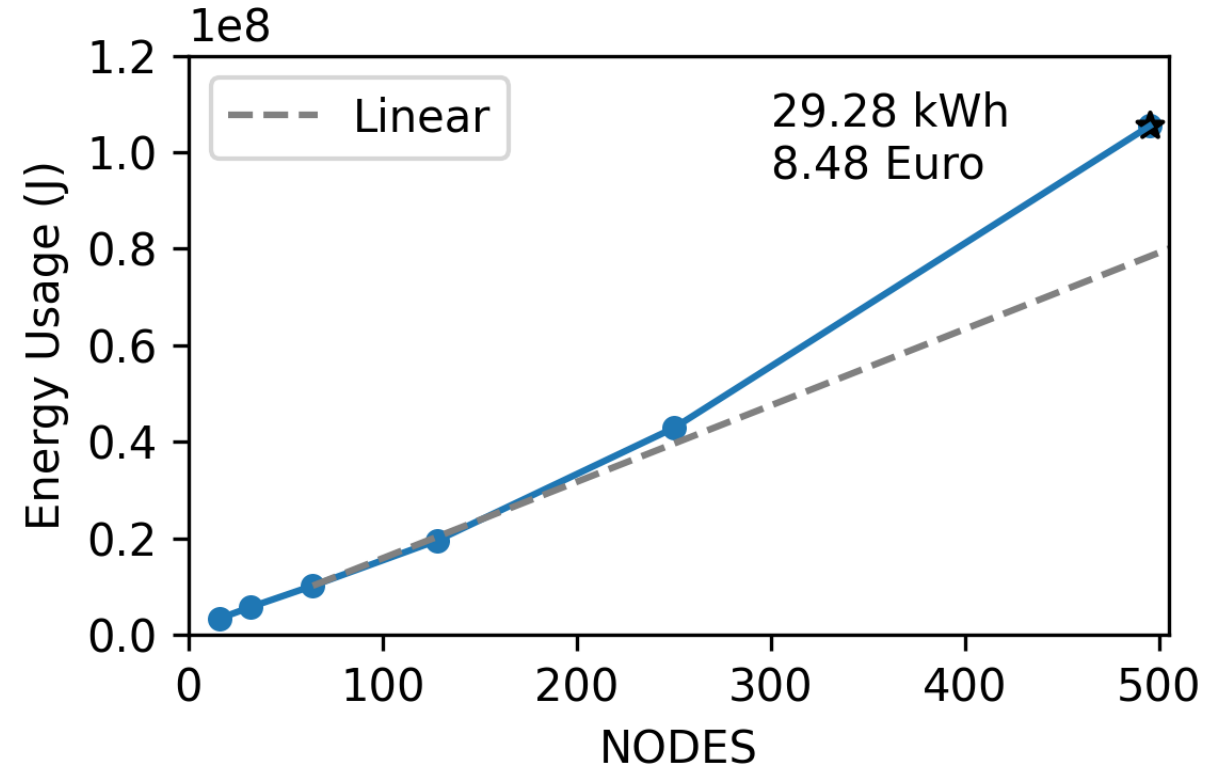
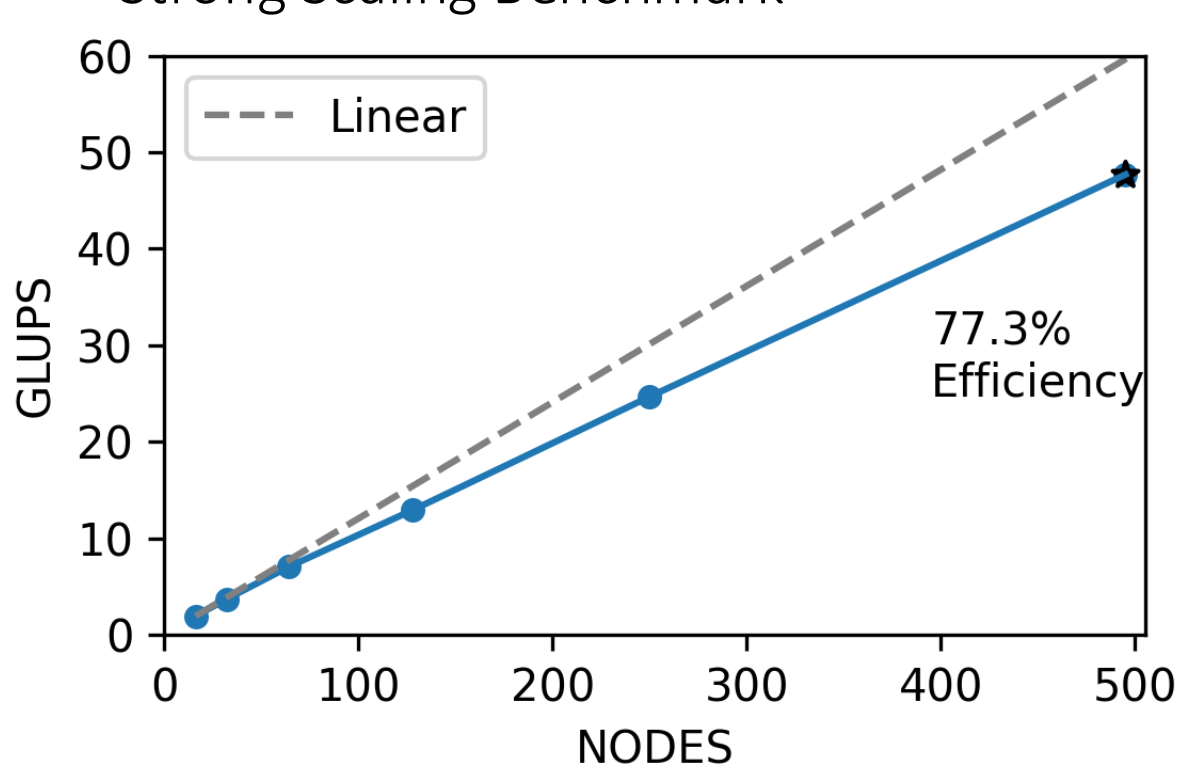
after collision kernel



after propagation, $t=t+1$

Palabos: Lattice-Boltzmann Solver

Strong Scaling Benchmark



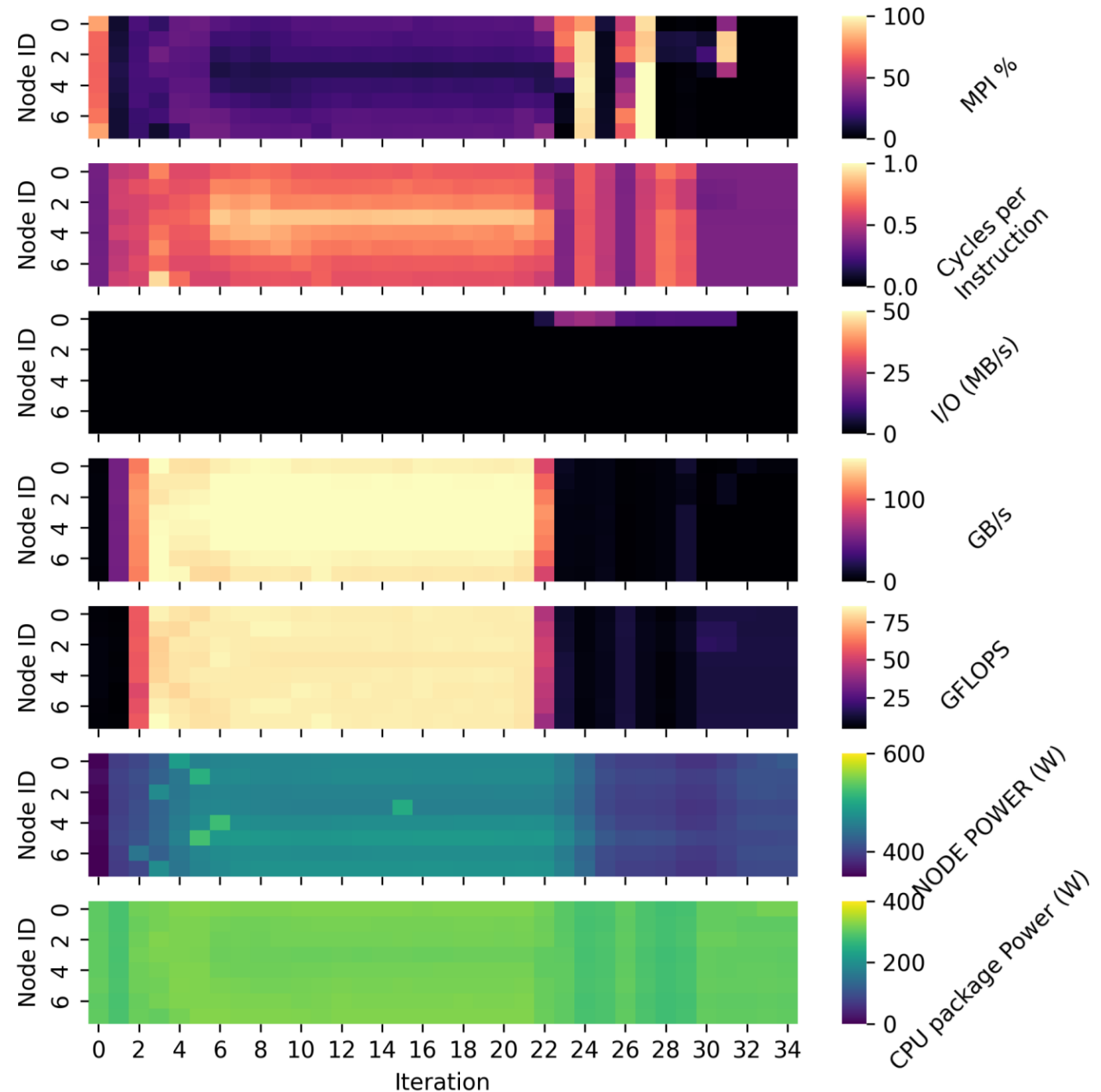
- An average electric car consumes about 0.2 kwh/km
- 495 node case (which ran for 9 minutes) just drove a car to Leeuwarden (149km from SP)!

Palabos:

Strong Scaling Benchmark

- Per-node, Per-iteration "traces"

- Node Power
- Avg CPU Freq (node)
- Main memory BW (GB/s)
- CPI (Cycles per instruction)
- MPI% (percentage spent in MPI calls)
- I/O (network communication)



Energy Aware Runtime (EAR)

Energy Aware Runtime (EAR) package provides an energy management framework for super computers.



Its Documented and available for use!!!

<https://servicedesk.surf.nl/wiki/display/WIKI/Energy>

Pages / ... / Energy

EAR example: GROMACS

❗ In this short example we will show you how to run a simple GROMACS benchmark with EAR enabled.

GROMACS (<https://www.gromacs.org>)

The HECBioSim Benchmarks (<https://www.hecbiosim.ac.uk/access-hpc/benchmarks>)

GROMACS A free and open-source software suite for high-performance molecular dynamics and output analysis.

HECBioSim benchmark suite consists of a set of simple benchmarks for a number of popular Molecular Dynamics (MD) engines, each of which is set at a different atom count. The benchmark suite currently contains benchmarks for the AMBER, GROMACS, LAMMPS and NAMD molecular dynamics packages.

- 1 Prepare the benchmark input
- 2 Prepare the SLURM job-script
- 3 Get energy and performance metrics report from your job

Prepare the SLURM job-script

Notice all that is special here is Lines 10 and 11. This is how you call the EAR runtime library (EARL).

Read more detail here [Energy Aware Runtime \(EAR\)](#) if you want more information on how EAR works.

```
1  #!/bin/bash
2
3  #SBATCH -p rome
4  #SBATCH -n 128
5  #SBATCH -t 00:20:00
6  #SBATCH --exclusive
7  #SBATCH --output=GROMACS_run.out
8  #SBATCH --error=GROMACS_run.err
9
10 #SBATCH --ear=on
11 #SBATCH --ear-policy=monitoring
12
13 module load 2022
14 module load foss/2022a
15 module load GROMACS/2021.6-foss-2022a
16
17 srun --ntasks=128 --cpus-per-task=1 gmx_mpi mdrun -s hEGFRDimer_benchmark.tpr
```

Obviously you need to submit it to the SLURM scheduler!!

So...

```
sbatch myjobscript.sh
```

Outlook

- Identify Energy footprint of users jobs/applications
- Dashboard, Ease of use for the average user to see the “profile” of their applications



Thank you!

- Contact us
 - <https://servicedesk.surf.nl/>
- EAR User Tutorial on Snellius
 - [https://servicedesk.surf.nl/wiki/display/WIKI/Energy+Aware+Runtime+\(EAR\)](https://servicedesk.surf.nl/wiki/display/WIKI/Energy+Aware+Runtime+(EAR))
- Energy Aware Runtime (EAR) --- Energy Aware Solutions
 - <https://www.eas4dc.com/solutions>
 - https://gitlab.bsc.es/ear_team/ear/-/wikis/home



<https://github.com/sara-nl/energy-efficient-computing/>

<https://ondemand.snellius.surf.nl/>