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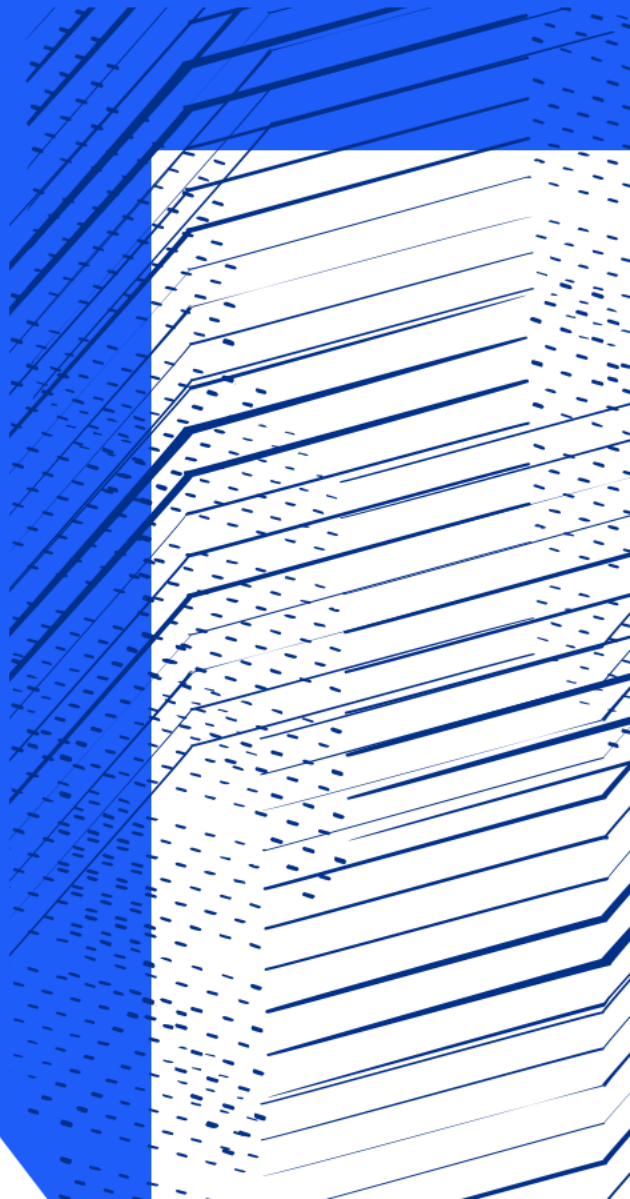
ISIS Neutron and Muon Source

Sustainable Computing

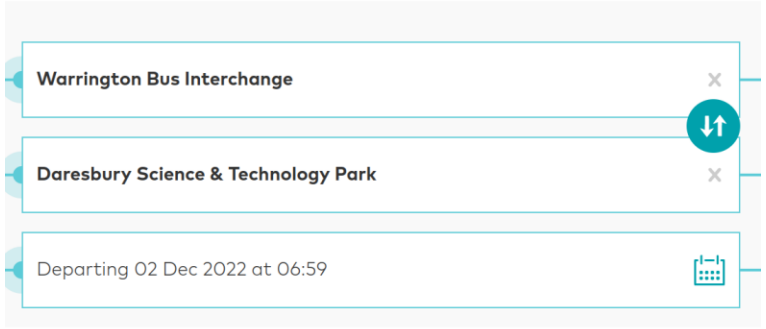
Sam Tygier
ISIS Computing Division

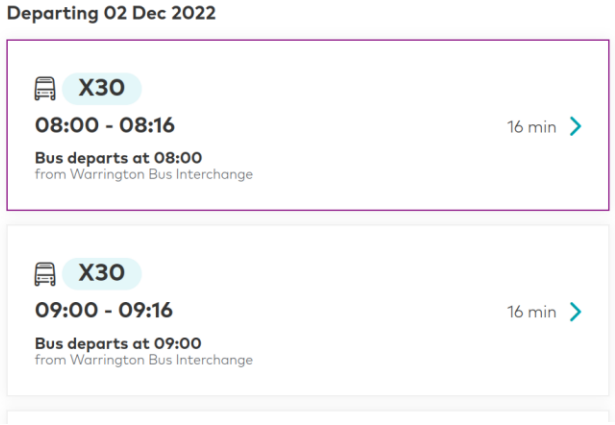
2 Dec 2022

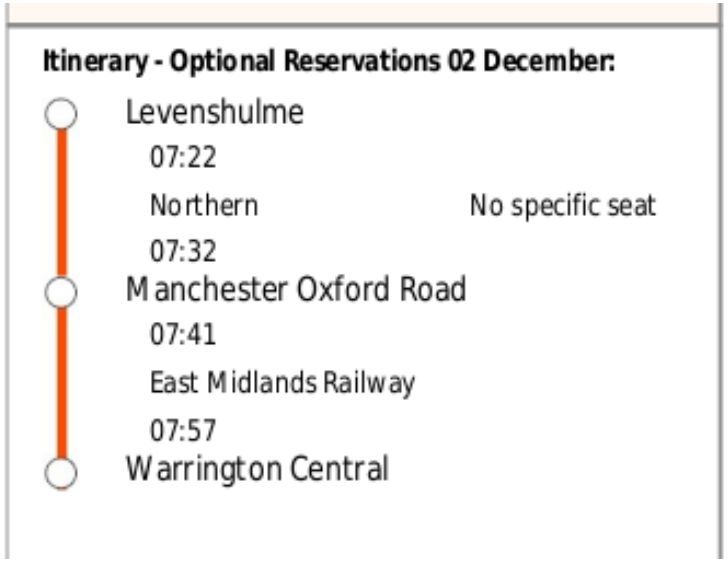


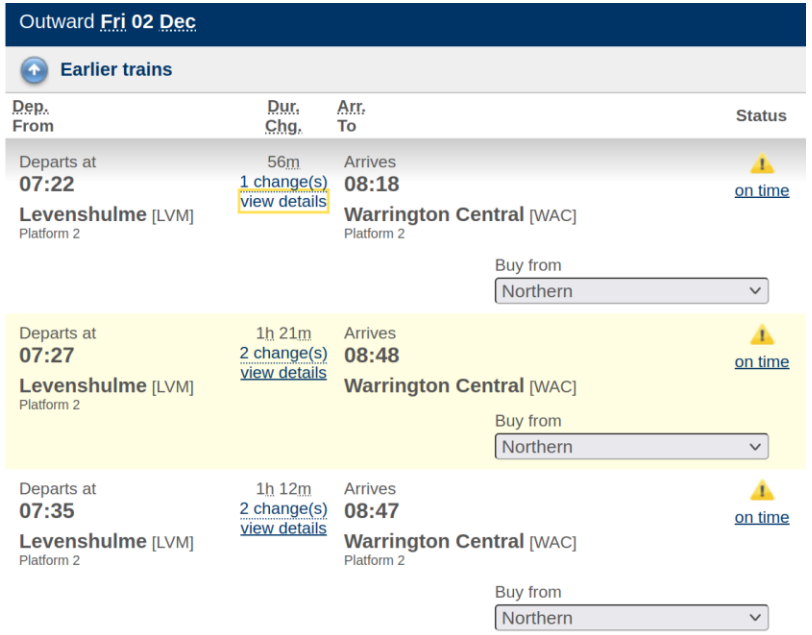
Getting to Daresbury

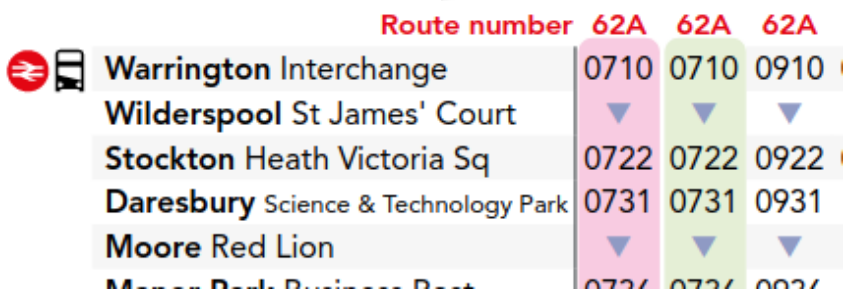
https://www.sci-techdaresbury.com/the-campus/travel-hub/travelling-by-bus/











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ISIS Computing division

Role of ICD

- Supports computing in ISIS
- Information, tools, software, hardware, clusters

Systems Operations

Service Desk
Infrastructure
Product Management
User & Authentication

User Programme Software

Proposals & Outcomes
Schedule & Operations

Scientific Software

Research Software Engineering
Systems Dev & R&D
Data Reduction

~80 Staff

Influence reaches further (ISIS, Users, RAL, ...)

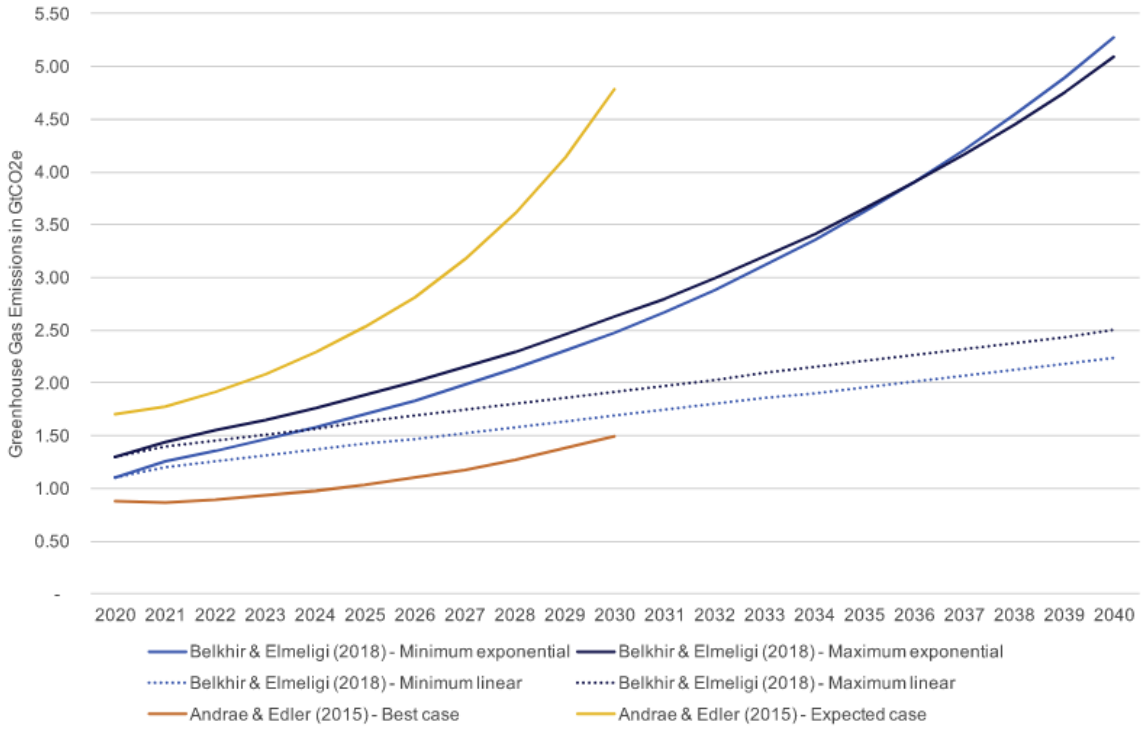
ICD Environmental Sustainability Working Group
Group of interested staff
Aim

- Understand current footprint
- Find opportunities for improvements
- Advice for staff

Links with SCD, CLF

Computing's footprint

- ICT ~2-4% of global CO_2 emissions[1] and growing
  - Steep improvements in efficiency
  - Steep growth in usage
- Footprint of computing in research is significant and growing[2]
- Not just electricity



Future ICT emission estimates - Freitag
(also cites estimate of decrease)

Jevons effect
Increase in efficiency can lead to an increase in demand
A long email has 1/20 footprint of a letter [3], but we send more emails than the letters they replaced

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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
[3] How Bad Are Bananas? 2020 M Berners-Lee, ISBN9781782837114

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

Facilities Council

10.5281/zenodo.5846587

1200 Laptops – 120 TCO_2 pa

* Electricity only

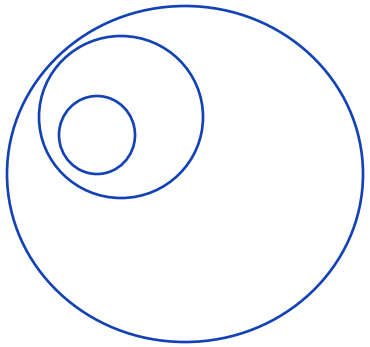
Software + Sustainability

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

Software Sustainability Institute

- Will this software project be usable in the future
  - Will there be an environment to run it 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

UKRI Science and Technology Facilities Council

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

Where can we improve

- Better software
  - Reduce resource usage for given work
- Smarter running
  - Improve where/when/how we compute
  - Better communication
- Hardware
  - Better procurement
  - Efficient use of hardware
- Driving efficiency with computing
  - Way to do science more efficiently

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ENERGY STAR

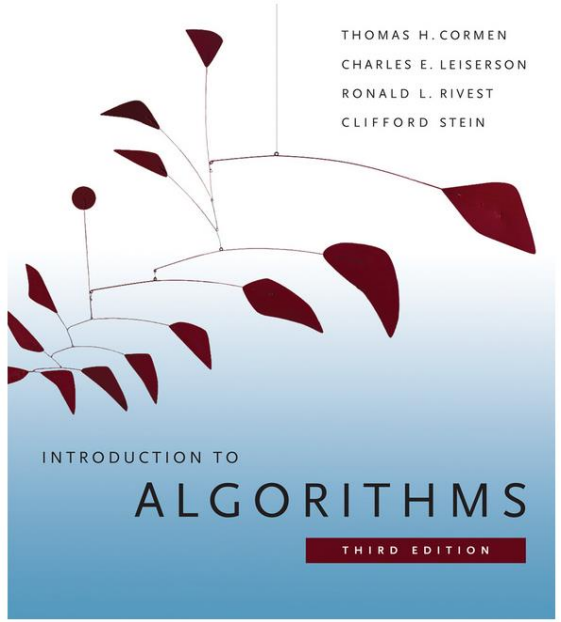
CEEDA

BREEAM®

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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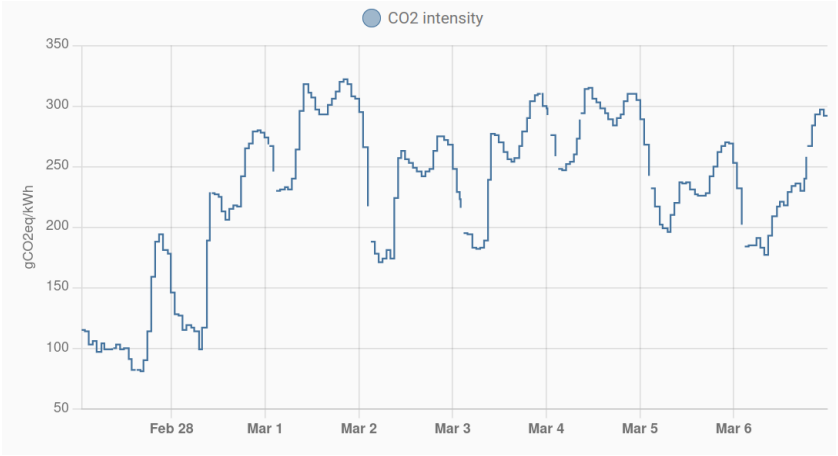
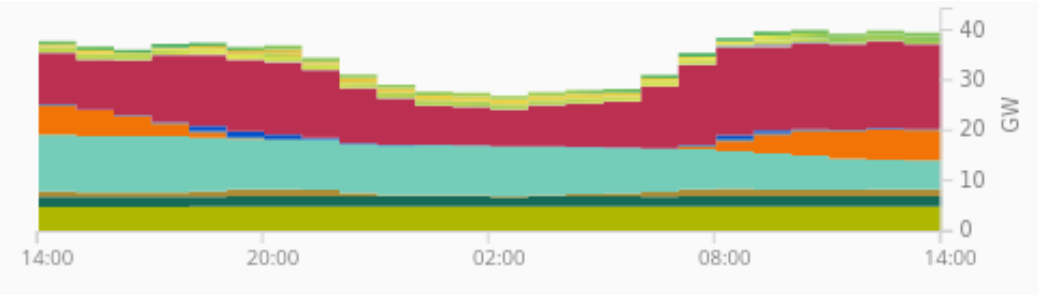
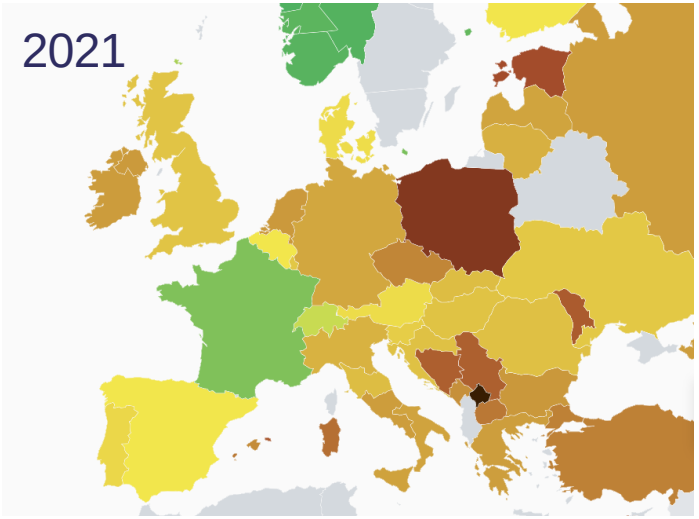
Time/Location shifting

- 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
- Cloud vs Local







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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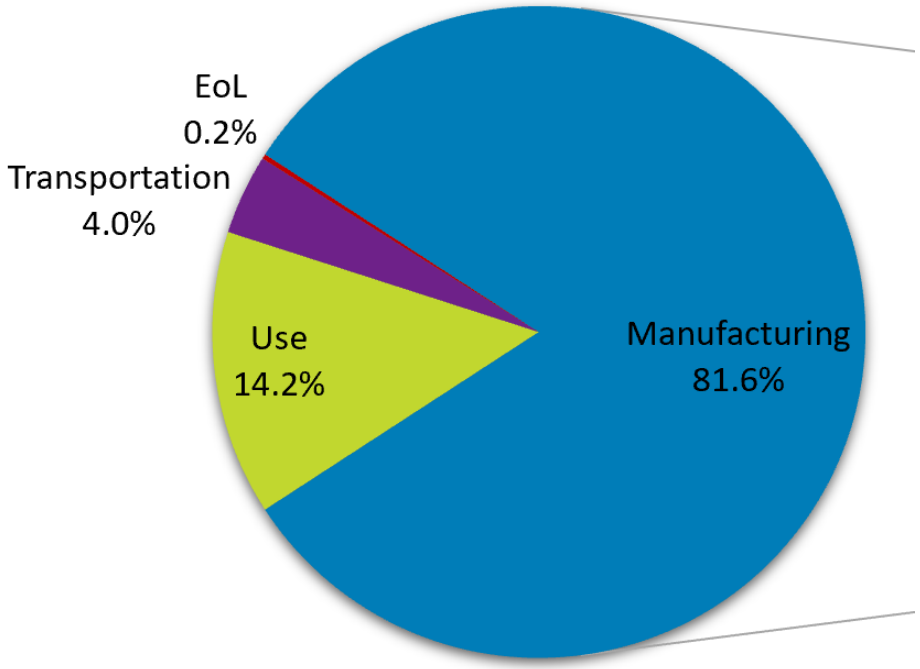
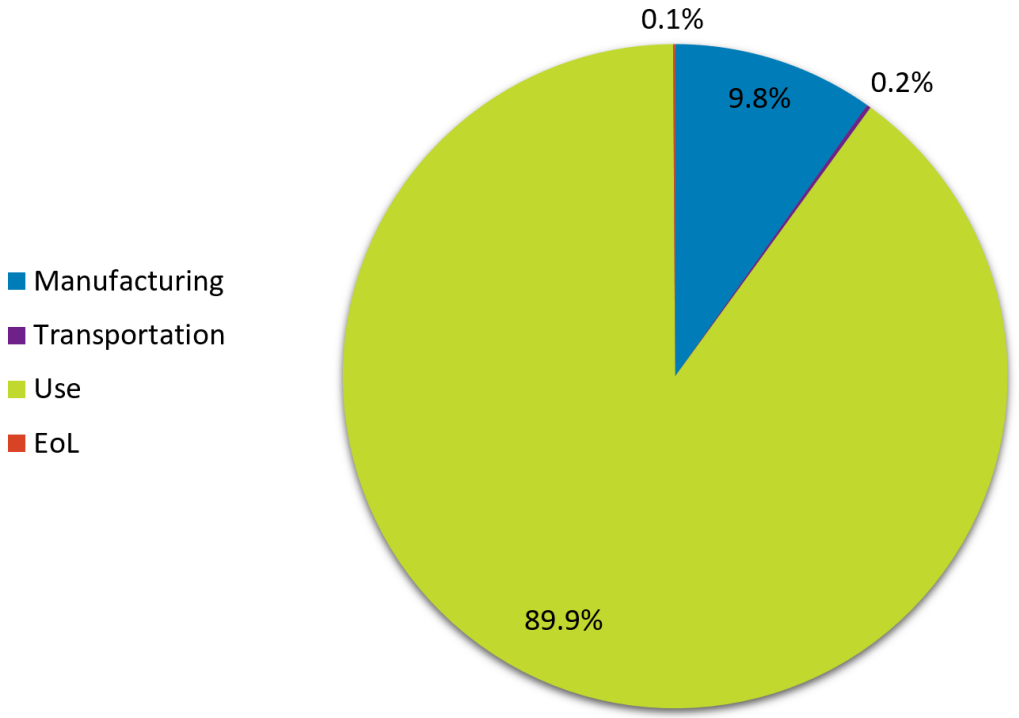
Product lifetime carbon footprints



Dell Precision 5550 Laptop



Dell PowerEdge R840 Server

* Base configs. A big SSD can make a difference

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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 - arxiv.org/abs/2207.10793

https://ukri.sharepoint.com/sites/thesource/SitePages/PC-Recycling-Scheme.aspx

More efficient science

SANS2D tube calibration script

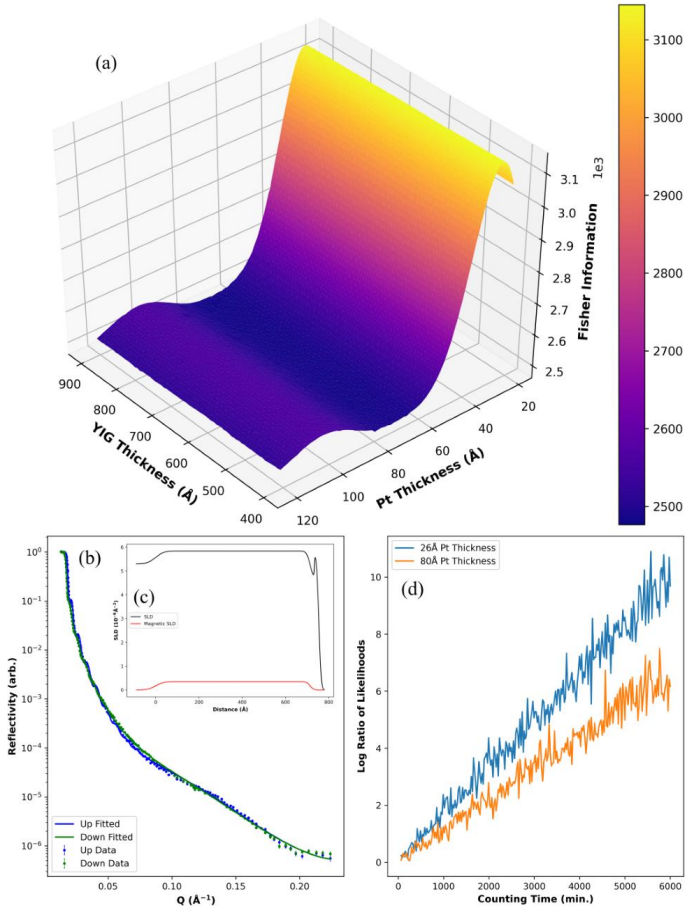
- 30 -> 3 mins per iteration (remove redundant IO)
- No longer need to leave running over night
- Save CPU, research time

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

Golden ratio scanning for tomography

- Currently number of images must be decided in advance
- With golden angle step can stop at any point
- Run until data quality is good enough



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

*David Fairbrother, Jos Cooper

More info

- UKRI Net Zero Digital Research Infrastructure Scoping Project
  - https://net-zero-dri.ceda.ac.uk/
- Sustainable computing workshop
  - 1-4pm, 5 and 6 December 2022
  - https://forms.office.com/r/QBwJjvna3W
- ICD sustainability WG
  - Sam.tygier@stfc.ac.uk
- ISIS sustainability hub
  - https://stfc365.sharepoint.com/sites/isis-sustainability

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Thank you

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