Sustainable Supercomputing: an overview of activities at EPCC

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About EPCC

- Part of the University of Edinburgh
- Established in 1990, now with 140 staff
- UK National HPC Service provider
  - Hosting site for UK Exascale
- Research activities range from Supercomputing to AI to Data Science
  - Reflected by wide range of systems – from HPE Cray EX to Cerebras CS-3
- MSc & PhD programme in HPC & HPC with Data Science

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EPCC hardware timeline

Sources of CO^2 emissions from supercomputing

Operation

- Power usage

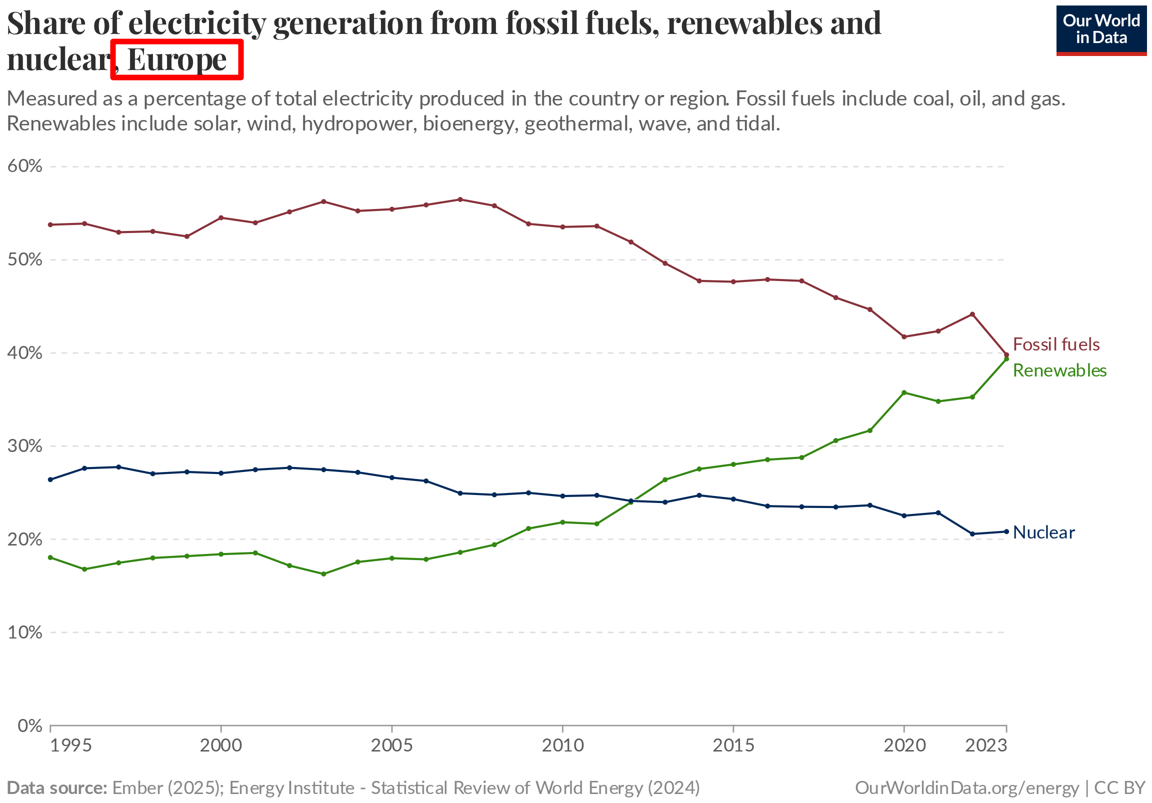
Manufacturing

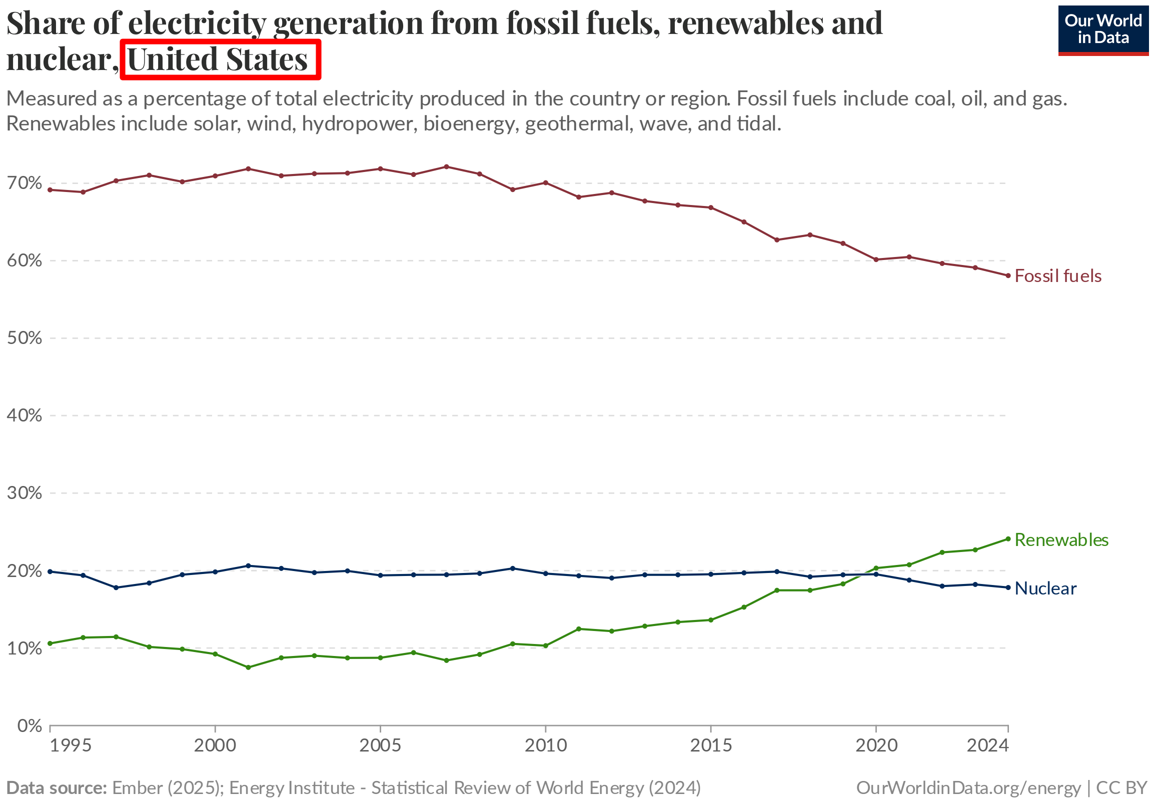
- Computer hardware
- Power & cooling infrastructure, e.g. transformers

Construction

- Data centres
- Supporting infrastructure

Grid decarbonisation





Hannah Ritchie (2017) - "Global renewables are growing, but have been partly offset by a decline in nuclear production"
Retrieved from: 'https://ourworldindata.org/global-renewables-are-growing-but-are-only-managing-to-offset-a-decline-in-nuclear-production' [Online Resource]

What are we doing at EPCC?

1. Power usage reduction
2. Better cooling infrastructure & reuse of waste heat
3. Optimisation of system utilisation
4. Experimentation with novel/bespoke hardware
5. Educating users

POWER USAGE REDUCTION

Energy efficiency

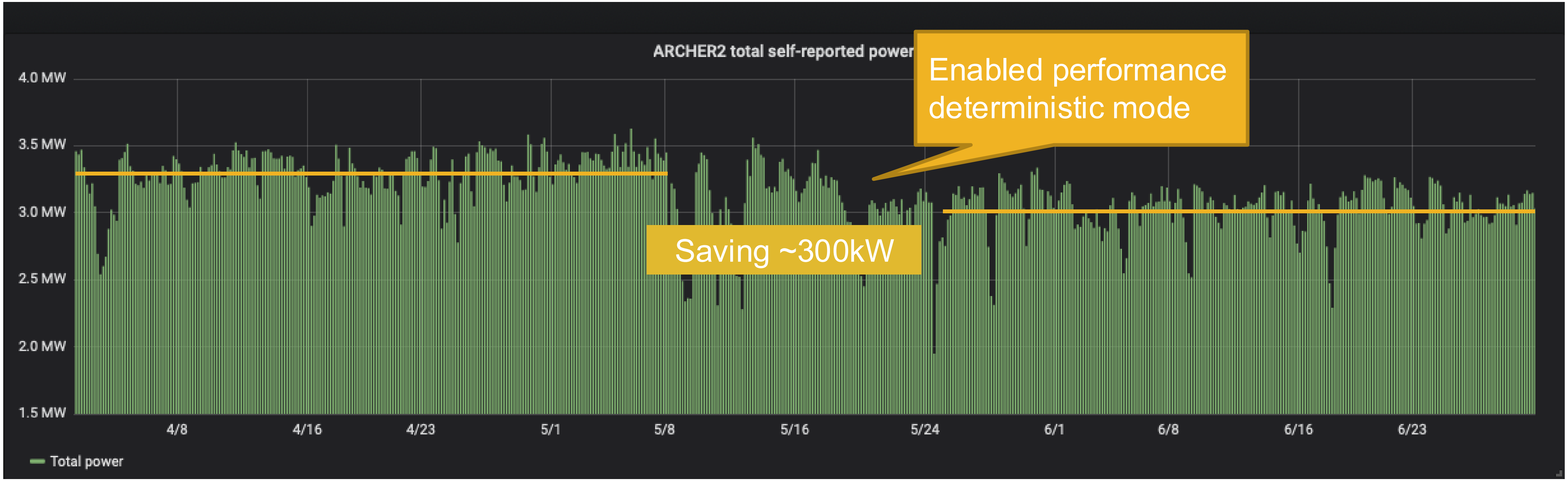
- Focus on system level and performance improvements
  - Biggest impact across large number of systems and applications

- Algorithmic/numerical improvements are also important
  - Mostly with a view to optimising performance (i.e. time to solution)

$$Energy\ (J) = Power\ (W) \times time(s)$$

AMD EPYC modes

- **Power** deterministic
  - CPU will run as fast as it can for given TDP (thermal design point) or power input – variable performance
  - Allows the highest possible performance
- **Performance** deterministic
  - Will deliver the same predictable performance across CPUs
  - Might result in slightly different power consumption across CPUs

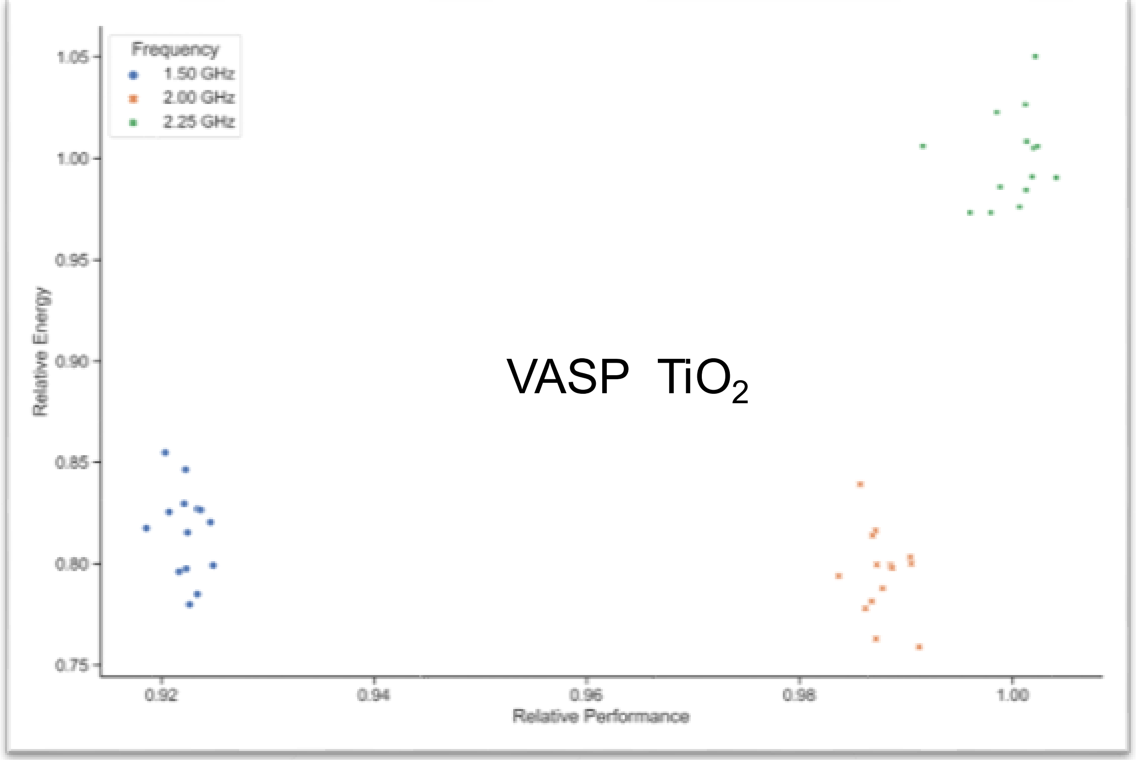


ARCHER2 CPU frequency reduction

Summary of relative energy and performance at 2.00 GHz, compared to 2.25 GHz

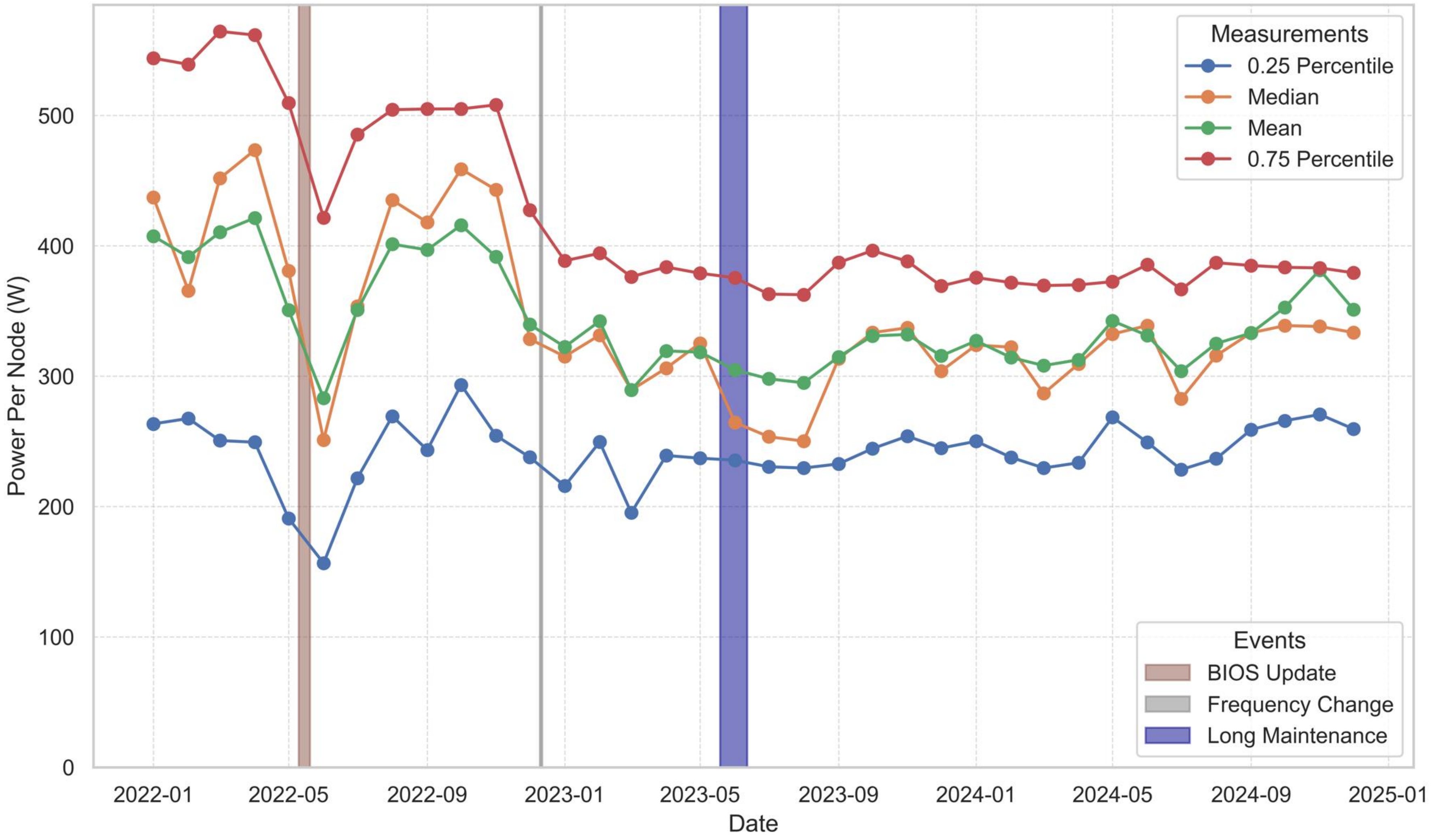
Benchmark (single node)	Energy	Performance
VASP (TiO_2)	-20%	-1%
CASTEP (Al Slab)	-13%	-1%
GROMACS (1400k atoms)*	-5%	-15%
OpenSBLI (TGV 512ss)	-20%	-5%
LAMMPS (LJ 8M atoms)**	-4%	-21%
NAMD (STMV 1M atoms)**	-5%	-33%

* Data from Laura Moran, EPCC
** Data from Douglas Shanks, HPE



- Default CPU frequency reduced from 2.25GHz to 2.0GHz
- User can override this default
    - Higher frequency defaults for some codes

Impact of changes over time



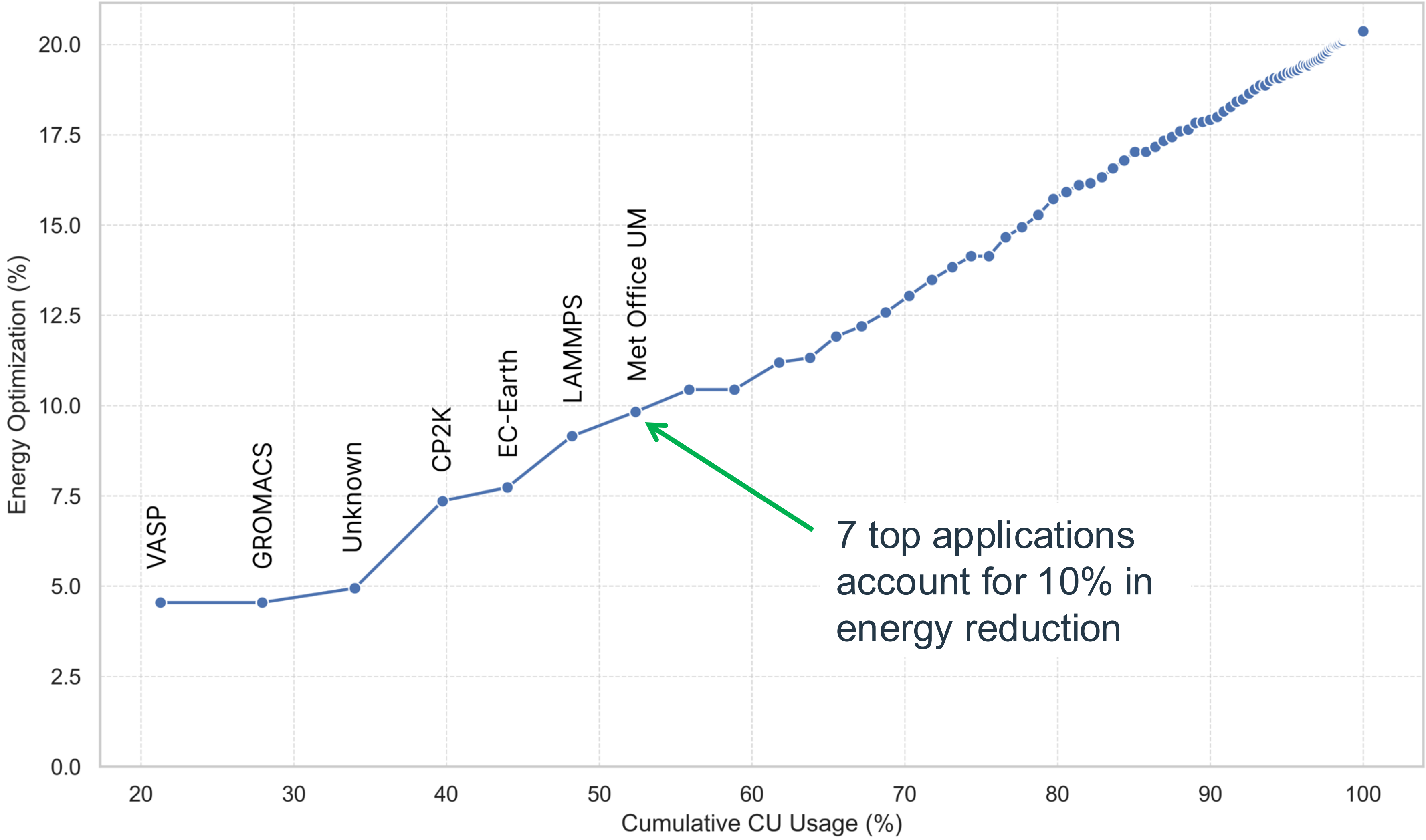
ARCHER2

5,860 nodes

2 x AMD EPYC™ 7742 64-core CPUs

750,080 cores

Impact of changes on application energy usage



CU = Compute Unit = 1 node hour

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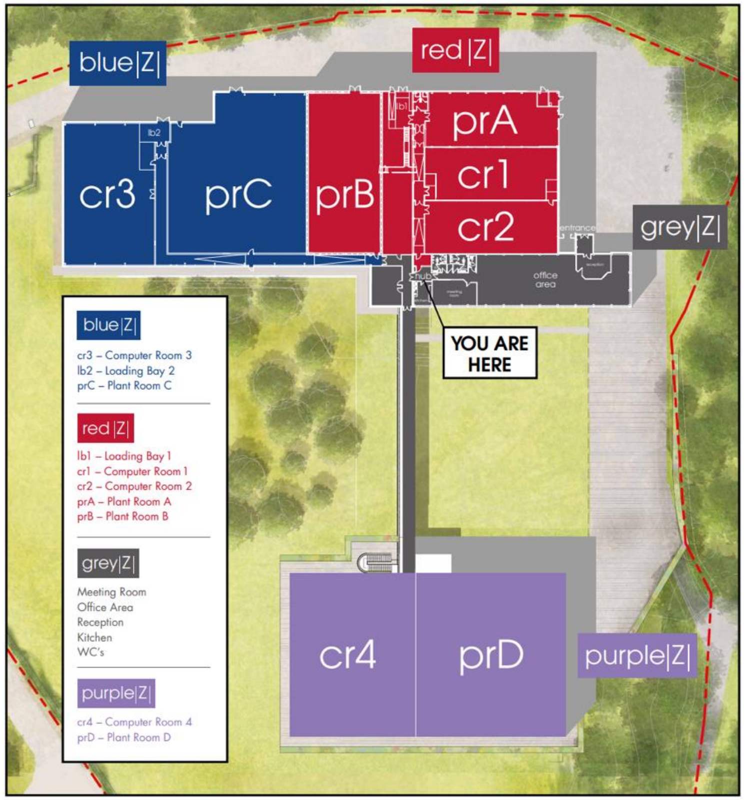
COOLING & WASTE HEAT

Long term investment

- Data centre efficiency requires **long term strategic** investment
  - There is an (inevitable) upfront cost in emissions
- At EPCC, oldest machine room from 1970s
- Infrastructure must support new developments in power and cooling
- Certified renewable energy



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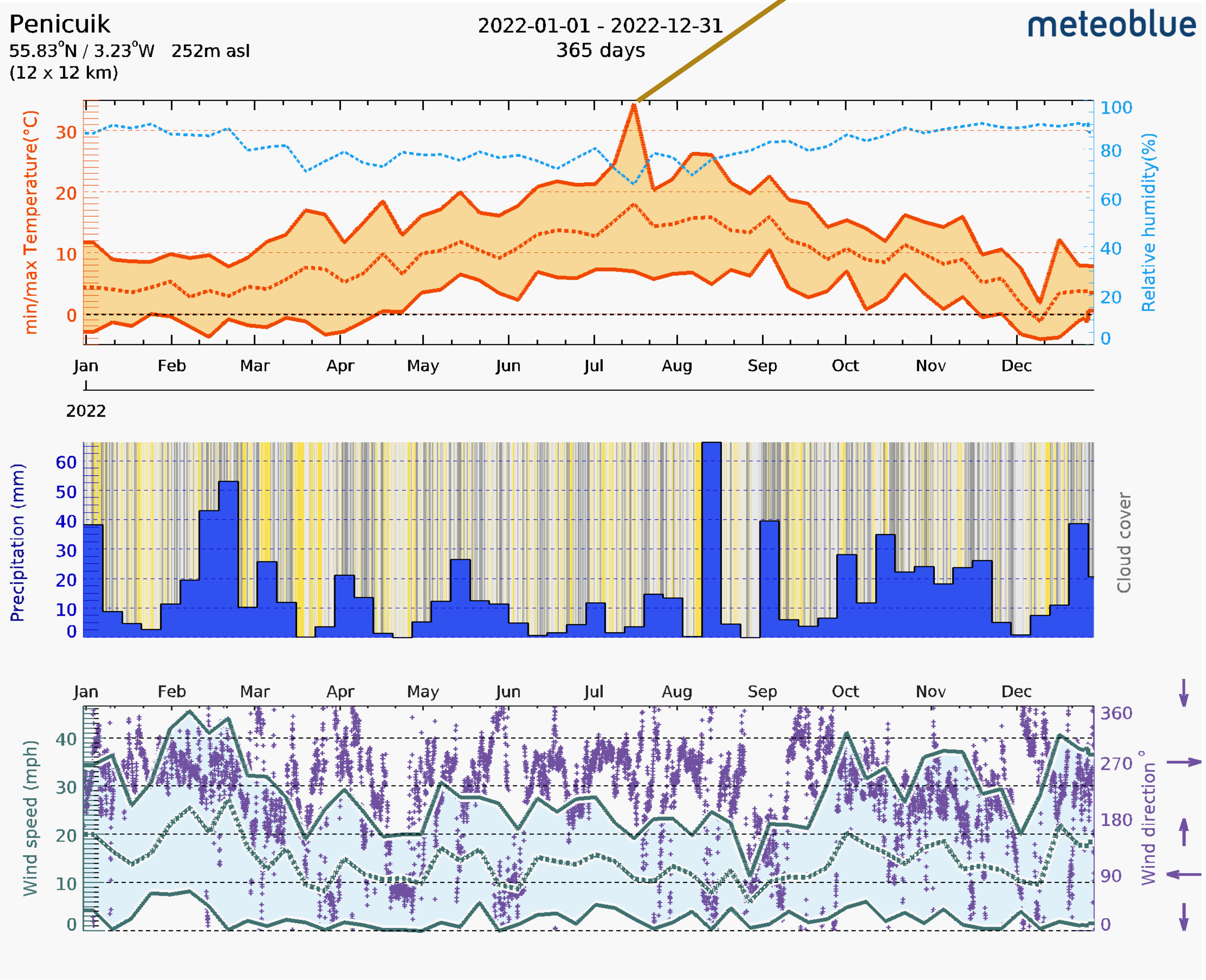
Climate

First time over 30C

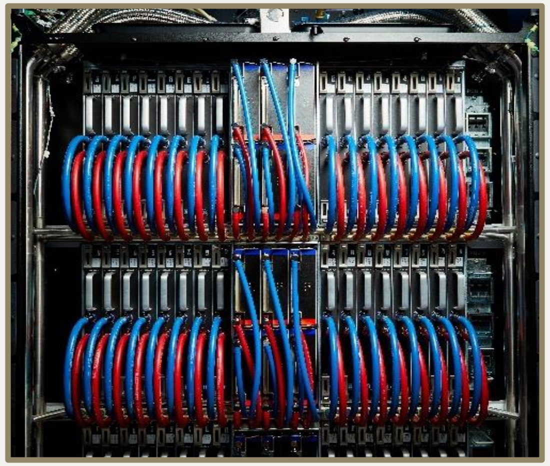


Free cooling!

Warm water is pumped to the roof, outside air & fans chill it

https://www.meteoblue.com/en/weather/historyclimate

Other forms of cooling



Direct liquid cooling

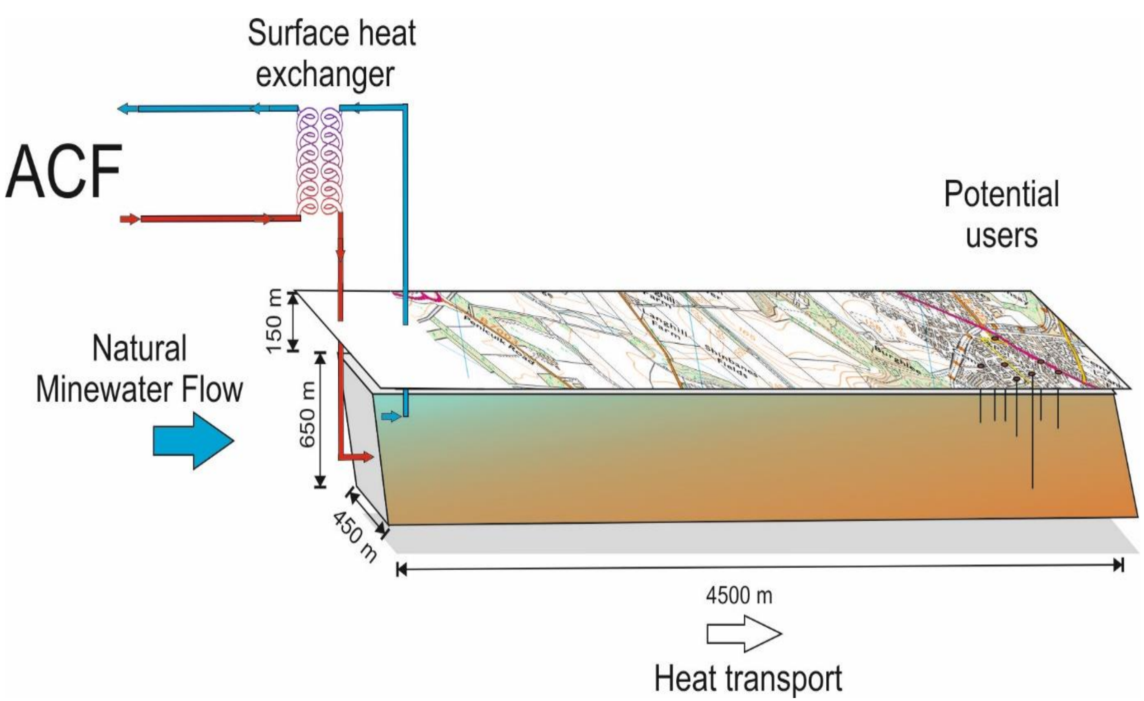
Adiabatic cooling

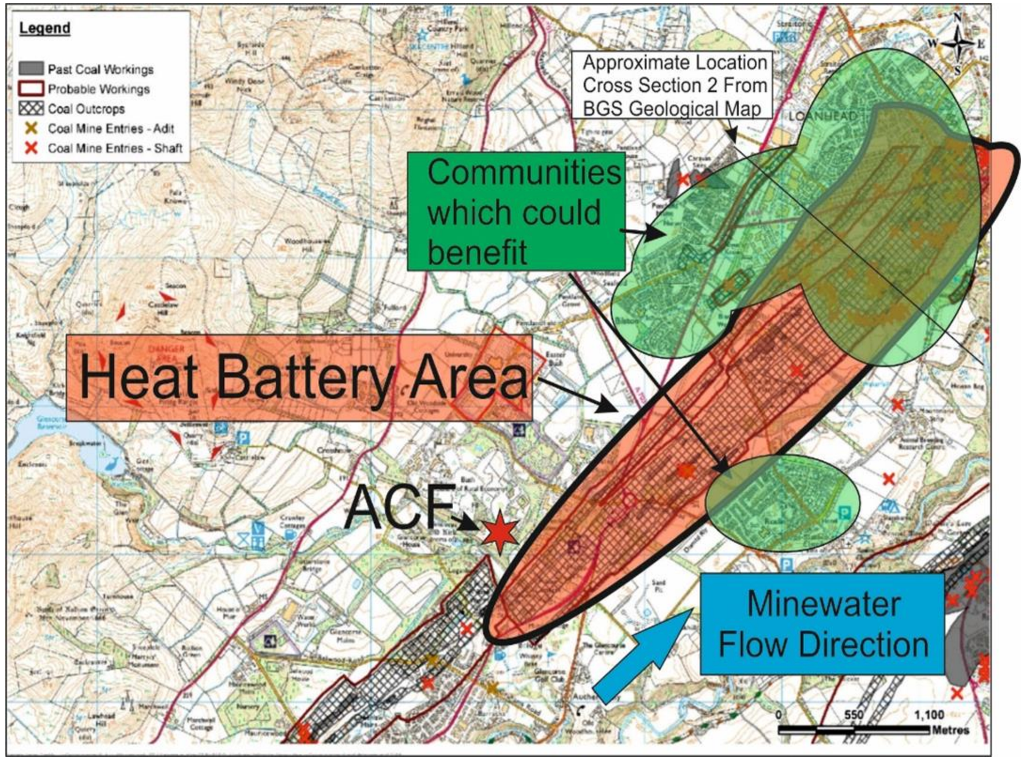
Temperature controlled racks

Geothermal battery feasibility project

Problem: We want to be able to reuse our excess heat, but nowhere nearby can use it

Solution: Move the heat to where it is useful





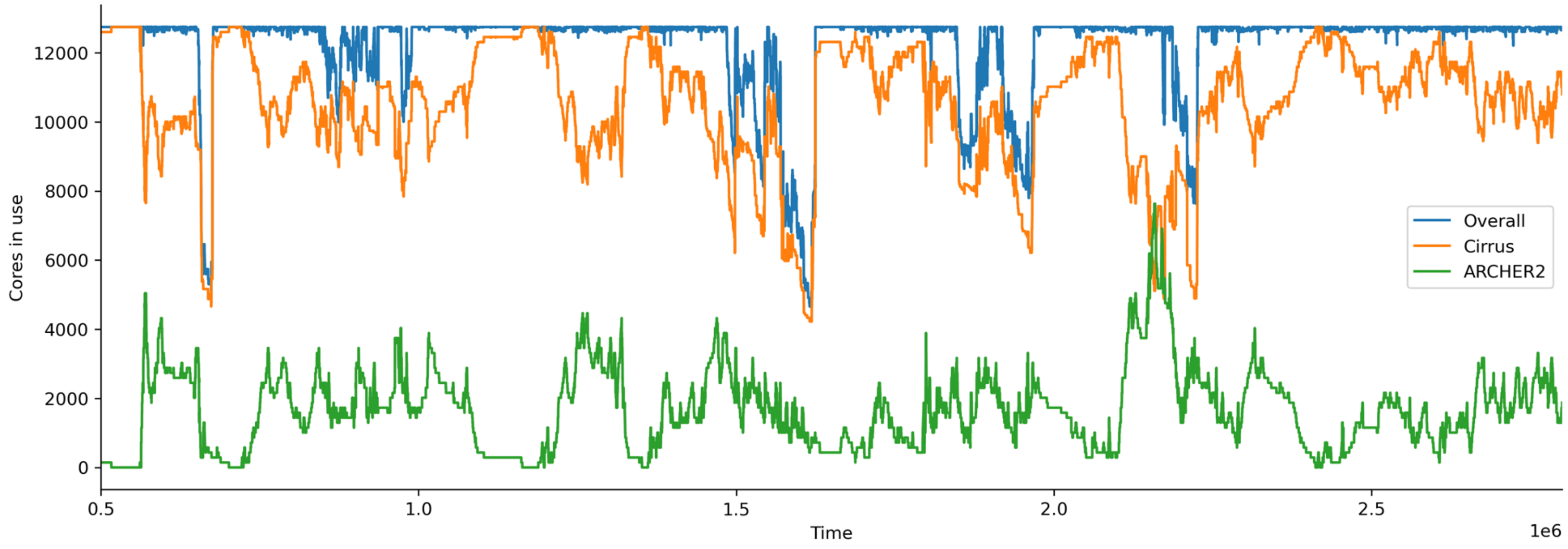
IMPROVING SYSTEM UTILISATION

Load balancing jobs across supercomputers

- Problem: Multiple systems, utilisation varies
  - Steady 95% for **ARCHER2** (Tier1 national facility)
  - Highly variable 50-90% for **Cirrus** (Tier2 regional facility)

- Basic premise: move jobs *from* busy system *to* less busy one
  - Should result in faster turnaround for users, better utilisation
  - Better utilisation means improved use of investment

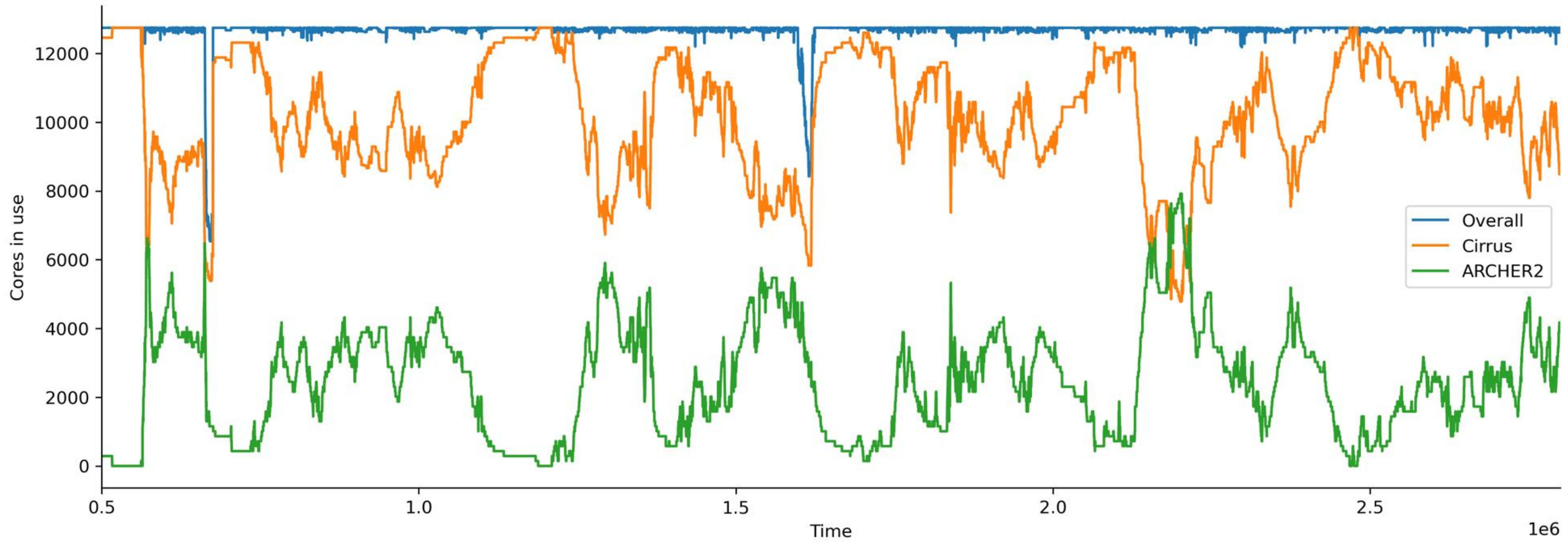
- Methodology:
  - Use ElastiSim simulator tool
  - Move single node jobs from ARCHER2 ➔ Cirrus (“mobile” jobs)
  - Make Cirrus jobs “moldable” (using SLURM)



Top: Moldable Cirrus jobs plus 20% of eligible ARCHER2 jobs

January 2024 - Cirrus base load 80%

Orange: Cirrus
Green: ARCHER2
Blue: Combined

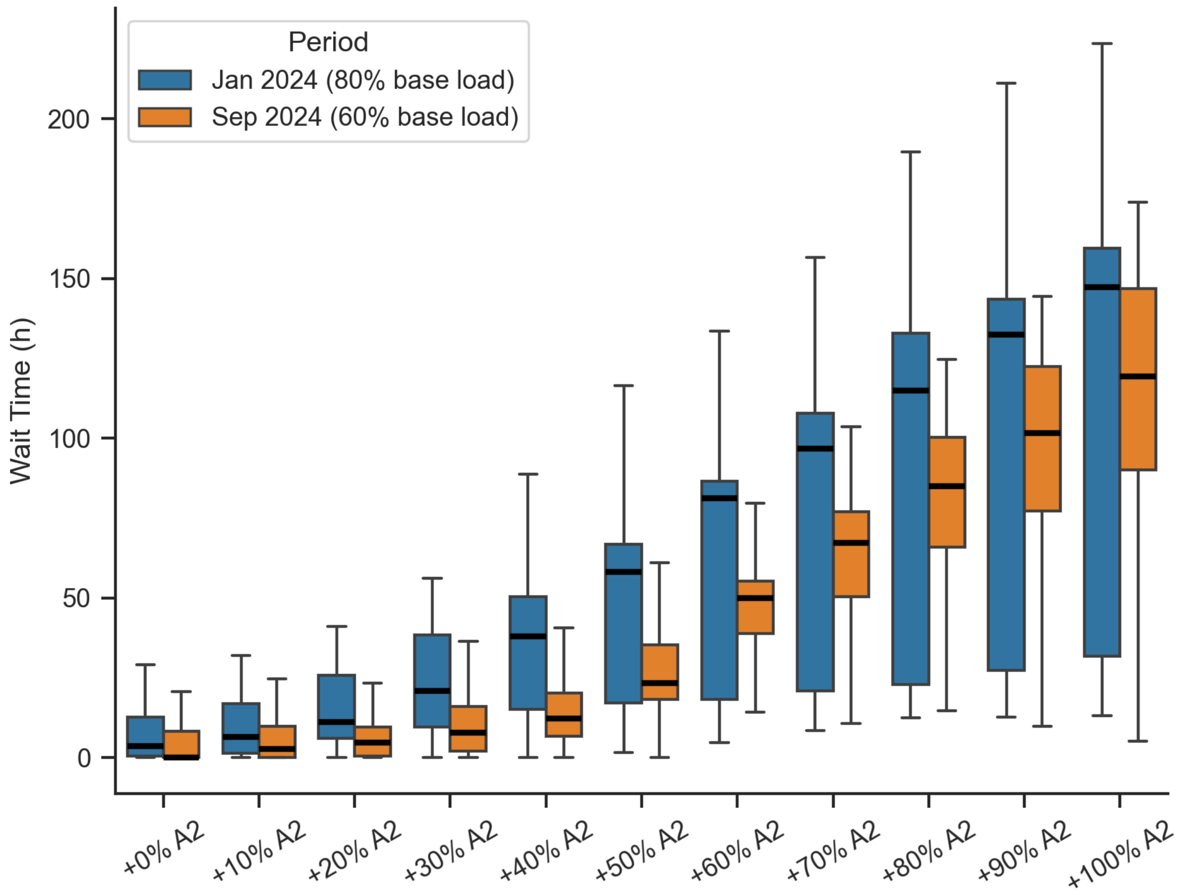


Bottom: Moldable Cirrus jobs plus 30% of eligible ARCHER2 jobs

Simulation of impact of moldable & mobile jobs

- Increased utilisation can result in prohibitively long wait times for users
- Sweet spot roughly at base load + mobile jobs ≅ 100%
- Assumptions
  - Perfect scaling
  - All single node jobs can be mobile
  - All jobs can be moldable

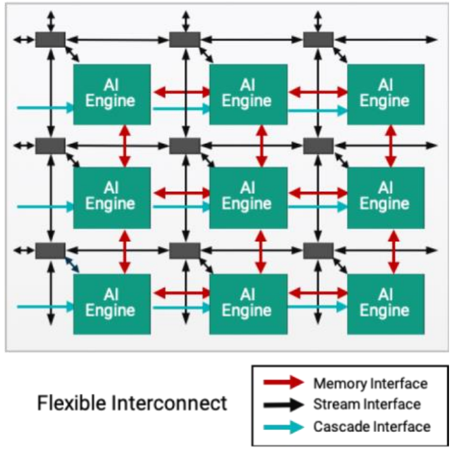
➔ Many more impact/feasibility analyses required before we can implement a proof-of-concept

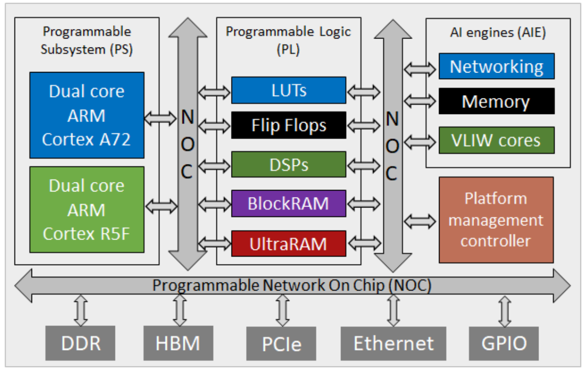


EXPERIMENTATION WITH NOVEL/BESPOKE HARDWARE

Efficient and specialised hardware

- New hardware solutions that promise improved energy to solution
  - Through better performance and/or reduced power draw
- Cerebras Wafer Scale Engine
  - AI-focussed, but with potential for HPC workloads
- RISC-V
  - Tenstorrent Grayskull can run stencil code at similar performance to Xeon Platinum, 5 times less energy
- AMD Xilinx FPGAs and AI engines
- AMD AI engines





EDUCATION

Education

Efficient software is important → the **developers**' responsibility

Efficient *use* of software is equally important → the **users**' responsibility

Deployment of software is important → the **system providers**' responsibility

Education is key – enable developers/users/system providers to understand implications of their choice

"Green software use on HPC"
https://epcced.github.io/2025-04-01_GreenHPC_Online

Final thoughts

Supercomputers are **scientific instruments** that are used to find solutions to many of the problems humanity faces

→ to discover new vaccines

→ to design new renewable energy solutions

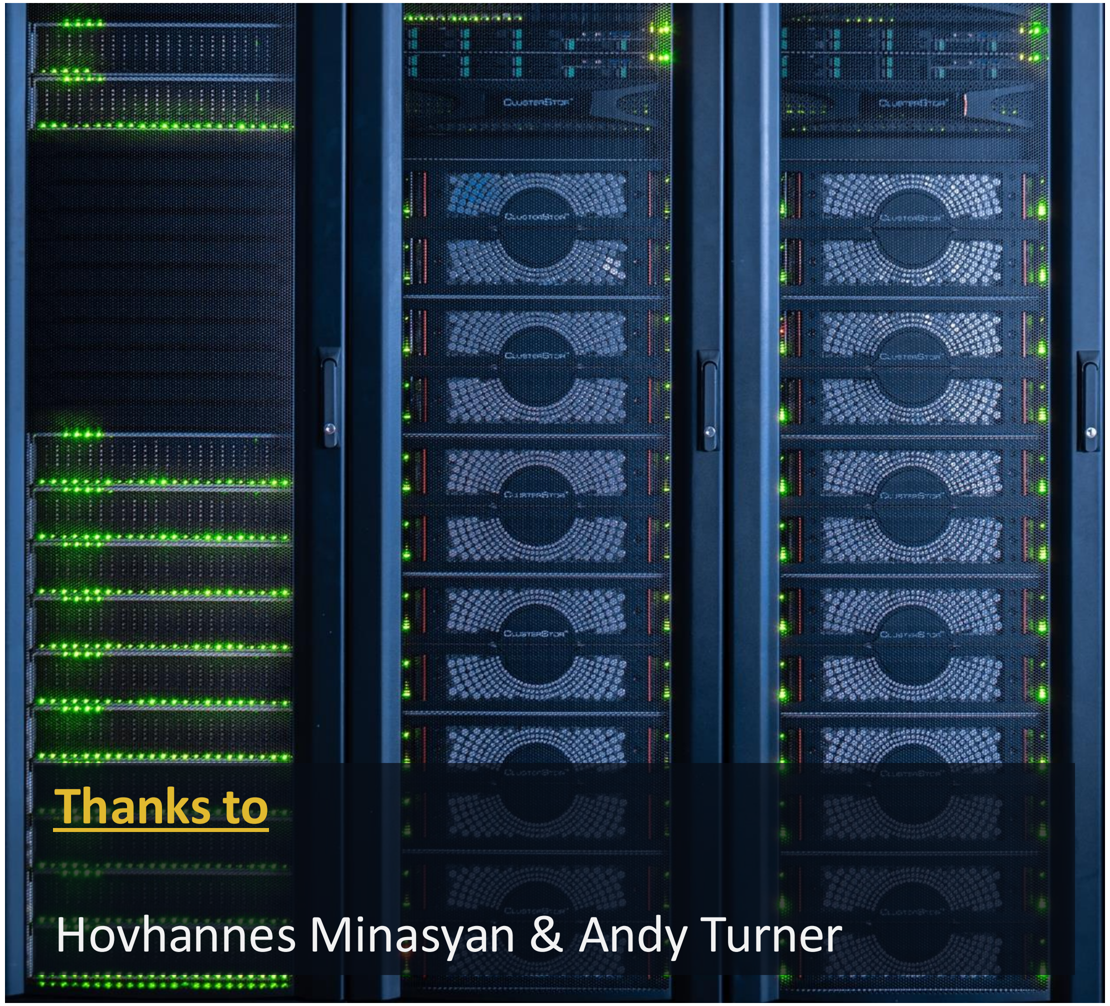
→ and even to model the climate, in order to more accurately predict climate change and its impact

Significantly reducing scientific throughput is a false economy

Net Zero HPC must be achieved while maintaining, or indeed increasing, the amount of science we do

Conclusions

- Sustainable supercomputing is about more than just energy efficiency
- Energy efficiency remains important even as national grids decarbonise - keep demand under control
- Other important factors are infrastructure optimisation, improved resource utilisation, exploring alternative hardware, education
- Many open research questions remain!



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