2024 Workshop on Phylogenomics

Green computing

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Český Krumlov – January 26, 2024

Green Computing: Challenges

- Extremely broad topic
  - From electric grid to CPU to software to users
  - Different cultures / mindsets / languages
  - “Divide-and-conquer” is problematic
- Many non-technical factors
  - Economics, politics, bureaucracy, psychology...

Agenda

- Energy monitoring
- Energy optimization
- Carbon-aware computing

Computing infrastructure survey

- What are you using for long analyses (>4h)?
  - Personal laptop or desktop
  - Dedicated desktop or server (lab-owned)
  - Shared server or cluster (institute-owned, external)
  - Cloud (e.g. AWS)

Our computing infrastructure

- Lab-owned: 4 desktops, 6 rack servers
- HITS institute cluster #1 (on premise)
- HITS institute cluster #2 (university)
- External resources (SCC Karlsruhe, LRZ Garching/Munich)

Motivation 2019: Climate crisis

- Back-of-the-napkin estimate:
  - 2 CPUs x 85W + peripherals + cooling >= 200W
  - 24h single-node job: 0.2 x 24 = 4.8 kWh
  - German energy mix 2019: ~400g CO2 / kWh
  - CO_2 emissions: 4.8 x 0.4 = 1.92 kg

10 km x

BMW X5 M50d: 190g/km

Software gets faster

New Results

Comment on this paper

A Fast and Memory-Efficient Implementation of the Transfer Bootstrap

Sarah Lutteropp, Alexey M. Kozl

doi: https://doi.org/10.1101/73

480x speedup

EPA-ng: Massively Parallel Evolutionary Placement of Genetic Sequences

Pierre Barbera, Alexey M Kozl

Tomáš Flouri, Alexandros St

30x speedup

Systematic Biology, Volume 68, ue 2, March 2019, Pages 365–369, https://doi.org/10.1093/sysbio/syy054

CORRECTED PROOF

RAxML-NG: a fast, scalable and user-friendly tool for maximum likelihood phylogenetic inference

Alexey M Kozlov, Die ndros Stamatakis

4x speedup

Bioinformatics, btz305,

Published: 09 May 2019 **Article history**

Multi-rate Poisson tree processes for single-locus species delimitation under maximum likelihood and Markov chain Monte Carlo

P Kapli, S Lutteropp, J Zhang, K Kobert, P Pavlidis, A Stam is, T Flouri

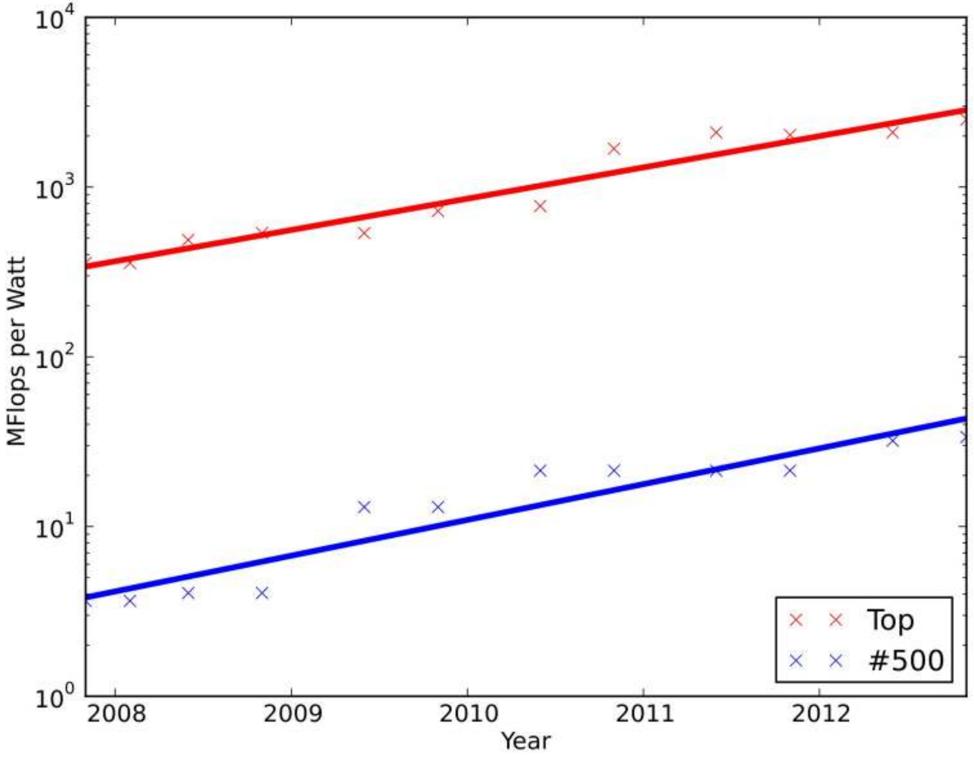
~1000x speedup

Bioinformatics, Volume 33, doi.org/10.1093/bioinformatics/btx025

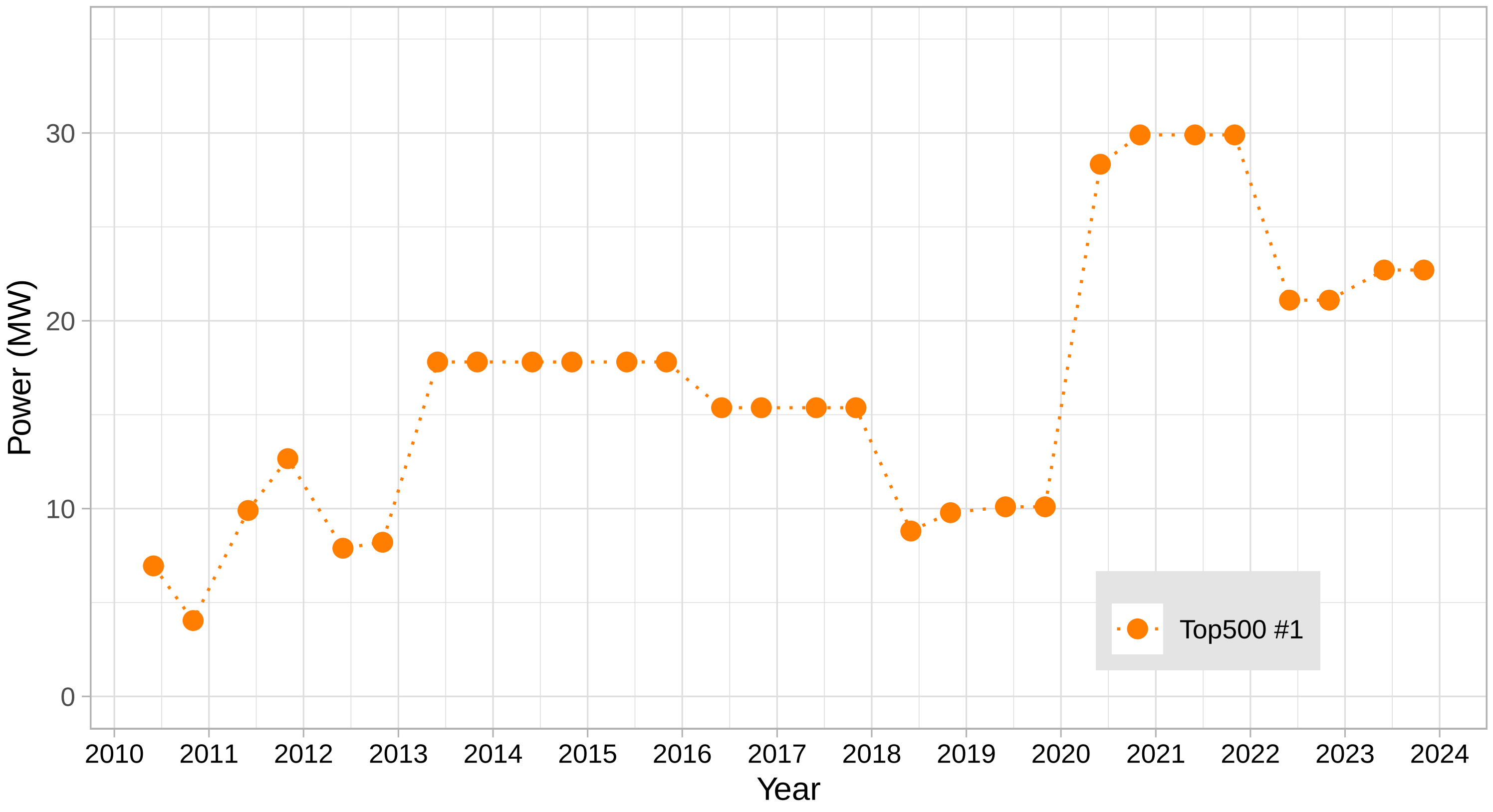
Published: 20 January 2017 **Article history**

Hardware gets better

- Green500: Exponential growth in FLOPS/Watt



Top500 power trend



The Jevons paradox

- W. S. Jevons „The Coal Question“ (1865):

Improved efficiency

Increased consumption rate

Lower cost

a.k.a. “rebound effect” or “induced demand”

Images: dpa, Wikipedia, techcrunch.com, https://www.busandmotorcoachnews.com

Energy monitoring

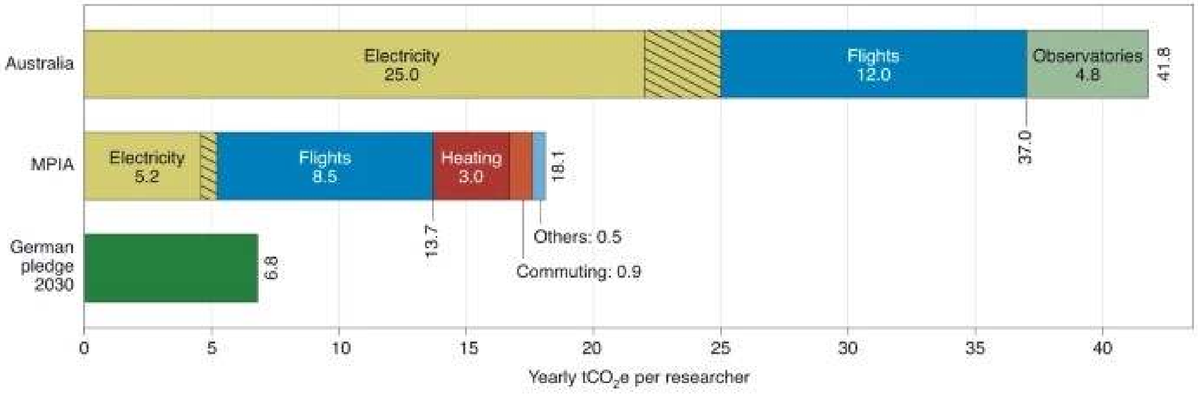
Energy monitoring: goals

- Measuring energy *accurately* is hard!
- Let’s be pragmatic
  - All measurements are wrong, but some are useful
  - Feasibility over Simplicity over Accuracy
  - Consistency important for comparability

Energy monitoring: use case #1

- General awareness
  - Impact vs. other areas, e.g. transportation
  - Averaged estimates are OK → W/core, CO_2/kWh ...

Fig. 1: Average annual emissions in 2018 for an Australian and MPIA researcher in $tCO_2e\ yr^{-1}$, broken down by sources.

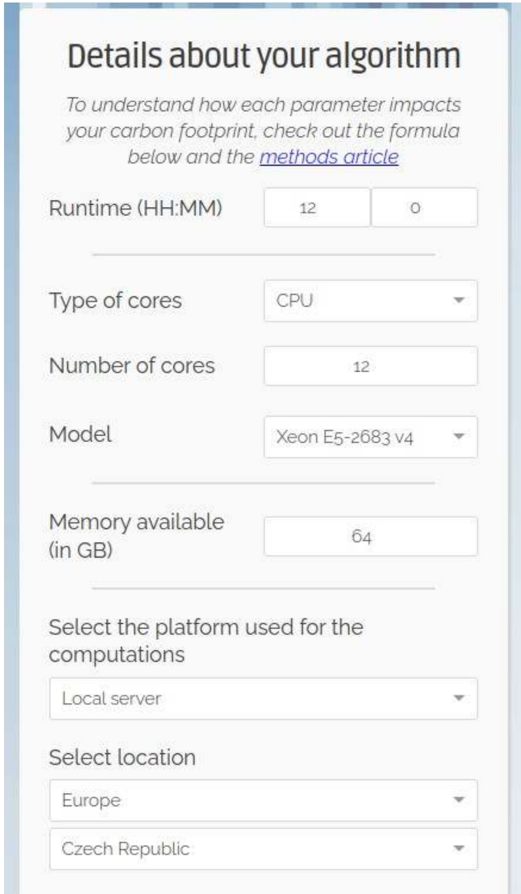


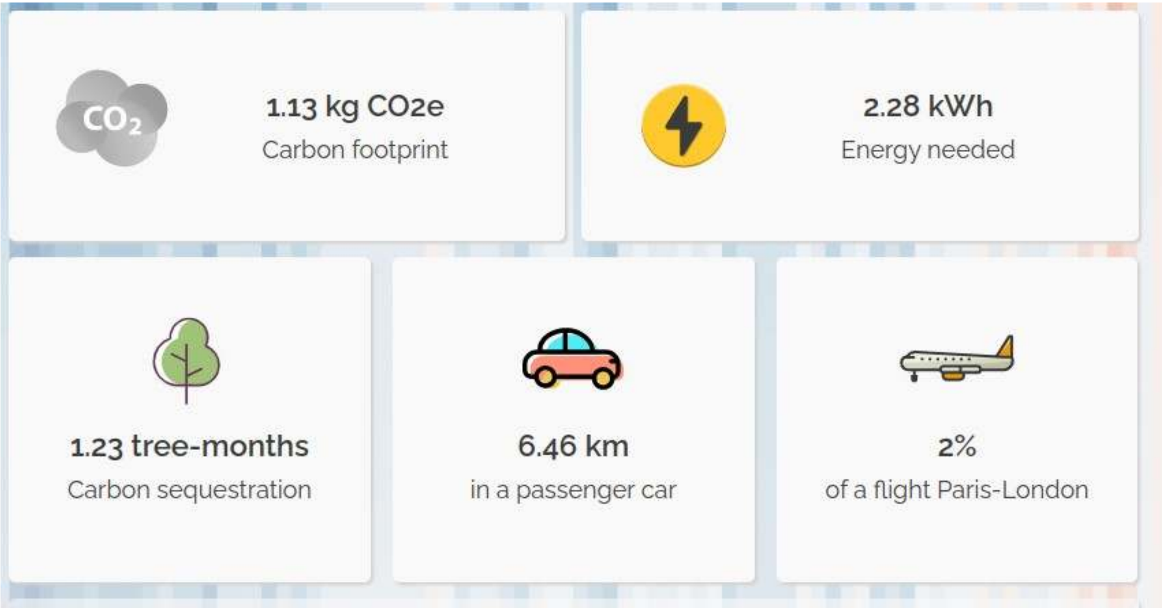
(Jahnke et al., Nat Astronomy 2020)

Top-down estimation

- The analysis took 1,200,000 CPU-hours on the SuperMUC-NG supercomputer (LRZ, Garching, Germany)
- In 2021, LRZ energy consumption was 32,632,950 kWh [LRZ1], and in total 2,308,500,000 CPU-hours were allocated to user jobs [LRZ2]
- On average, this corresponds to roughly 14 Wh per CPU-hour, or 17,000 kWh for the full analysis
- This translates to ~7,200 kg of CO2 based on carbon intensity of the German electricity mix (0.425 kgCO2/kWh in 2021 [UBA])
- This is roughly equivalent to 17 NY->London flights (one-way) [Google]

Bottom-up estimation



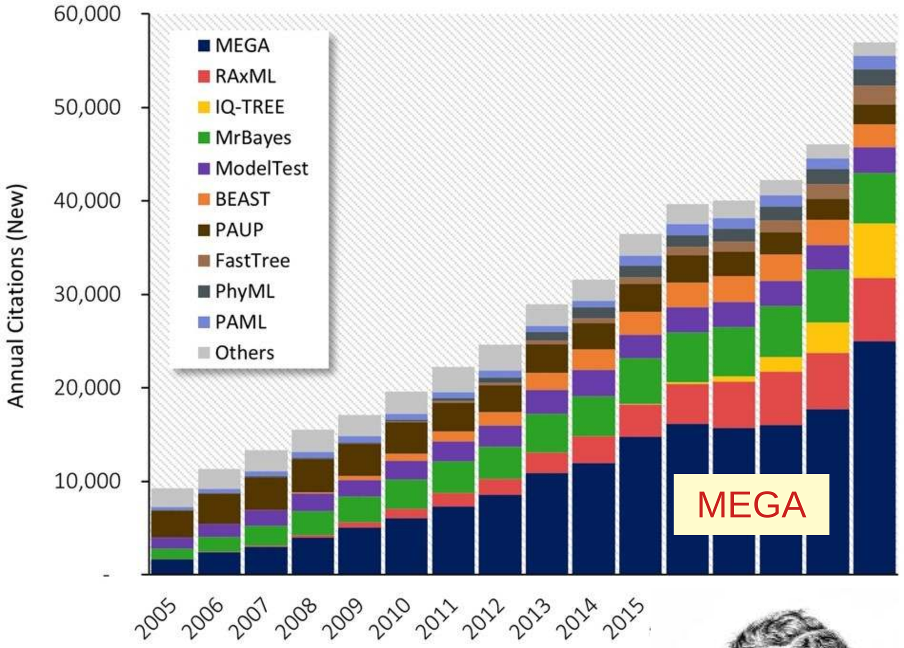


http://calculator.green-algorithms.org/

NJ for Future?

		Computer Resources			Environmental Impact	
		Time	Memory	Energy	C-footprint	Trees
Function	Method/Tool	(h)	(peak, MB)	(kWh)	(g)	(days)
(c) Phylogeny inference						
c1.	Maximum likelihood	8.1	4,000	0.11	41	1.2
c2.	FastTree	0.7	700	0.01	3	0.1
MEGA	Neighbor-joining	0.1	8	<0.01	<1	<0.1

(Kumar, 2022 MBE)



can raxml-ng handle 6 million genomes of SARS-CoV-2? #172

Closed I [redacted]pened this issue last week · 4 comments

Energy monitoring: use case #2

- Comparative analysis / benchmarking
  - Year-to-year, programs, parameters etc.
  - Actual measurements needed
  - Systematic under-/overestimation is OK

Energy measurement levels

- Building / Datacenter → smart meters
- Server room, rack → smart PDUs
- Node / Server
- CPU / GPU
- Job
- User

Energy monitoring: Toolbox

	IPMI / DCMI	NV-SMI	ROcM-SMI	RAPL
Platform	Servers	GPU (Nvidia)	GPU (AMD)	CPU (Intel, AMD)
Scope	Full system	GPU	GPU	CPU+DRAM
Power	✔	✔	✔	✘
Energy	✘	✘	✔	✔
Resolution	low	medium	medium	very high
Low latency	✘	depends?	???	✔
Reliability	✘	???	???	✔
Non-root access	✘	✔	✔	✔ / ✘
Power limiting	✔ / ✘	✔	✔	✔

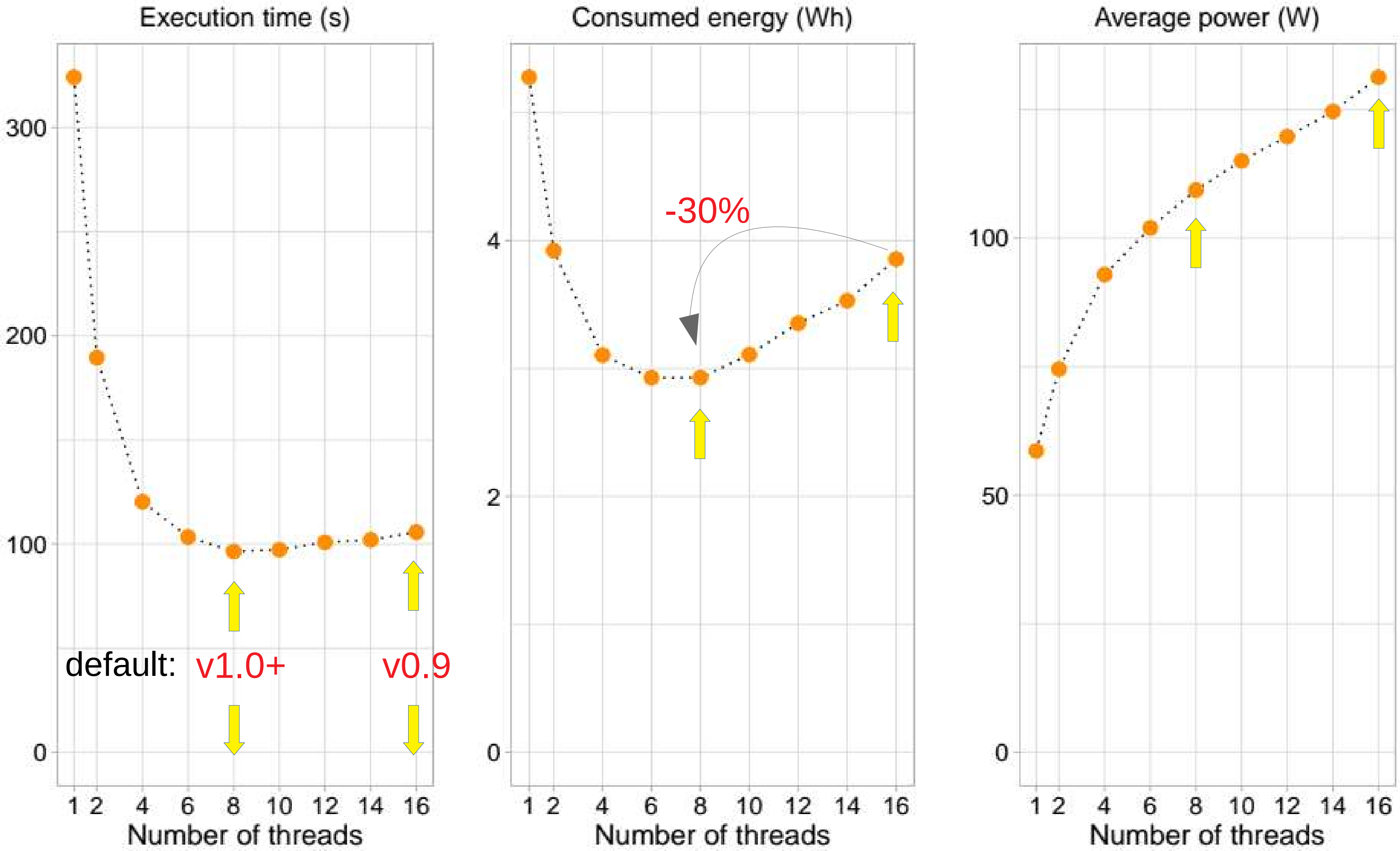
Energy monitoring: RAxML-NG

- New in RAxML-NG v1.0: energy usage report
  - Measured with Intel RAPL → CPU+DRAM only
  - Supported on Linux systems only
  - To disable, add: --extra energy-off

```
Elapsed time: 42846.287 seconds

Consumed energy: 162370.469 Wh (= 812 km in an electric car, or 4059 km with an e-scooter!)
```

Energy-to-solution

Automatic parallelization tuning



Experiment Impact Tracker

- Energy&CO2 tracking library for Python
  - Code: https://github.com/Breakend/experiment-impact-tracker
  - Paper: https://jmlr.csail.mit.edu/papers/volume21/20-312/20-312.pdf

```
from experiment_impact_tracker.compute_tracker import ImpactTracker

experiment1 = tempfile.mkdtemp()
experiment2 = tempfile.mkdtemp()

with ImpactTracker(experiment1):
    do_something()

with ImpactTracker(experiment2):
    do_something_else()
```

```
$ generate-carbon-impact-statement experiment1_log_dir experiment2_log_dir
```

Energy monitoring in SLURM

- Plugins for RAPL, IPMI...
- Node power
- Job energy

```
[user@cascade-login ~]$ scontrol show node cascade-149
NodeName=cascade-149 Arch=x86_64 CoresPerSocket=20
   CPUAlloc=0 CPUTot=40 CPULoad=0.00
   AvailableFeatures=cpu6230,ram96,rtx2080
   ActiveFeatures=cpu6230,ram96,rtx2080
   Gres=gpu:2,cpuonly:1
   NodeAddr=cascade-149 NodeHostName=cascade-149 Version=20.11.7
   OS=Linux 4.18.0-147.8.1.el8_1.x86_64 #1 SMP Thu Apr 9 13:49:54 UTC 2020
   RealMemory=95000 AllocMem=0 FreeMem=92900 Sockets=1 Boards=1
   MemSpecLimit=2048
   State=IDLE ThreadsPerCore=2 TmpDisk=0 Weight=1 Owner=N/A MCS_label=N/A
   Partitions=debug.p
   BootTime=2021-06-09T11:20:43 SlurmdStartTime=2021-06-09T15:02:11
   CfgTRES=cpu=40,mem=95000M,billing=40,gres/gpu=2
   AllocTRES=
   CapWatts=n/a
   CurrentWatts=18 AveWatts=14
   ExtSensorsJoules=n/s ExtSensorsWatts=0 ExtSensorsTemp=n/s
   Comment=(null)
```

```
[user@cascade-login ~]$ sacct -j 880244 -o ConsumedEnergy
ConsumedEnergy
--------------
        70.11K
        70.11K
        70.10K
```

Energy in SLURM: problems

- Poor visibility, no summary stats
- RAPL broken on Intel Haswell and later
  - Fixed on HITS clusters
  - Bug opened upstream: https://bugs.schedmd.com/show_bug.cgi?id=9956
- No support for NVIDIA GPUs (yet?)
  - But: AMD GPUs via ROCm-SMI library

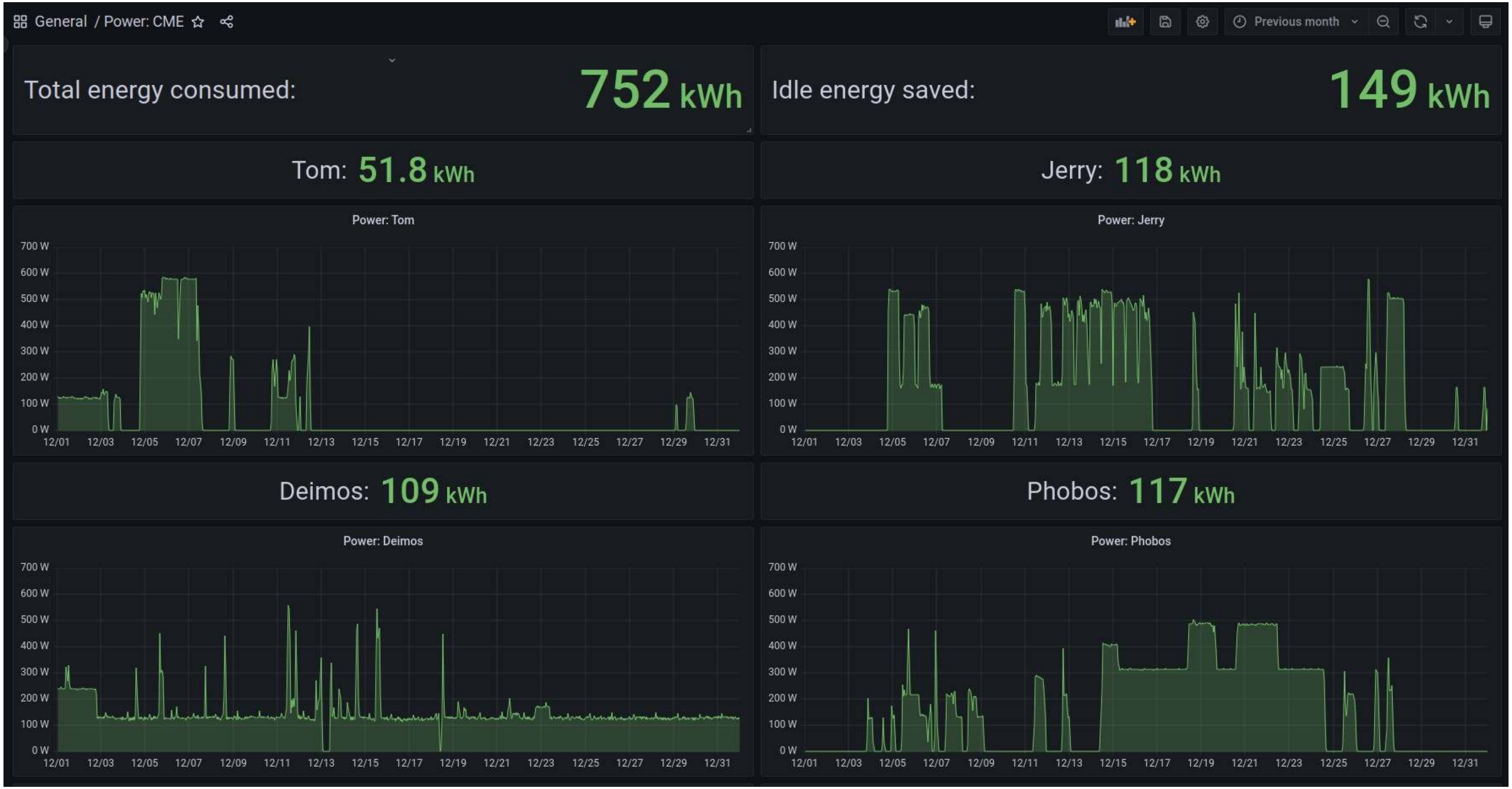
Per-application energy

- What if nodes are shared?
- Perfect attribution problematic
- Heuristic: use CPU usage ratio (proc/sys)

Guerilla monitoring @ HITS

- Group servers
  - IPMI → telegraf → influxDB → Grafana
  - Resolution: 30 s
  - HowTo: https://github.com/amkozlov/ipmi-grafana
- HITS clusters
  - IPMI → checkmk → CSV → influxDB → Grafana
  - Resolution: 1 min

Group servers power



Cluster nodes power: aggregated

+ storage + network + cooling + PSU conversion losses

Energy optimization

Idle consumption

- Example: Intel i7-7800X, 6 cores, 64GB RAM
  - sleep: 5W, idle: 55W, under load: 150W
  - 50% utilization → 25% savings (219 kWh/a)
  - 30% utilization → 42% savings (306 kWh/a)
- Example: Xeon Platinum 8260, 48 cores, 764GB RAM
  - standby: 20W, idle: 120 W, under load: 500 W
  - 50% utilization → 16% savings (438 kWh/a)
  - 30% utilization → 30% savings (613 kWh/a)

Sleep-on-Idle

- Desktops
  - Suspend-on-idle + Wake-on-LAN
  - Used by several groups, no centralized solution yet
- Rack servers
  - No suspend to RAM :(
  - PowerOff-on-idle + PowerOn-over-IPMI
  - https://github.com/amkozlov/idle-sleep

PowerOff-on-Idle

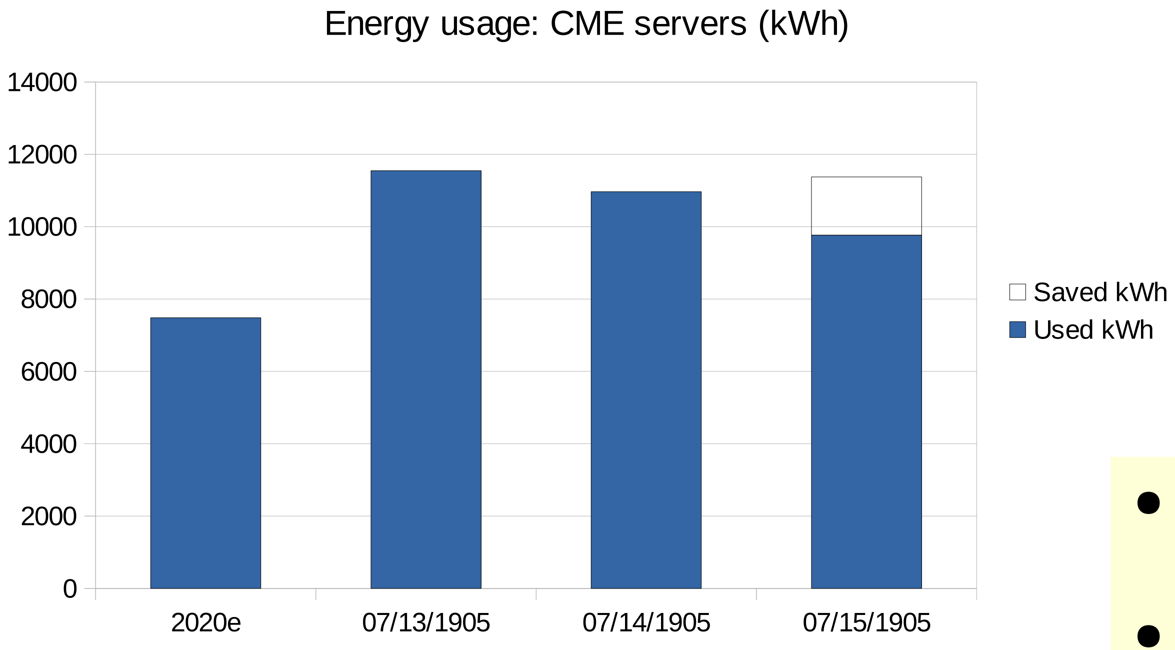
- Idle detection cron job
  - No active sessions + CPU utilization < 0.5 → idle
  - Idle since 1 hour → poweroff
  - Can be temporarily disabled:

```
deimos$ ecosleep disable 12h
Server will not be powered off until: Di 16. Mai 10:13:34 CEST 2023
```

- PowerOn via SSH

```
laptop$ alias | grep ecowake
alias ecowake='ssh kozlovay@XXXX.h-its.org sudo /hits/fast/cme/ecosleep/wakeup.sh'

laptop$ ecowake deimos
kozlovay@XXX.h-its.org's password:
Chassis Power Control: Up/On
waiting for deimos .......................................................
Server is back online!
```

Idle power savings 2023



- 1600 kWh (16%)
- -11% vs. 2022

Problems / Improvements

- screen/tmux sessions lost
  - tmux-resurrect might help
- Boot delay 1-2 min.

Power scaling

Power scaling on CPU and GPU

- Widely available: Intel/AMD/NVIDIA
- Power and/or frequency limits
- Typical range: 50% - 100% TDP
- Easy-to-use, transparent to workload

NVIDIA GeForce RTX 2080 SUPER

```
$ nvidia-smi -q -d POWER,CLOCK
  Power Management                     : Supported
  Power Draw                           : 4.24 W
  Power Limit                          : 250.00 W
  Default Power Limit                  : 250.00 W
  Enforced Power Limit                 : 250.00 W
  Min Power Limit                      : 125.00 W
  Max Power Limit                      : 250.00 W
```

```
$ sudo nvidia-smi -pl 200
Power limit for GPU 00000000:17:00.0 was set
to 200.00 W from 300.00 W.
```

Intel Xeon Platinum 8260

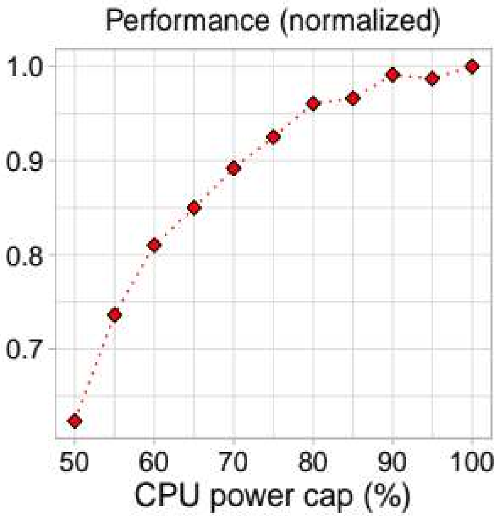
```
$ sudo cpupower frequency-info
  hardware limits: 1000 MHz - 3.90 GHz
  available cpufreq governors: performance powersave
  current policy: frequency should be within 1000 MHz and 3.90 GHz.
```

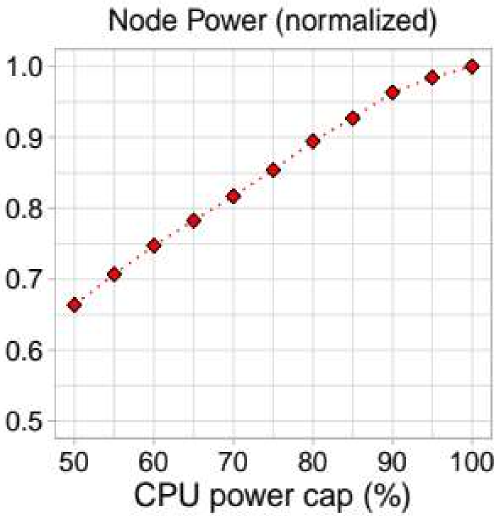
AMD EPYC 7452

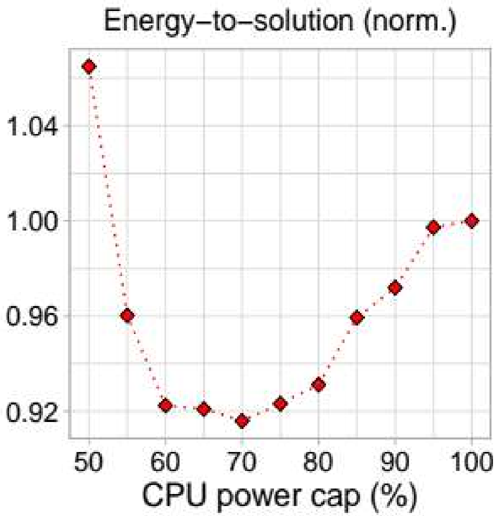
```
$ sudo cpupower frequency-info
  hardware limits: 1.50 GHz - 2.35 GHz
  available frequency steps:  2.35 GHz, 2.00 GHz, 1.50 GHz
```

```
$ sudo cpupower frequency-set -u 2000000
Setting cpu: 0
...
```

Energy efficiency “sweet spot”

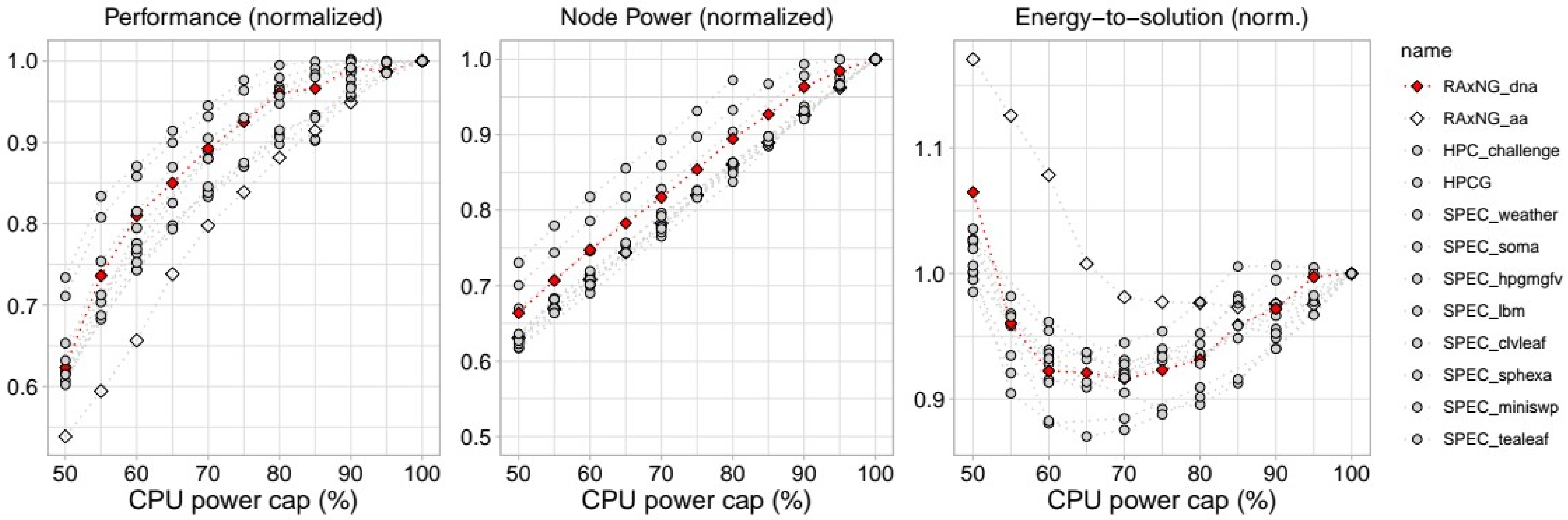




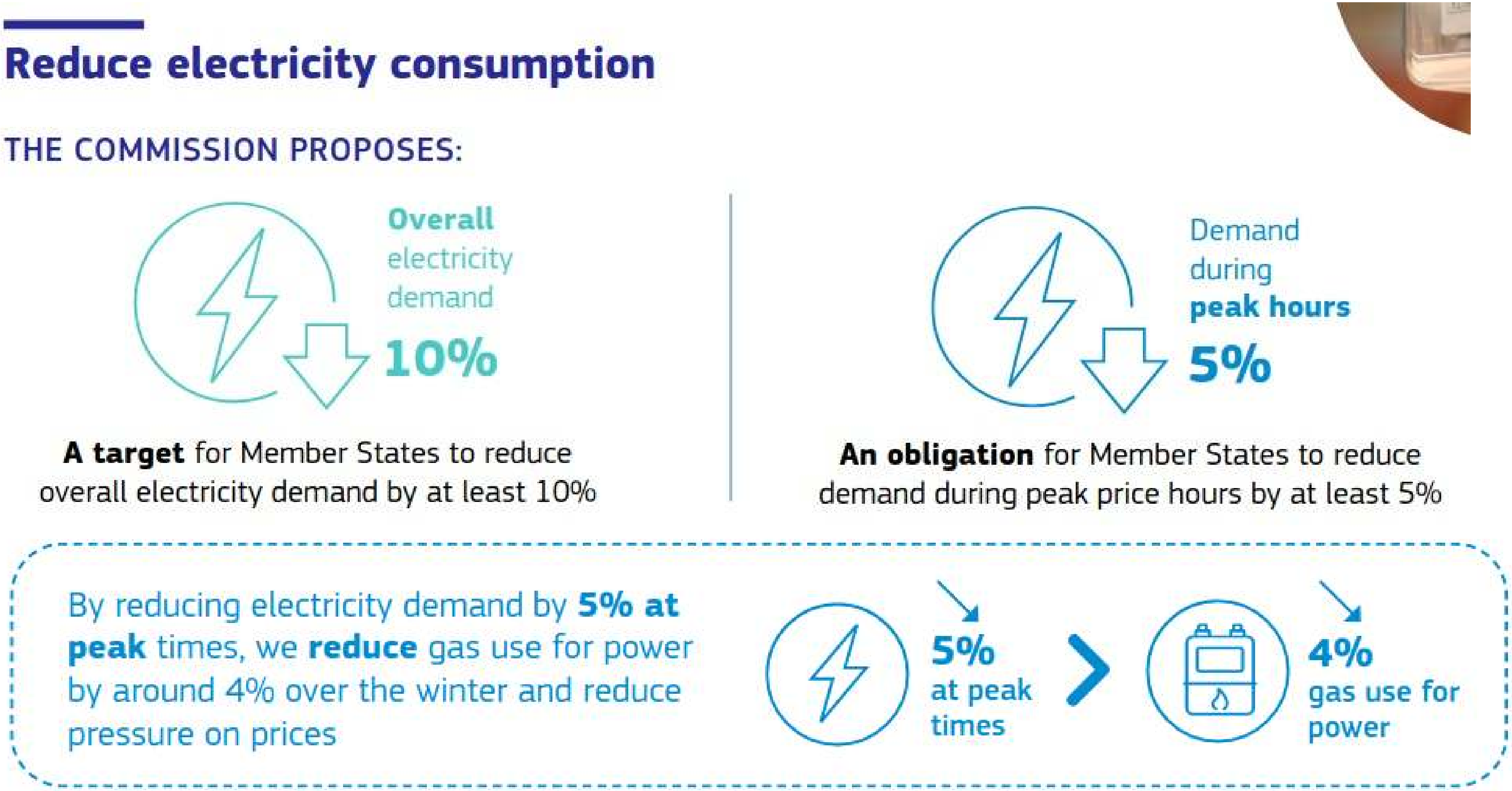


(RAxML-NG 1.1, 2x Intel Xeon Platinum 8260, 48T)

Workload variation



Motivation 2022: Energy crisis



Source: https://ec.europa.eu/commission/presscorner/detail/en/fs_22_5491

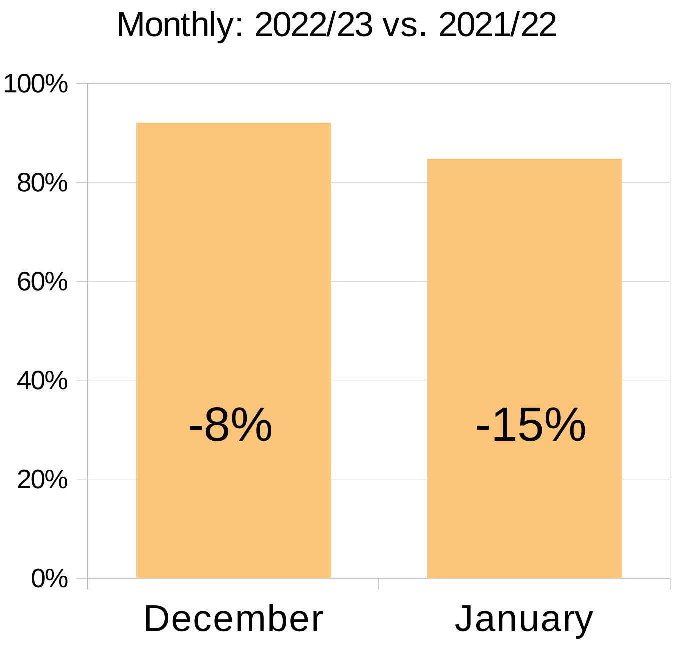
HPC community reaction

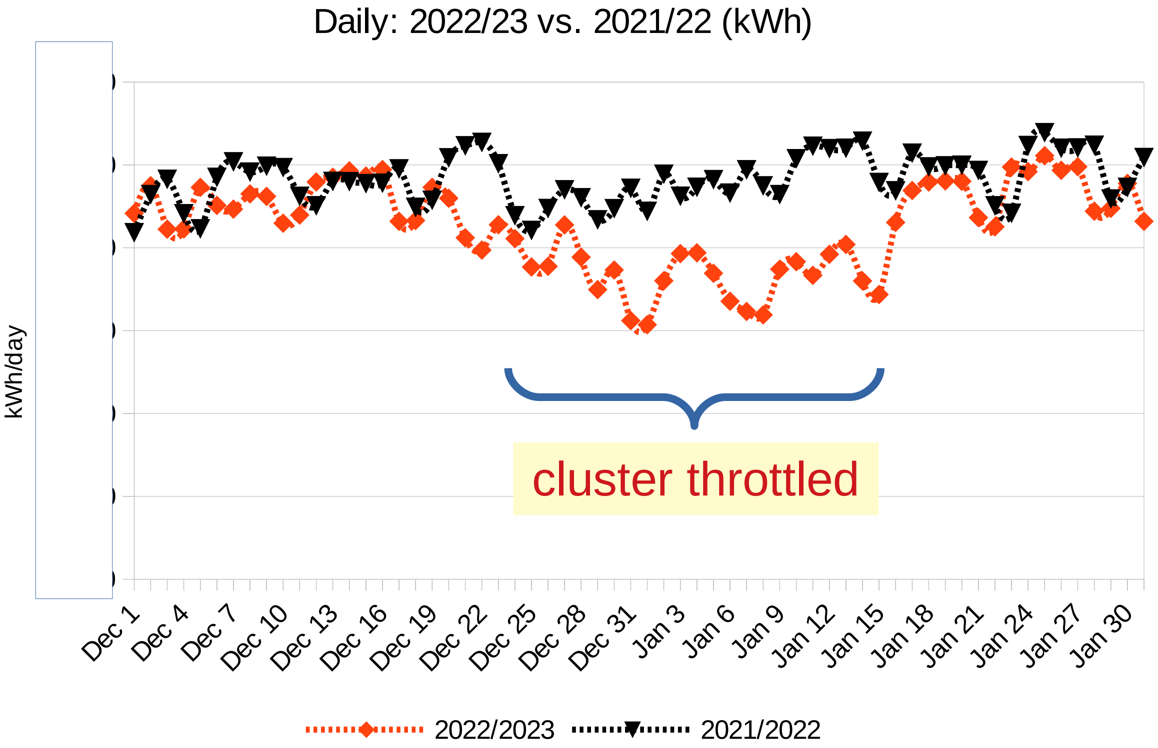
(biased subjective perception, limited sample size)

“Christmas experiment”

- 23.12.2022 → Apply power throttling
  - Haswell cluster (URZ): CPU 2000 MHz
  - Cascade cluster (HITS): CPU 90 W / GPU 175 W
- 16.01.2023 → Back to normal power
- 16.01. – 29.01. → Baseline data collection

Energy consumption: HITS campus





Energy consumption: Clusters

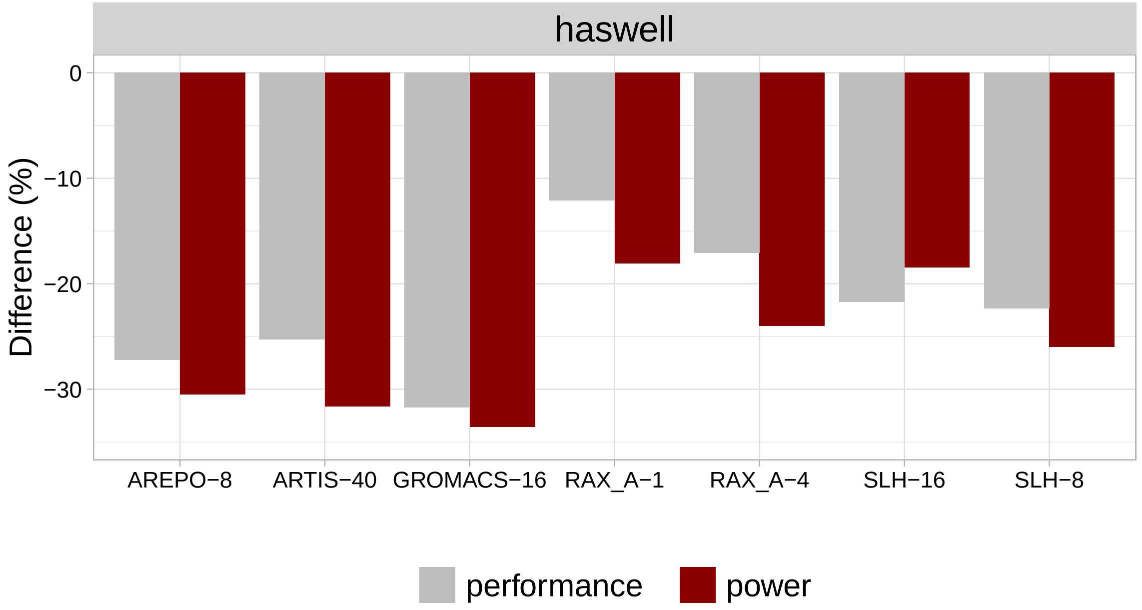
	Avg. node power (excl. idle)			Energy saved	Performance reduction (min … max)
	Regular 16.01 – 29.01	Reduced 23.12 – 15.01*	Diff.		
Haswell / URZ	150 W	100 W	-33 %	5110 kWh	-12 % ... -32 %
Cascade / HITS	294 W	220 W	-25 %	4791 kWh	-10 % ... -25 %

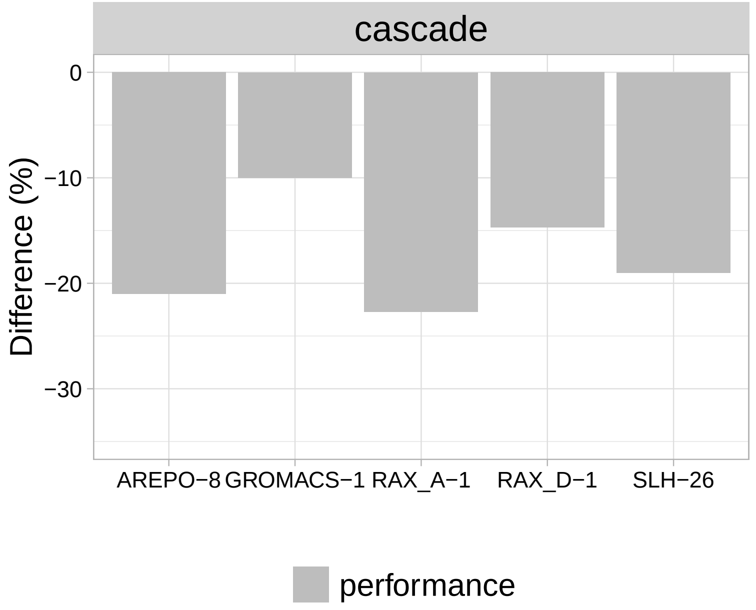
* cascade: 07.01-11.01 excluded due to storage failure

Estimated total savings (3 weeks):

 10,000 kWh =  5-7 years =  50,000 km

Performance vs. power reduction

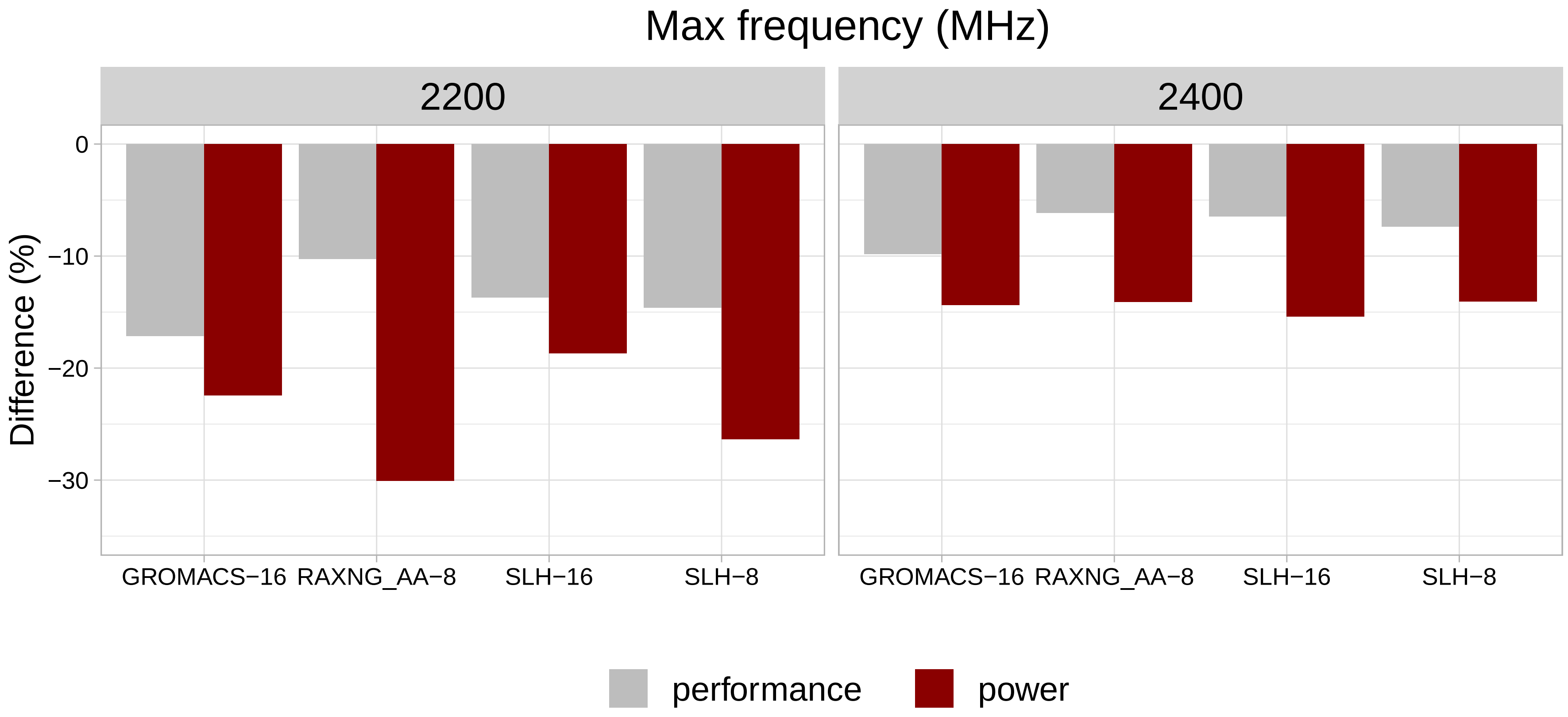




- performance loss is sublinear w.r.t. power

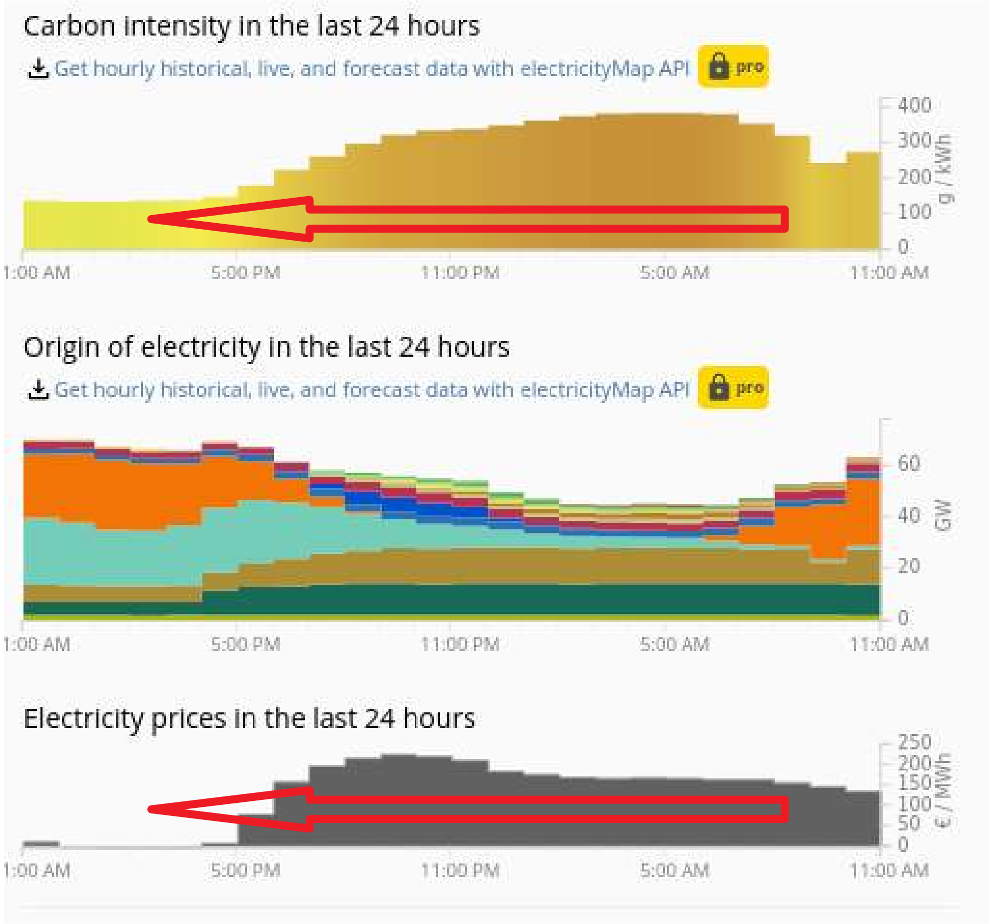
- BUT: for many workloads, “free lunch” is small: 2000 MHz below efficiency sweet spot?

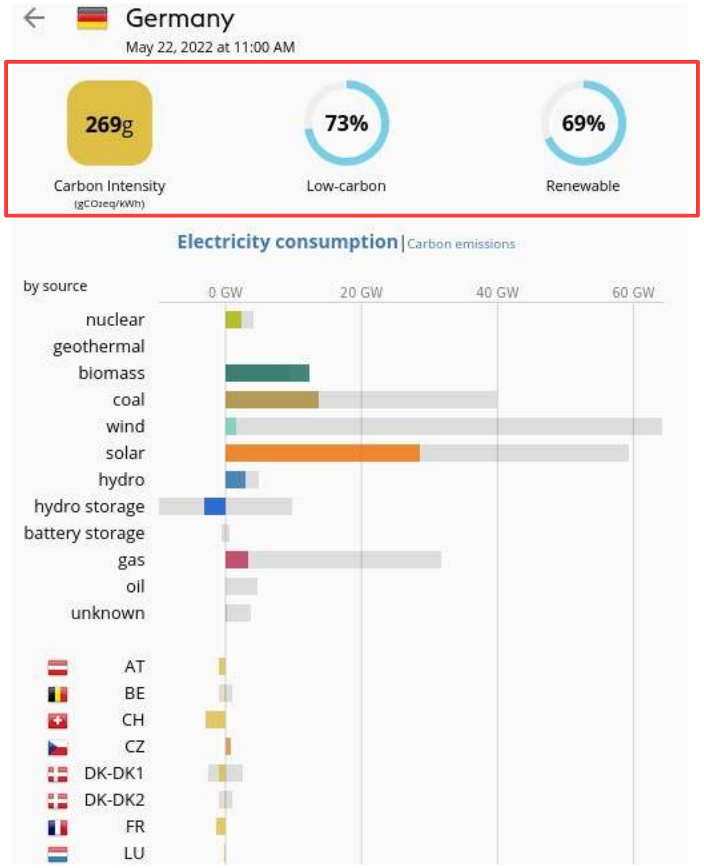
Searching for the sweet spot



Carbon-aware computing

Real-time energy mix





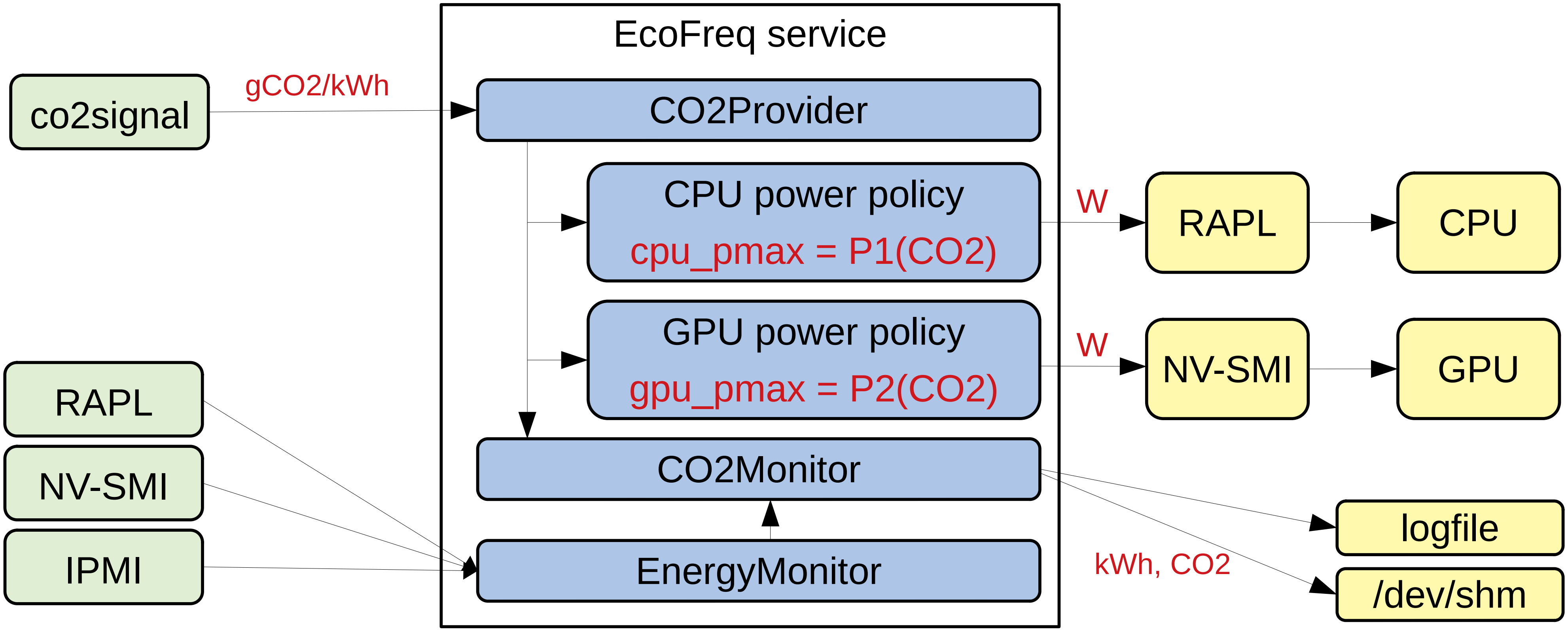
https://app.electricitymaps.com

Signal: Local, marginal, CO2, price

https://www.stromgedacht.de/

https://tibber.com

Compute with cleaner energy



- Proof-of-concept implementation: https://github.com/amkozlov/eco-freq

Power scaling: techniques

- RAPL / DVFS
  - Dynamic power / frequency limits → ~50% - 100% TDP
  - Supported by most CPUs/GPUs (Intel, AMD, NVIDIA)
- Utilization capping
  - e.g. Linux cgroup
- Adaptive parallelization
  - Adjust # threads / MPI ranks
- Freeze / suspend / turn off nodes

RAPL: advantages

- Transparent to the workload
  - No profiling, recompilation etc.
  - Long jobs are fine (no interruption / restart)
- Also works without job queue / scheduler
- No generation forecast needed
  - But can be used if available

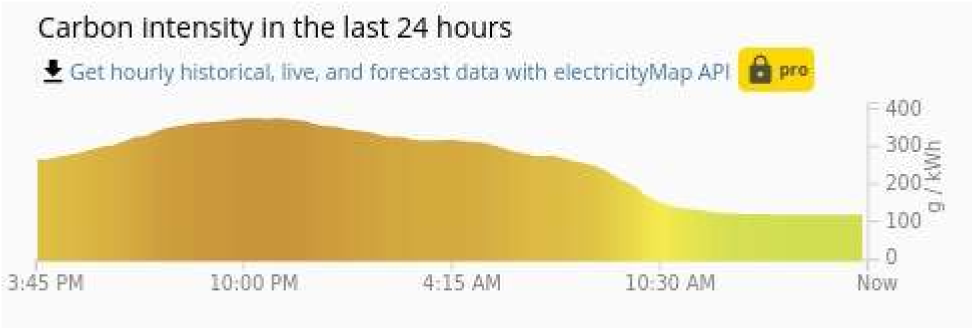
EcoFreq: Demo

```
$ sudo ./ecofreq.py

#Timestamp              gCO2/kWh     CPU_Pmax [W]    GPU_Pmax [W]    SYS_Pavg [W]    Energy [J]        CO2 [g]
2021-06-11T23:14:18          380          223.000              NA         398.650    358785.000         37.874
…
2021-06-12T09:44:48          262          275.750              NA         529.639    476675.000         34.632
…
2021-06-12T13:44:59          133          330.000              NA         594.097    534687.500         19.778
```

```
$ ./ecostat.py
EcoStat v0.0.1

Loading data from log file: /var/log/ecofreq.log

Time interval:                 2021-05-18 - 2021-06-11
Duration active:               23 days, 23:15:57
Duration inactive:             17:06:18
CO2 intensity range [g/kWh]:   108 - 449
CO2 intensity mean [g/kWh]:    284
Energy consumed [J]:           657629645.0
Energy consumed [kWh]:         182.675
CO2 emitted [kg]:              51.701283
```

```
$ ./ecorun.py -p linear raxml-ng

[...]


time_s:       882.708
pwr_avg_w:    553.422
energy_j:     488510.0
energy_kwh:   0.136
co2_g:        51.112
```

EcoFreq: Evaluation

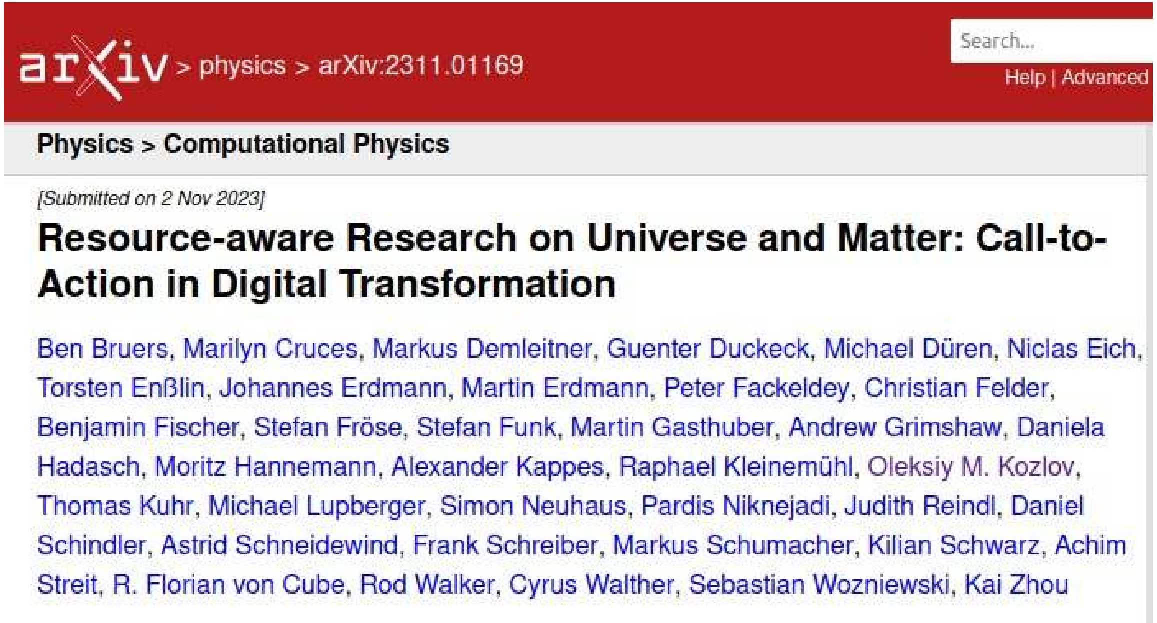


Germany, June 11-12, 2021

RAxML-NG v1.0.2 @ Intel Xeon Platinum 8260, 48C			
	Baseline	EcoFreq	Diff. %
Time [s]	58502	62257	+6.4 %
Energy [kWh]	9.533	9.082	-4.7 %
CO2-to-solution [g]	2590	2307	-10.9 %
CO2-per-hour [g] (100% utilization)	153	133	-13.1 %

Further topics

- Cooling
- Heat re-use
- UPS
- Datacenter location
- Embodied carbon
- E-waste
- ...



arXiv > physics > arXiv:2311.01169

Search...

Help | Advanced

Physics > Computational Physics

[Submitted on 2 Nov 2023]

Resource-aware Research on Universe and Matter: Call-to-Action in Digital Transformation

Ben Bruers, Marilyn Cruces, Markus Demleitner, Guenter Duckeck, Michael Düren, Niclas Eich, Torsten Enßlin, Johannes Erdmann, Martin Erdmann, Peter Fackeldey, Christian Felder, Benjamin Fischer, Stefan Fröse, Stefan Funk, Martin Gasthuber, Andrew Grimshaw, Daniela Hadasch, Moritz Hannemann, Alexander Kappes, Raphael Kleinemühl, Oleksiy M. Kozlov, Thomas Kuhr, Michael Lupberger, Simon Neuhaus, Pardis Niknejadi, Judith Reindl, Daniel Schindler, Astrid Schneidewind, Frank Schreiber, Markus Schumacher, Kilian Schwarz, Achim Streit, R. Florian von Cube, Rod Walker, Cyrus Walther, Sebastian Wozniewski, Kai Zhou

https://arxiv.org/abs/2311.01169

Take-home messages

- Familiarize yourself with energy
  - measured in kWh, not “average households”
- Look for absolute consumption numbers
  - Not hypothetical “savings”
- Don’t wait for management or IT
  - Find motivated colleagues, build horizontal links