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Environmental sustainability for scientific software

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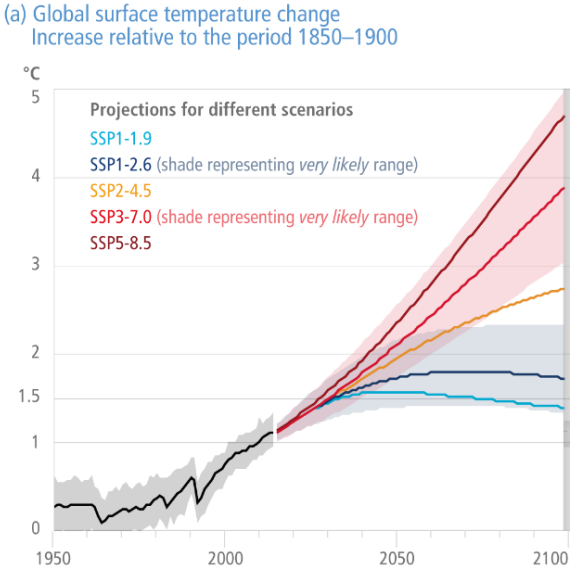
ICD Environmental Sustainability Working Group

22 Sep 2022

NOBUGS 2022

Why

- Things are bad and getting worse
- Passed 1°C warming, 400ppm CO_2
- Staying within CO_2 budgets for 1.5°C needs rapid changes
- Net zero policies: Gov, UKRI, STFC
- ICT ~2-4% of global CO_2 emissions [1] and growing
- Footprint of computing in research is significant and growing [2]



www.ipcc.ch

"Today's IPCC Working Group 1 report is a **code red for humanity**. The alarm bells are deafening, and the evidence is irrefutable: greenhouse-gas emissions from fossil-fuel burning and deforestation are choking our planet and putting **billions of people at immediate risk**. Global heating is affecting every region on Earth, with many of the changes becoming irreversible."
-- UN Secretary-General António Guterres

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[1] The real climate and transformative impact of ICT, C. Freitag 10.1016/j.patter.2021.100340
[2] UKRI Net Zero Digital Research Infrastructure Scoping Project 10.5281/zenodo.7016951

UK research's big emitters

Context

JASMIN
CO_2: 410 tonnes pa (1.5gWh y-1 + ~ 16% supply chain)

ARCHER
CO_2: 2,200 tonnes pa (8gWh y-1 + ~ 16% supply chain)

NERC SHIPS
CO_2: 35,000 tonnes pa

FAAM: 2,400 tonnes pa (fuel only)

STFC ISIS: 24,000 * tonnes pa (88 gWh pa)

---> ARCHER2 : ~ 6,000 tonnes per year
---> Next Generation : ?????

UK Research and Innovation

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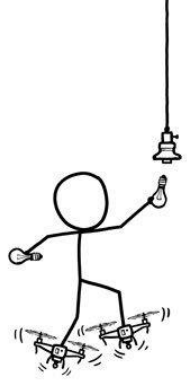
https://doi.org/10.5281/zenodo.5846587

* Electricity only



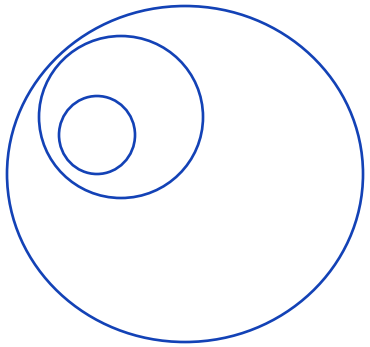
Software + Sustainability

- Will this software project be usable in the future
  - Maintainability, documentation, availability, licensing, standards

Software Sustainability Institute

- Will there still be an environment to run this software in
  - Social, individual, environmental, economic, and technical

KARLSKRONA MANIFESTO FOR SUSTAINABILITY DESIGN



SUSTAINABLE DEVELOPMENT GOALS

13 CLIMATE ACTION

- Climate is urgent issue that interacts with all others
- Electricity is the simple bit
  - Easy to measure, easy to switch sources, efficiency gains
  - Still complicated

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https://www.software.ac.uk/about
https://www.sustainabilitydesign.org/ http://arxiv.org/abs/1410.6968

*xkcd.com

CO_2 footprint of a software engineer

Office
- Heating
- AC

Laptop/Desktop
- Manufacture
- Electricity

Commuting

Trips
- To labs
- Conferences

Dev Infrastructure
- Hosting
- Version control
- Testing/CI
- Local/cloud

Software use
- Hardware
- Electricity
- HPC

Effects of software
- Experiment control
- Experiment design
- Replace physical process
- Science impact
- Societal impact

Non-work
- Food
- Home
- Lifestyle

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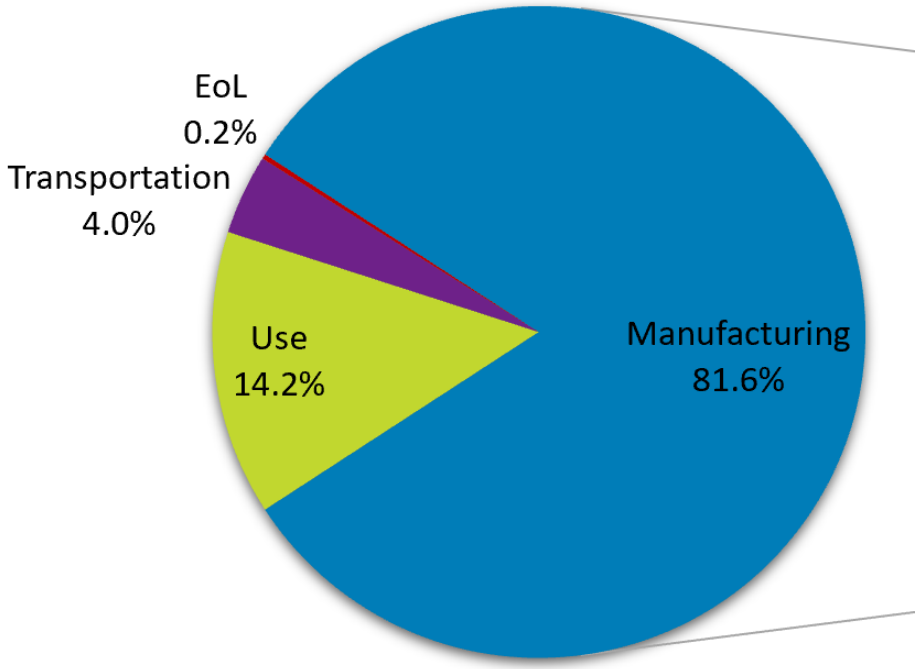
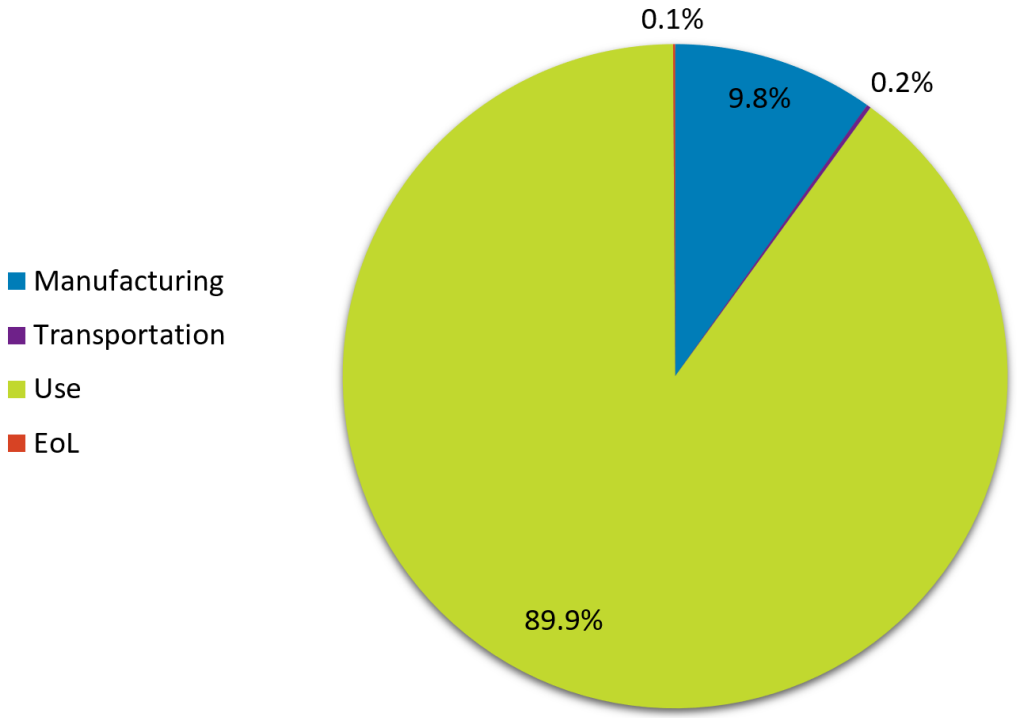
Product lifetime carbon footprints



Dell Precision 5550 Laptop



Dell PowerEdge R840 Server

* Base configs, a big SSD can make a difference

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ISIS Neutron and Muon Source

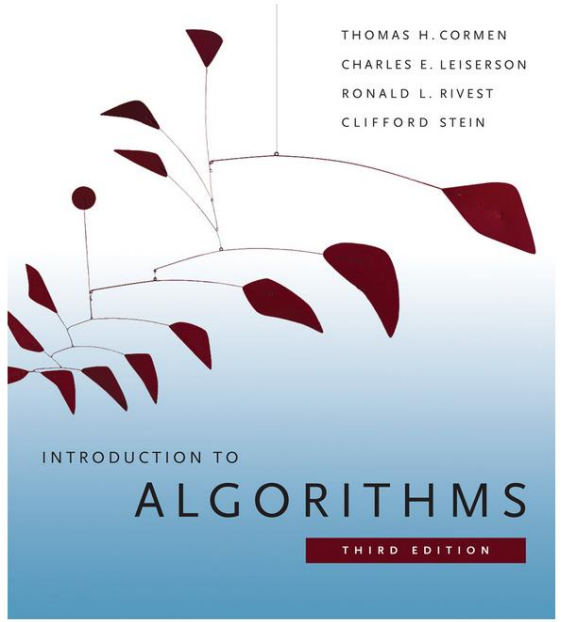
https://corporate.delltechnologies.com/en-us/social-impact/advancing-sustainability/sustainable-products-and-services/product-carbon-footprints.htm

The Dirty Secret of SSDs: Embodied Carbon - https://arxiv.org/abs/2207.10793

Efficiency

- Energy use = power × time
- Good algorithms & data structures
- Good languages
  - Or optimized libraries
- Avoid un-need work
  - Caching
  - Do you need to invert matrix, sort a list?
  - Loops
  - IO
- Compression

$O(1) < O(n) < O(n \log n) < O(n^2) < O(2^n)$



http://green-algorithms.org/
https://codecarbon.io/

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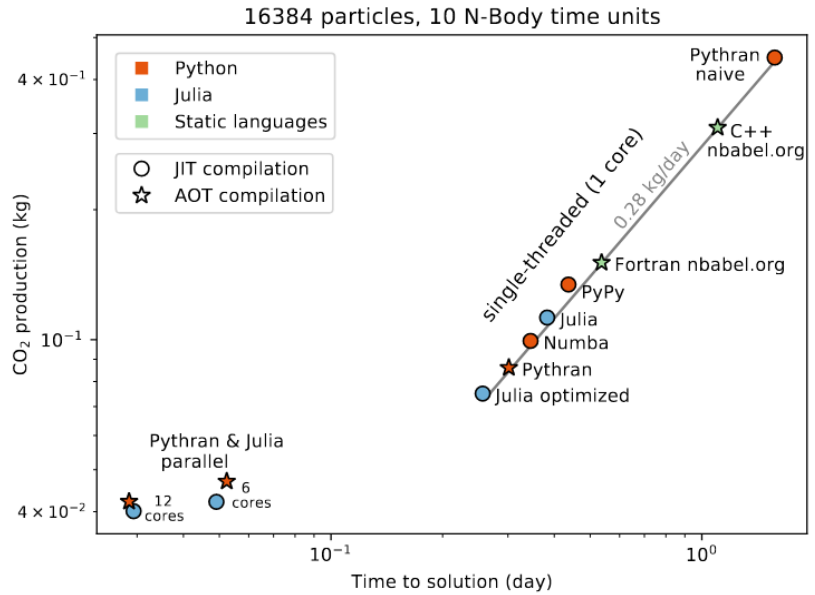
Should we stop using python?

- Python is slow compared to compiled languages
- For similar code 10-100x more CPU time
- But not hard to make python fast
  - Numpy (or scipp) vs loops
  - Scipy (algors in C/Fortran)
  - Python compilers (cython, numba, pythran, pypy)
  - Call compiled libraries
- 80/20 rule

	Energy
(c) C	1.00
(c) Rust	1.03
(c) C++	1.34
(c) Ada	1.70
(v) Java	1.98
(c) Pascal	2.14
...	
(i) Lua	45.98
(i) Jruby	46.54
(i) Ruby	69.91
(i) Python	75.88
(i) Perl	79.58



Don't use raw naïve python implementations of algorithms*

* Most python devs already don't

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Energy efficiency across programming languages, R. Pereira 10.1145/3136014.3136031
Reducing the ecological impact of computing through education and Python compiler, P. Augier 10.1038/s41550-021-01342-y

Examples

Mantid release notes

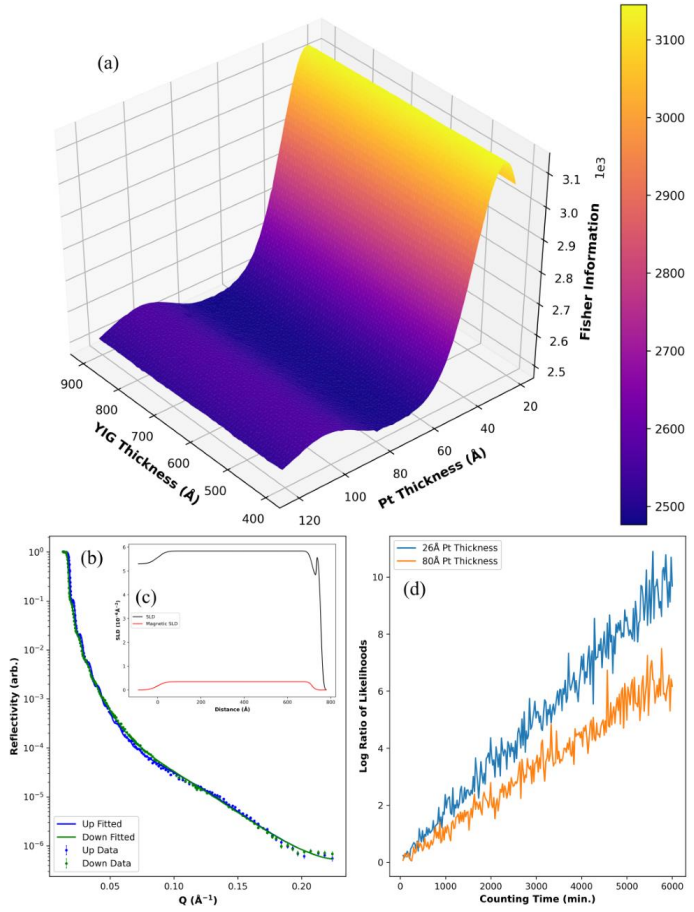
- One big file -> File per change
- Prevents conflicts, extra merges, extra test runs
- Saves CPU and developer time

SANS2D tube calibration script

- 30 -> 3 mins per iteration (remove redundant IO)
- No longer need to leave running over night
- Save CPU, research time

Holistic Optimization for Generating Better Experimental Neutrons

- Optimization of neutron reflectometry experiments
- Choose parameters that maximize Fisher information and minimize beam time
- Save beam time, same confidence results 2/3 time



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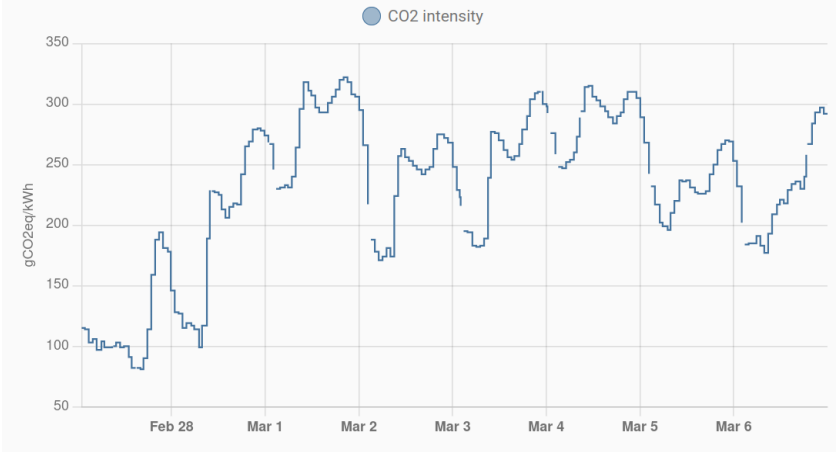
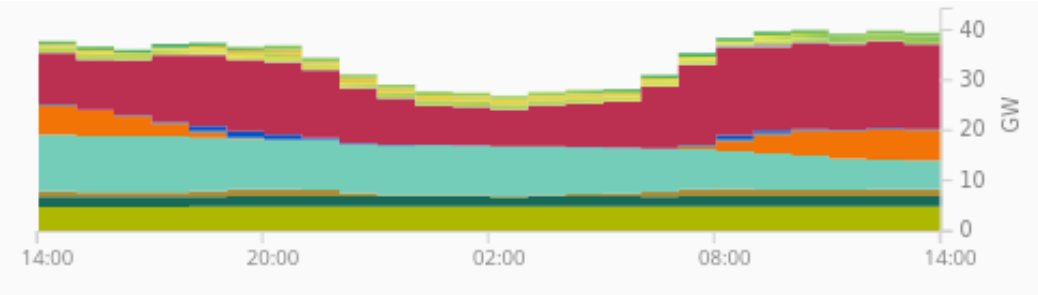
arXiv:2108.05605 - J Durant, L Wilkins, J Cooper

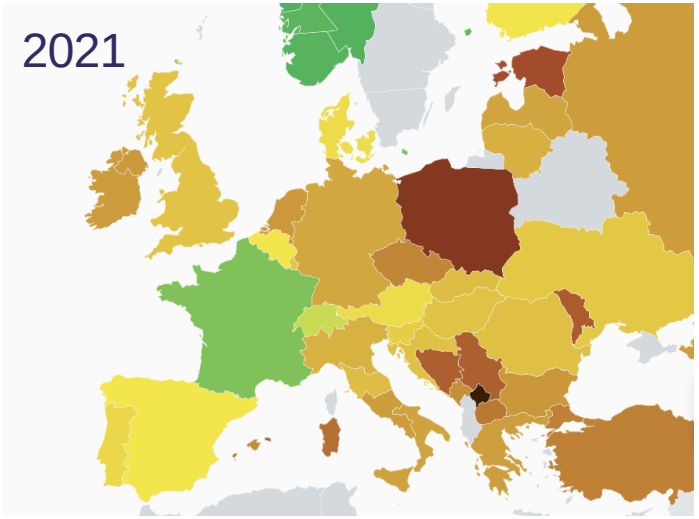
*David Fairbrother, Sarah Foxley, Jos Cooper

Time/Location shifting

- Carbon intensity of electricity g/kWh
  - Varies by place
  - Time of day, day of week
  - Weather/season
- Demand side response
  - Schedule work based on grid conditions
- Peak load shifting
  - Peaks in electricity use fossil fuels







Coal 820 g/kWh
Oil 650
Gas 490
Biomass 230
Solar 45
Hydro 24
Nuclear 12
Wind 11

co2signal.com
home-assistant.io
Electricitymap.org
IPCC

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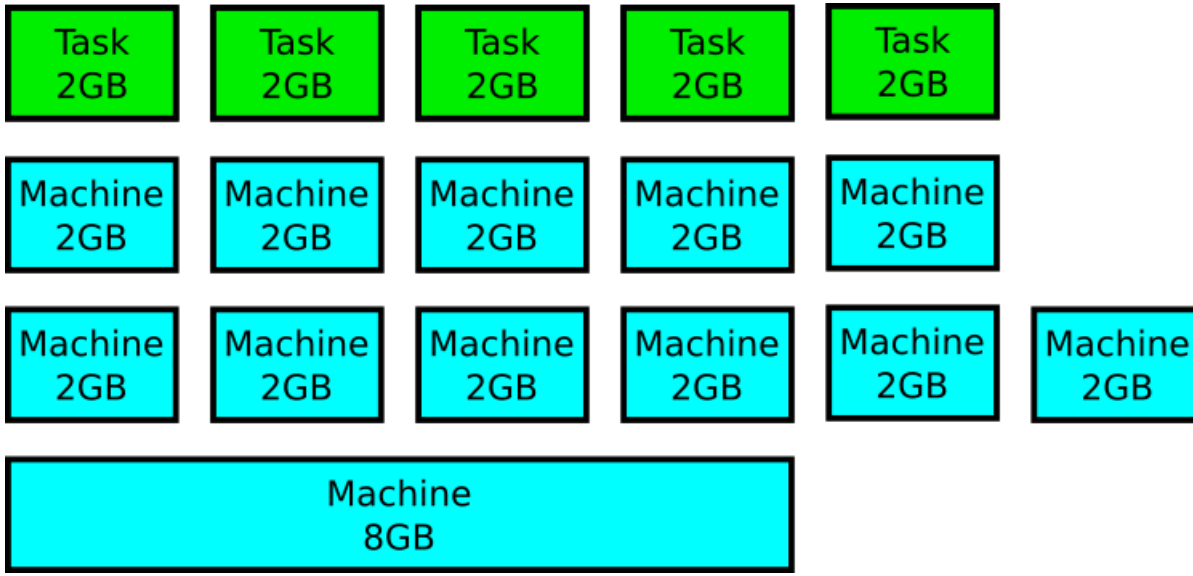
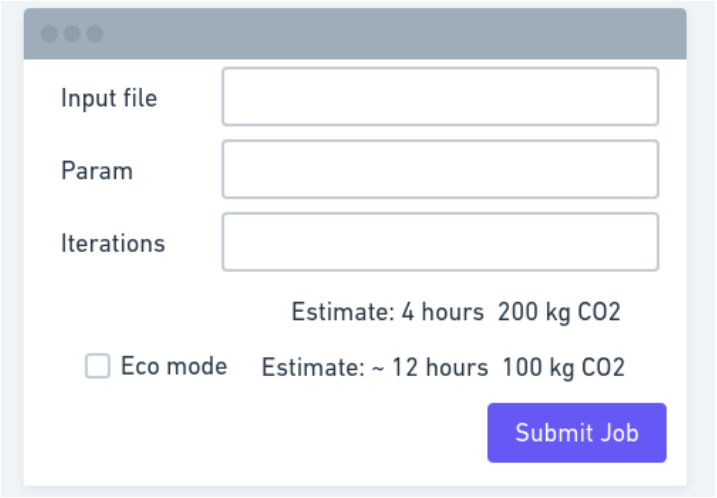
Infrastructure

- How many machines for X users
- Over and under provisioning
- CPU, RAM, Disk, network, GPU
- Availability
  - 99.999% uptime
  - Ok to wait in a queue
- Containers, VMs
- Resource
  - estimation
  - communication





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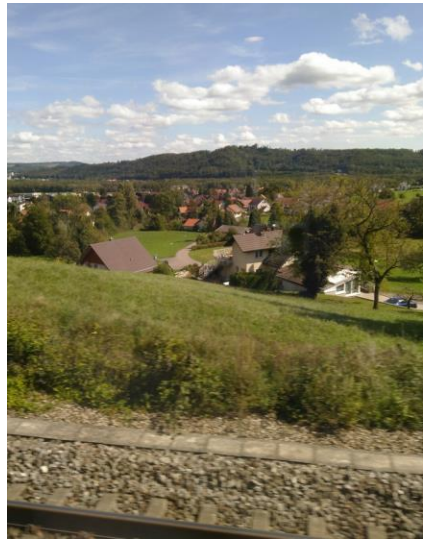
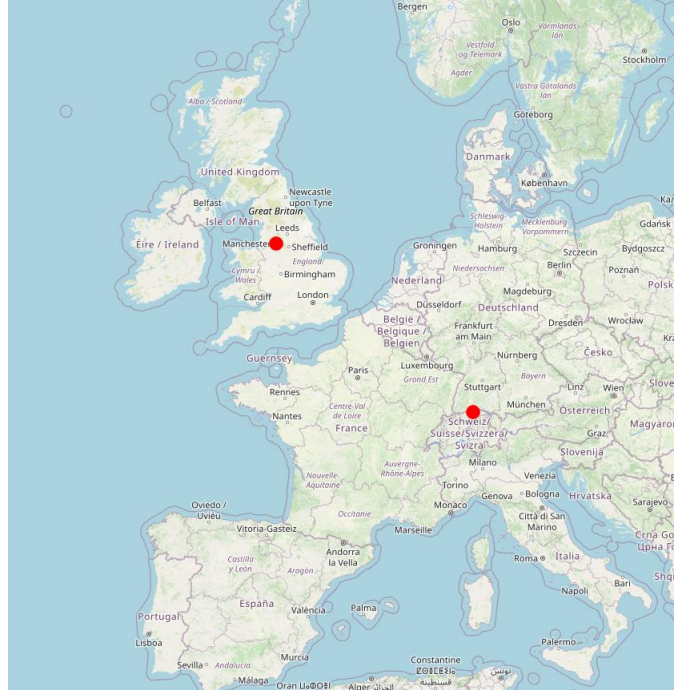
Travel

- Manchester to Zurich – 1000 km
- Air – 281 kg CO_2e
- My route
  - Train + Night Bus
  - 56 kg CO_2e
  - ~ 20 hour





Remote participants
~ 24 hours of HD video
~ 24 GB
~ 0.36 kWh for networks
~ 0.1 kg CO_2e

Aviation and Climate Change – the continuing challenge, A. Bows-Larkin - 10.1002/9780470686652.eae1031
Are technology myths stalling aviation climate policy?, P. Peeters - 10.1016/j.trd.2016.02.004
Zoom, video conferencing, energy, and emissions – D. Mytton - https://davidmytton.blog/zoom-video-conferencing-energy-and-emissions/

CO2e calculation

- Train + bus

Leg	mode	distance km	co2e kg/km	co2e kg
Manchester → London	Train	265	0.03549	9.40
London → Dover	Coach	126	0.02733	3.44
Dover → Calais	Ferry	40	0.129517	5.18
Calais → Paris	Coach	289	0.02733	7.90
Paris → Brugg	Train	559	0.00446	2.49
Total return				56.8

- Air

Leg	mode	distance km	co2e kg/km	co2e kg
Manchester → Zurich	Air	1000	0.140625	140.63
Total return				281.2

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Using UK gov values

https://www.gov.uk/government/publications/greenhouse-gas-reporting-conversion-factors-2022

Tips for rail travel

- The Man in Seat Sixty-One https://www.seat61.com/
  - Routes, booking advice
- Train is nicer than bus (but more expensive)
- If you have time take a walk outside the stations
- No silly airport restrictions
  - You can carry water, wine, food, shampoo, Swiss army knife*
- Check time for changes
  - Your travel bookers may not know how long it takes to get from Gare du Nord to Gare de Lyon

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*Check local laws

Summary

- Big topic – Big impacts
- Good software reduces energy consumption
  - Of the software
  - Other processes
- Does it need to run? does it need to run now?
- What resources does it need?
- What can you influence?
- Does you group have a sustainability team?
  - Join it or create it

Thanks

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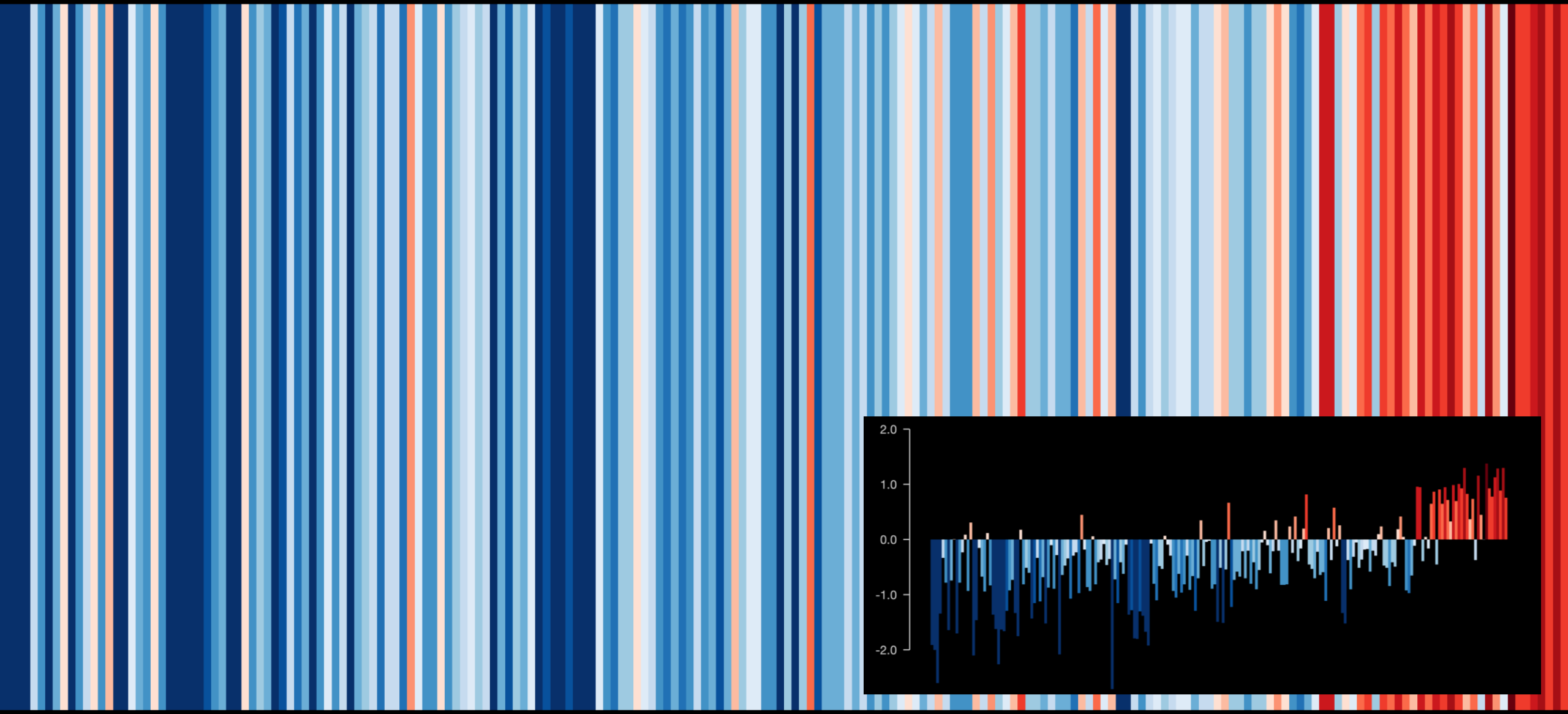
Further reading

- IPCC
  - Reports all have short readable Summary for Policymakers and Headline Statements
- UKRI Net Zero Digital Research Infrastructure Scoping Project
  - https://net-zero-dri.ceda.ac.uk/
- Without the Hot Air books
  - Food (S. Bridle) and Energy (D. MacKay) books free online
- How Bad Are Bananas - Mike Berners-Lee

Temperature change in Oxford since 1814



https://showyourstripes.info