

UNIVERSITY OF

Department of Public Health and Primary Care

Foundation

NIHR Cambridge Biomedical Research Centre

2023 EIC Workshop







Software Sustainability Institute



ESTIMATING THE CARBON FOOTPRINT **OF COMPUTING IN SCIENCE**

Loïc Lannelongue, PhD

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WHAT ABOUT THE SCIENCE WE DO? BIOLOGY

GWAS of 1,000 traits in UK Biobank

(225h / 100 GB per trait)

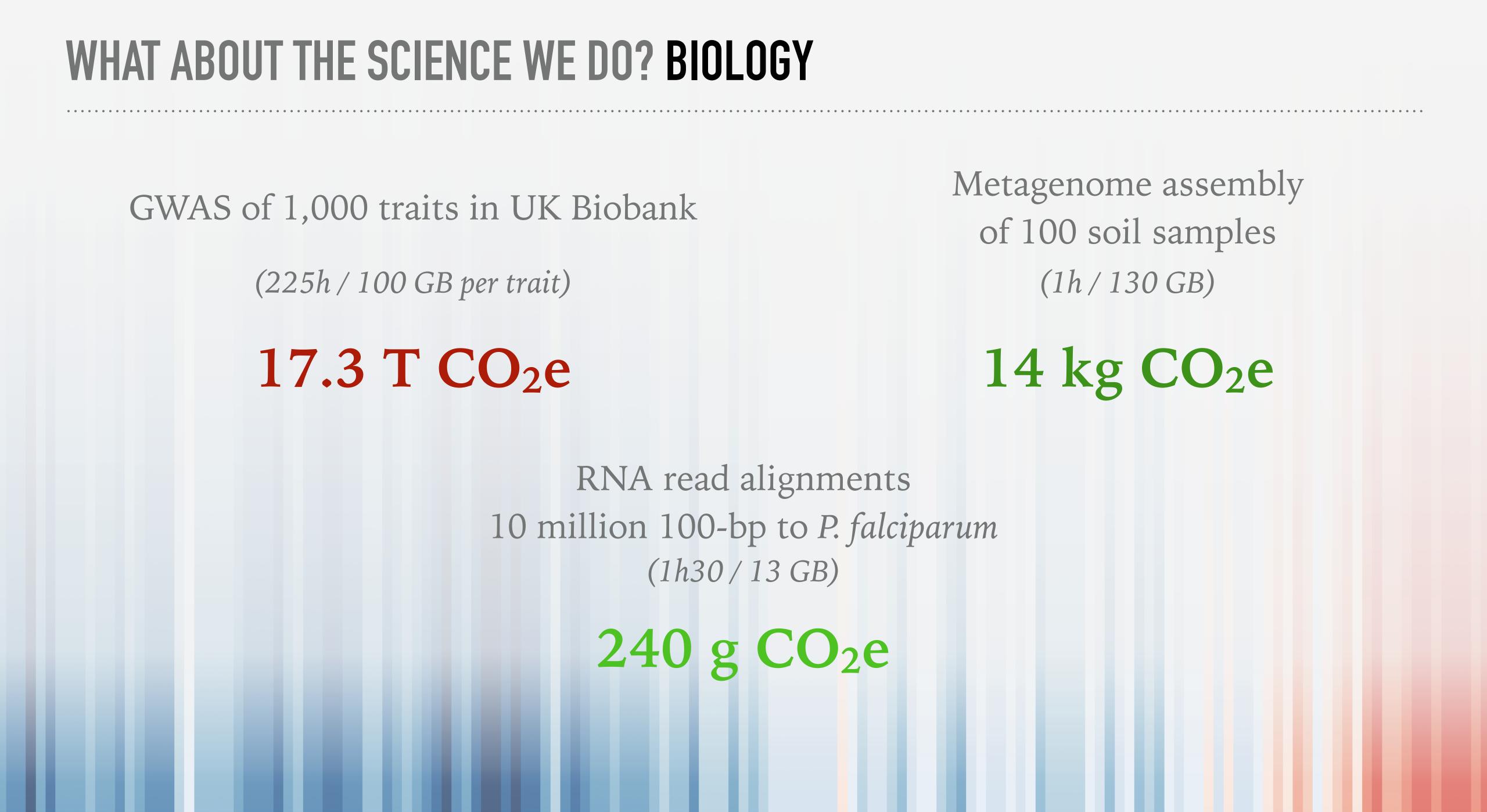
17.3 T CO₂e

RNA read alignments 10 million 100-bp to P. falciparum (1h30 / 13 GB)

Metagenome assembly of 100 soil samples (1h / 130 GB)

14 kg CO₂e

240 g CO₂e



WHAT ABOUT THE SCIENCE WE DO? AI + BIOLOGY

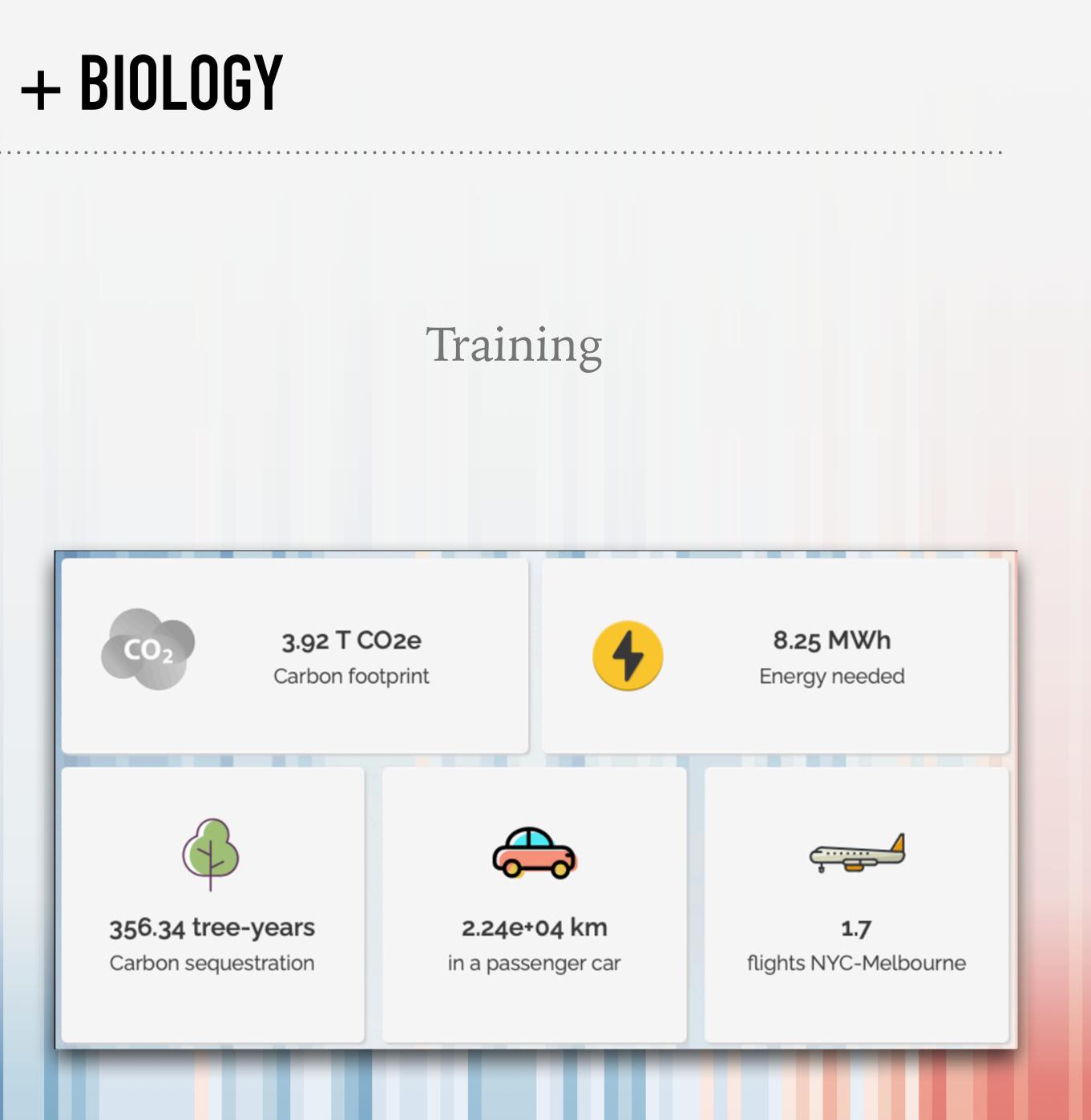
Article Open Access Published: 15 July 2021

Highly accurate protein structure prediction with AlphaFold

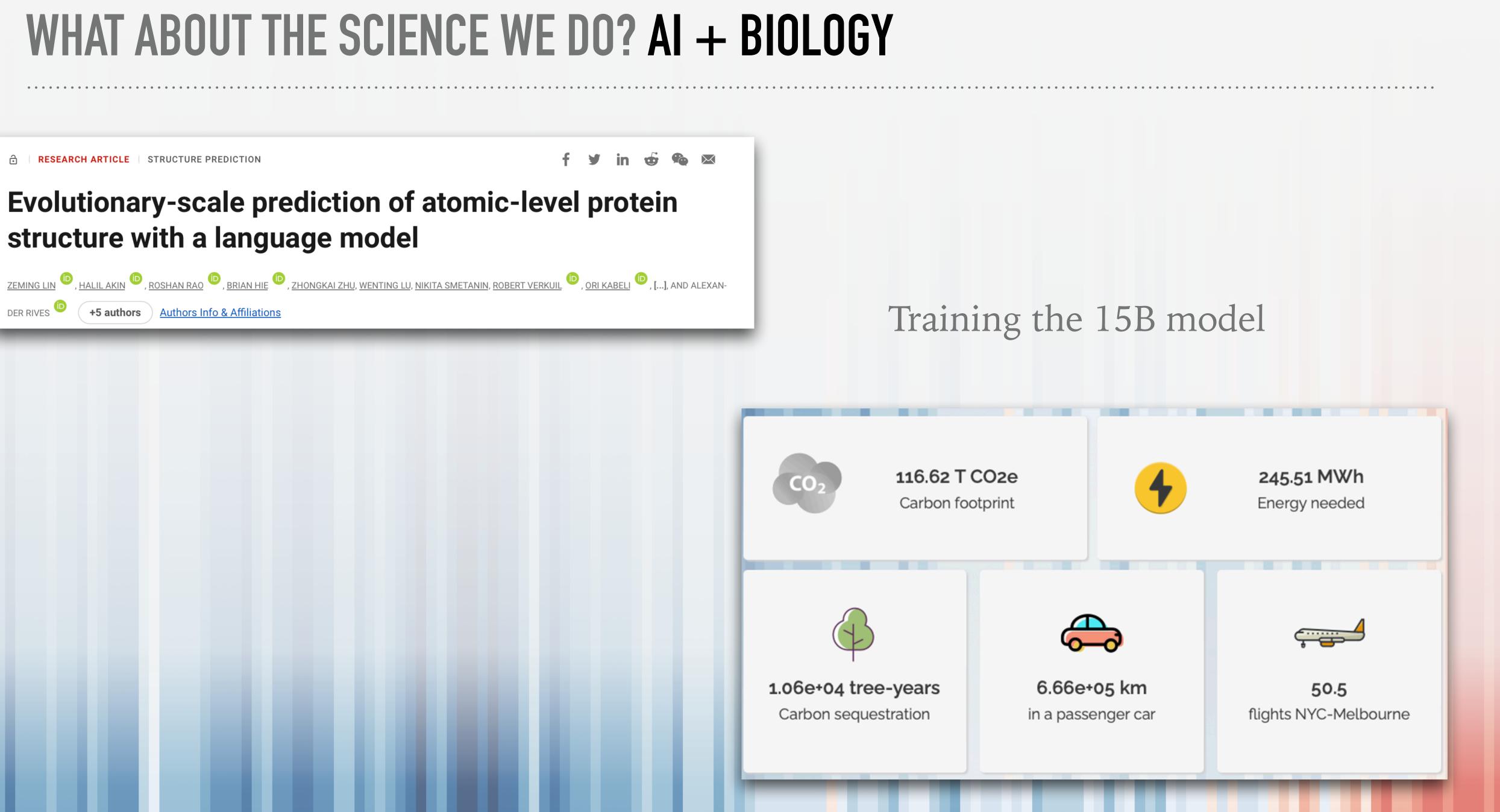
John Jumper 🗠, Richard Evans, Alexander Pritzel, Tim Green, Michael Figurnov, Olaf Ronneberger, Kathryn Tunyasuvunakool, Russ Bates, Augustin Žídek, Anna Potapenko, Alex Bridgland, Clemens Meyer, Simon A. A. Kohl, Andrew J. Ballard, Andrew Cowie, Bernardino Romera-Paredes, Stanislav Nikolov, Rishub Jain, Jonas Adler, Trevor Back, Stig Petersen, David Reiman, Ellen Clancy, Michal Zielinski, ... Demis Hassabis 🖂 + Show authors

<u>Nature</u> 596, 583–589 (2021) Cite this article

1.13m Accesses | 7287 Citations | 3435 Altmetric | Metrics



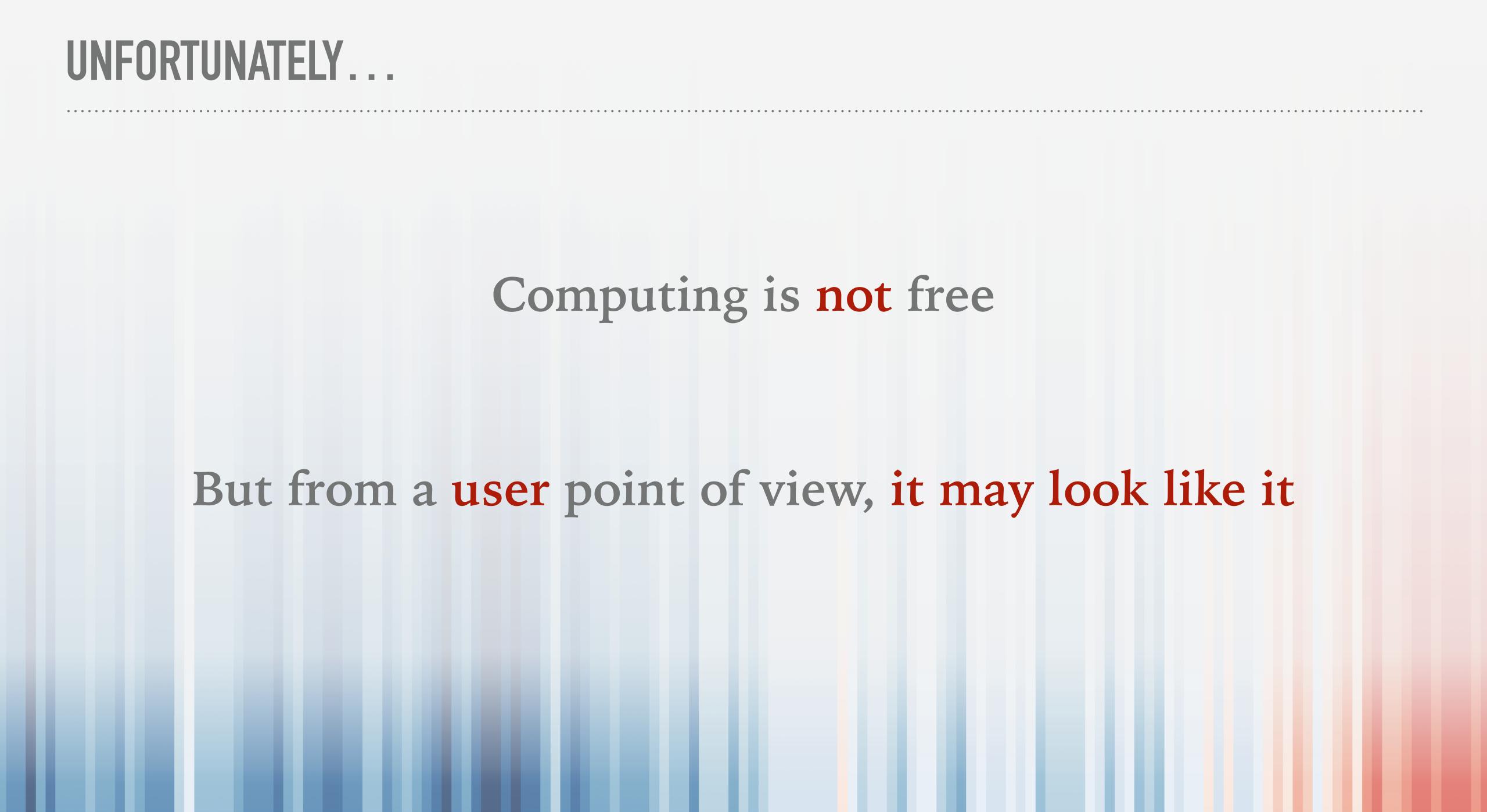
RESEARCH ARTICLE STRUCTURE PREDICTION



UNFORTUNATELY...

Computing is not free

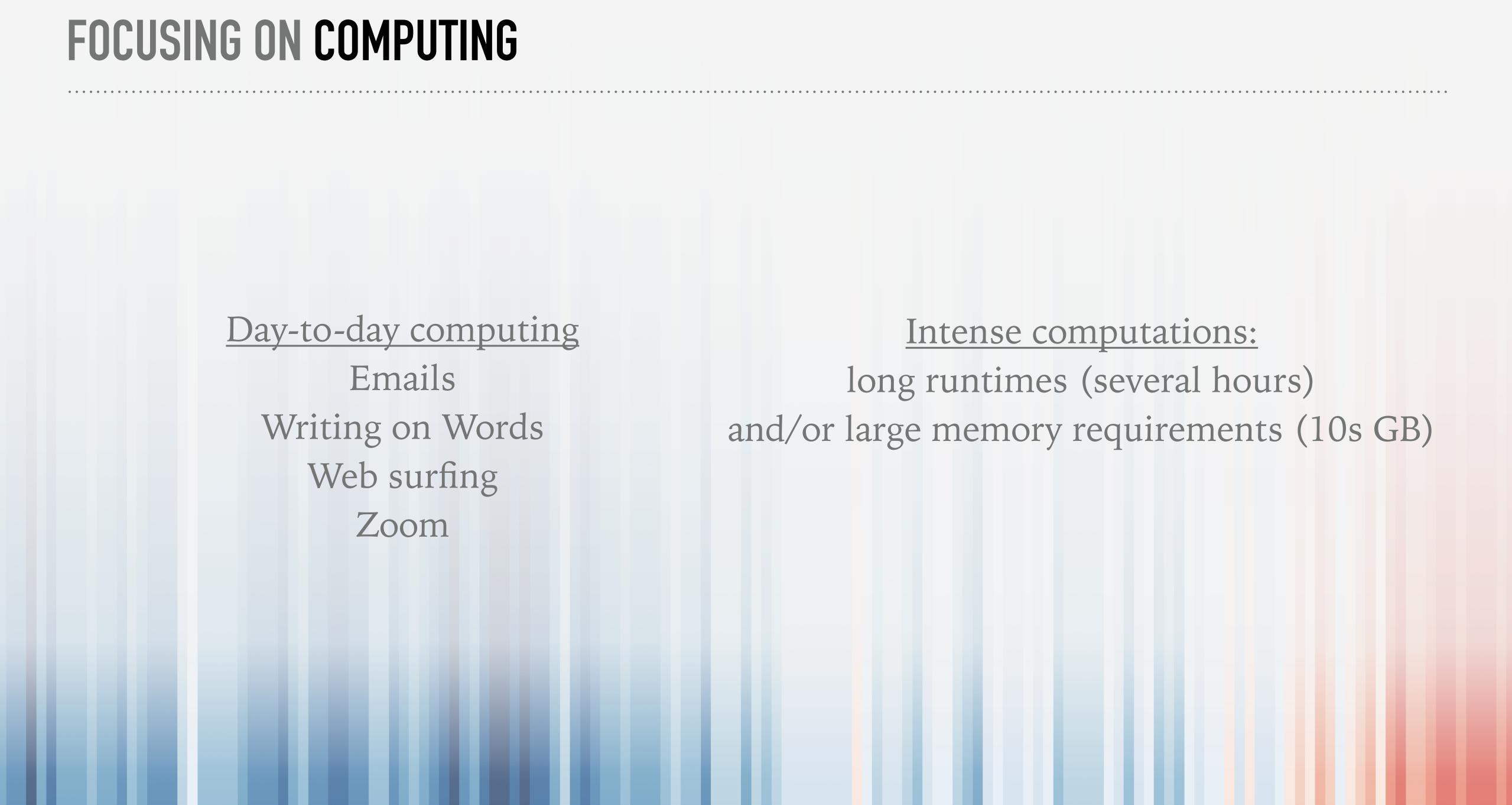
But from a user point of view, it may look like it



FOCUSING ON COMPUTING

Day-to-day computing Emails Writing on Words Web surfing Zoom

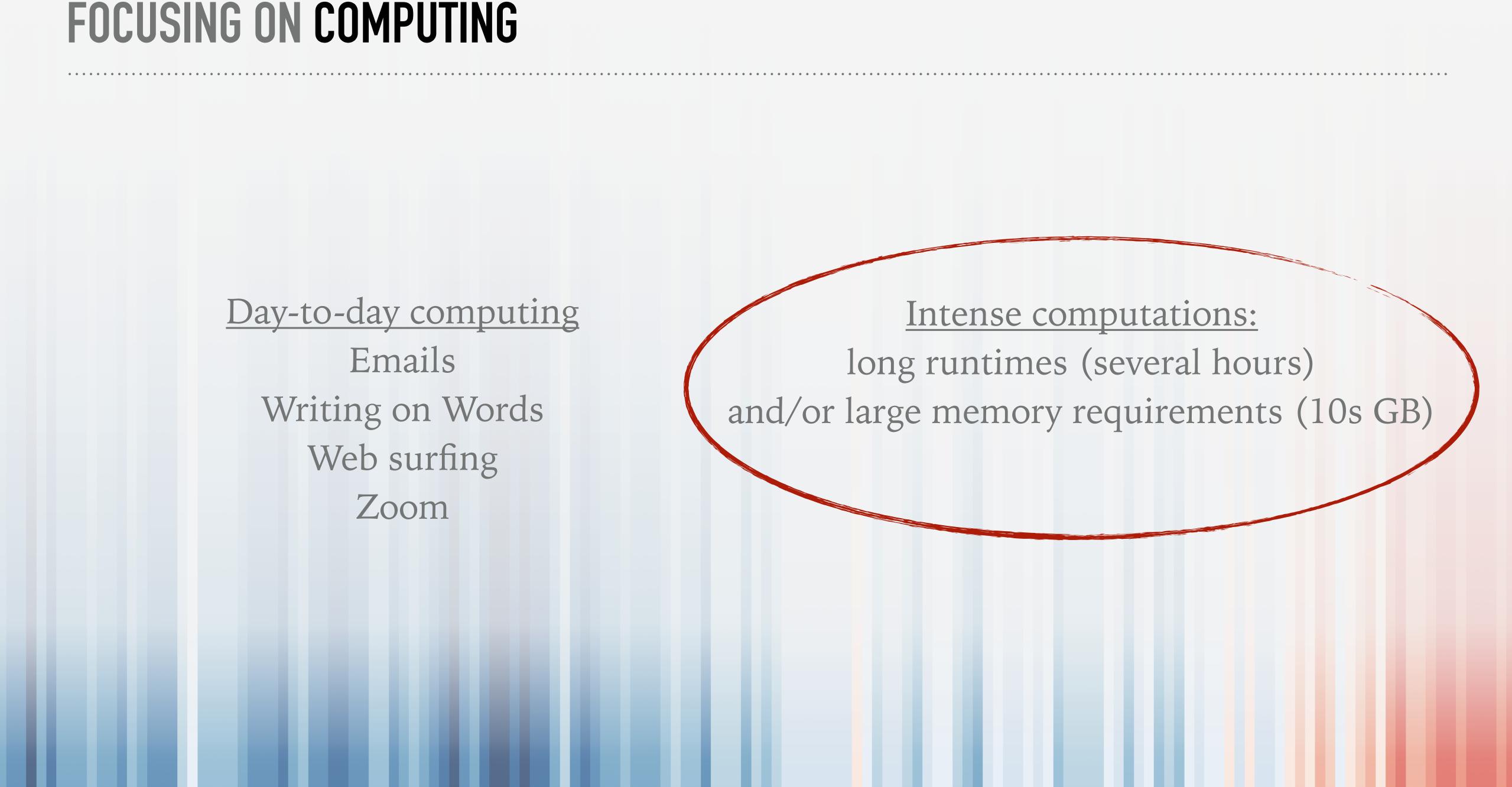
Intense computations: long runtimes (several hours) and/or large memory requirements (10s GB)



FOCUSING ON COMPUTING

Day-to-day computing Emails Writing on Words Web surfing Zoom

Intense computations: long runtimes (several hours) and/or large memory requirements (10s GB)



IT'S ALL THE SAME (ISH)





File Edit View Search Terminal Help
mark@linux-desktop:~\$ mkdir /tmp/tutorial
mark@linux-desktop:~\$ cd /tmp/tutorial
mark@linux-desktop:/tmp/tutorial\$ mkdir dir1 dir2 dir3
mark@linux-desktop:/tmp/tutorial\$ mkdir
mkdir: missing operand
Try 'mkdir --help' for more information.
mark@linux-desktop:/tmp/tutorial\$ cd /etc ~/Desktop
bash: cd: too many arguments
mark@linux-desktop:/tmp/tutorial\$ ls
dir1 dir2 dir3
mark@linux-desktop:/tmp/tutorial\$

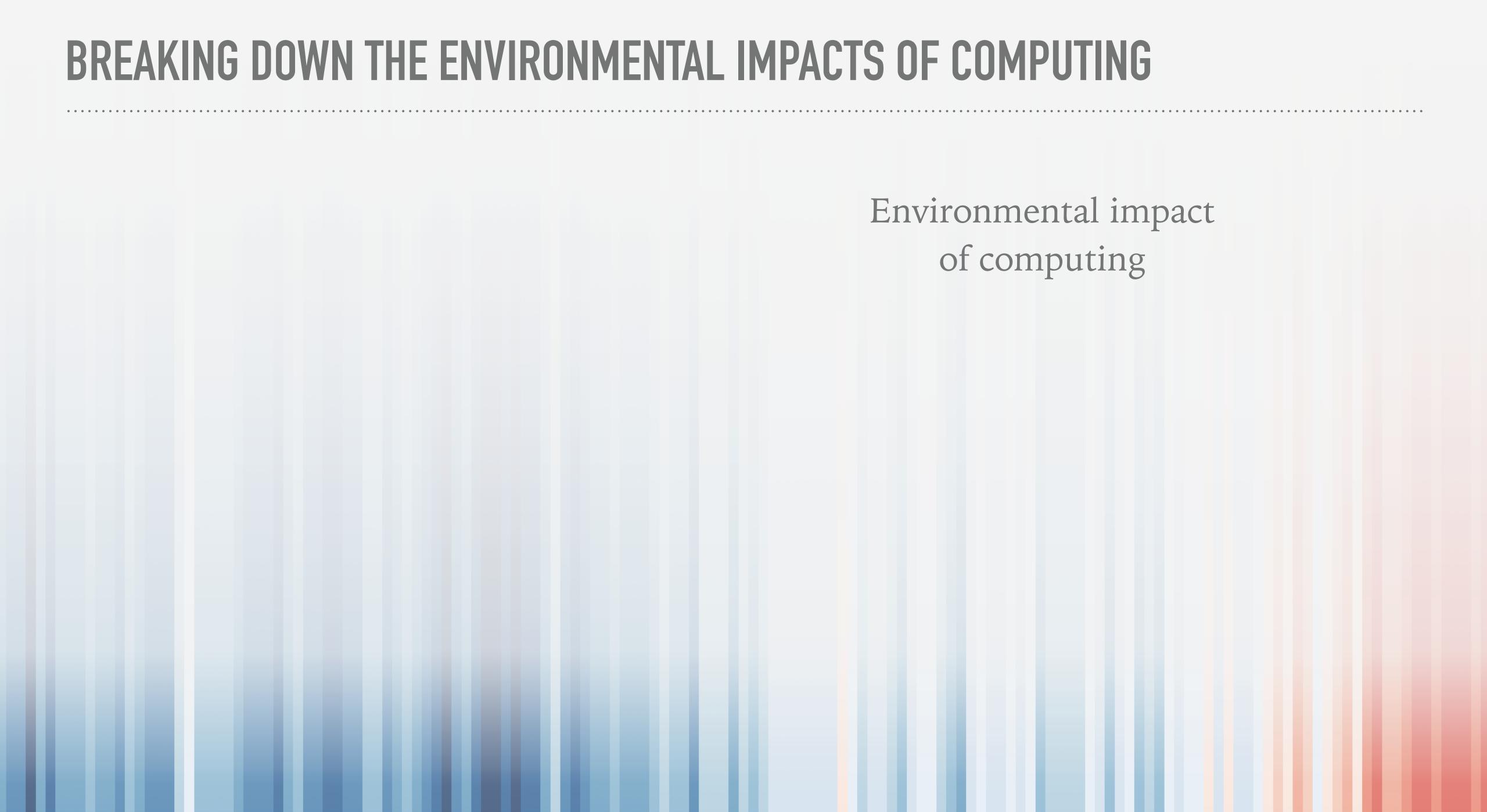


mark@linux-desktop: /tmp/tutorial





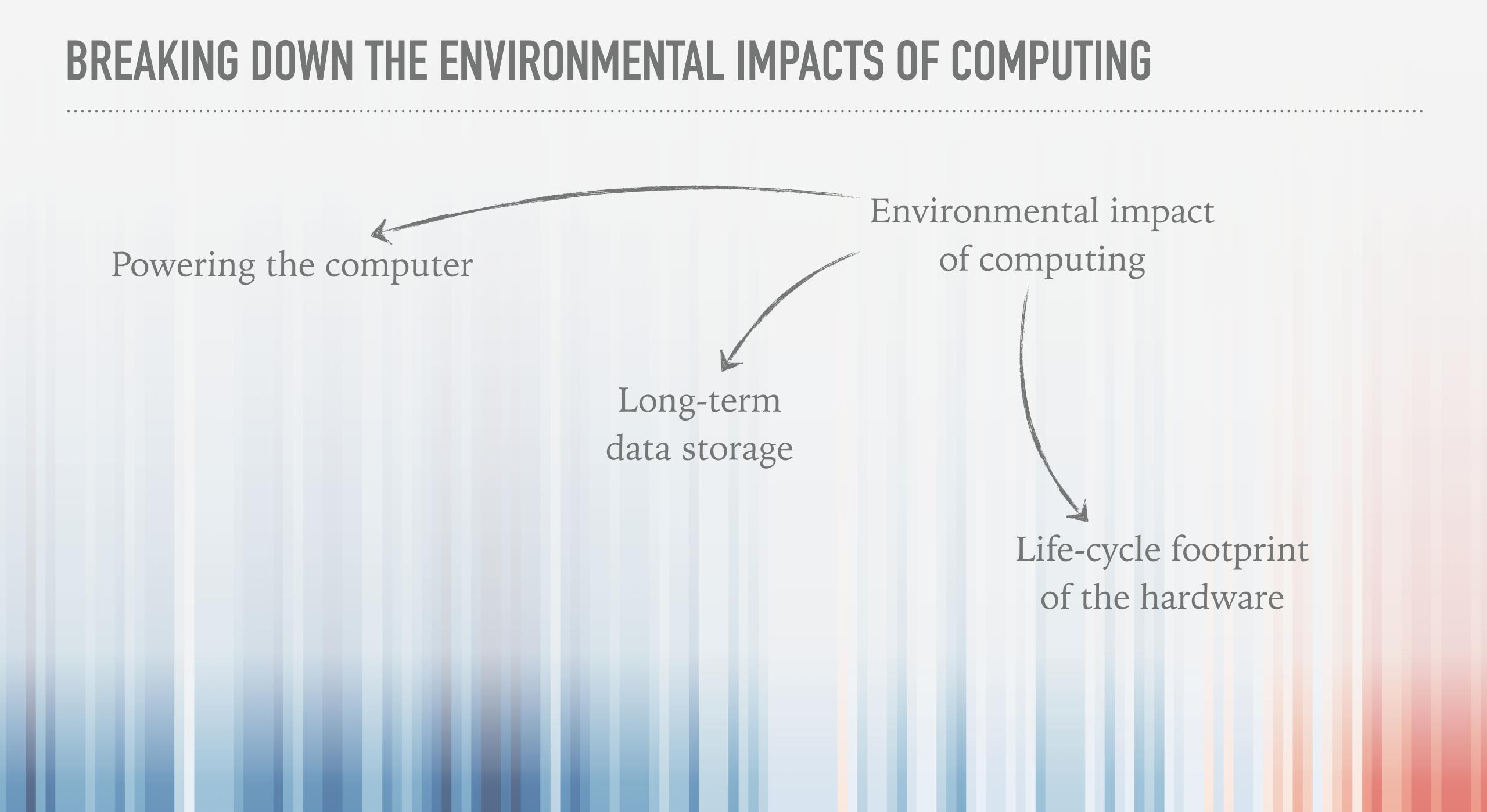
Environmental impact of computing



Powering the computer

Long-term data storage

Environmental impact of computing



Powering the computer

Long-term data storage

70-90% of the cradle-to-grave impact is from production (consumer devices)

Environmental impact of computing

Keep, Repair, Reuse



Powering the computer

Sustainability should be accounted for in renewing policies

Long-term data storage

15-40% for servers in data centres

70-90% of the cradle-to-grave impact is from production (consumer devices)

Environmental impact of computing





Children and digital dumpsites

E-waste exposure and child health

World Health Organization Long-term data storage

>82% of the 54m of tonnes of e-waste are handled by 12-56m informal waste workers worldwide

omputer

18m children work in industries involving waste processing

Environmental impact of computing

Keep, Repair, Reuse

Life-cycle footprint of the hardware

E-waste are predicted to raise by 40% by 2030



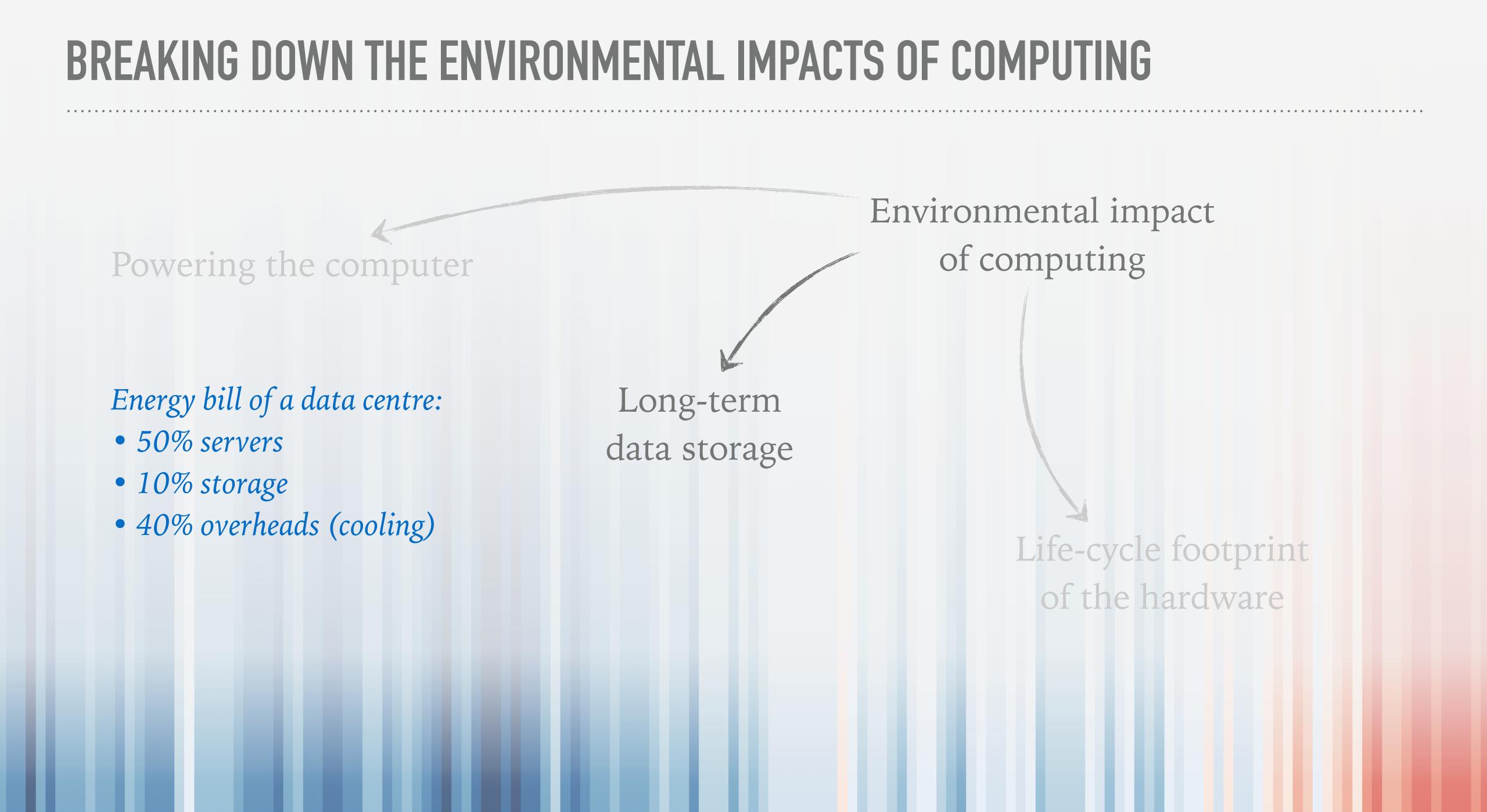
Powering the computer

Energy bill of a data centre:

- 50% servers
- 10% storage
- 40% overheads (cooling)

Long-term data storage

Environmental impact of computing



Powering the computer

Energy bill of a data centre:

- 50% servers
- 10% storage
- 40% overheads (cooling)

Long-term data storage



Environmental impact of computing

Don't store useless data

~10 kgCO₂e/TB/year

Life-cycle footprint of the hardware

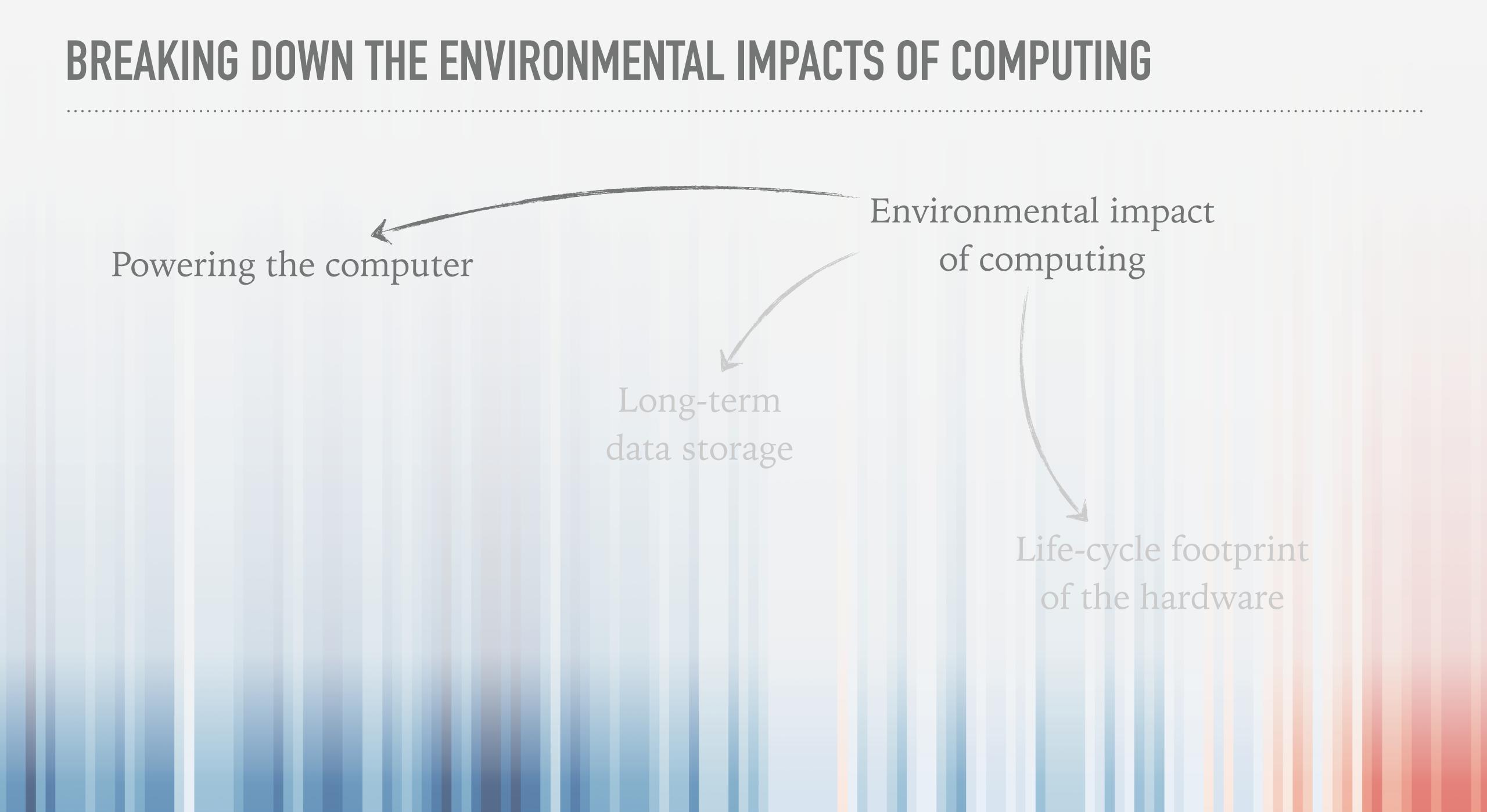
https://www.seagate.com/gb/en/global-citizenship/product-sustainability/



Powering the computer

Long-term data storage

Environmental impact of computing



THE CARBON FOOTPRINT OF COMPUTATION

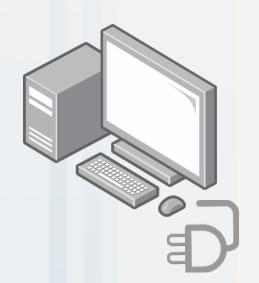
Carbon footprint = energy used x carbon intensity

 gCO_2e

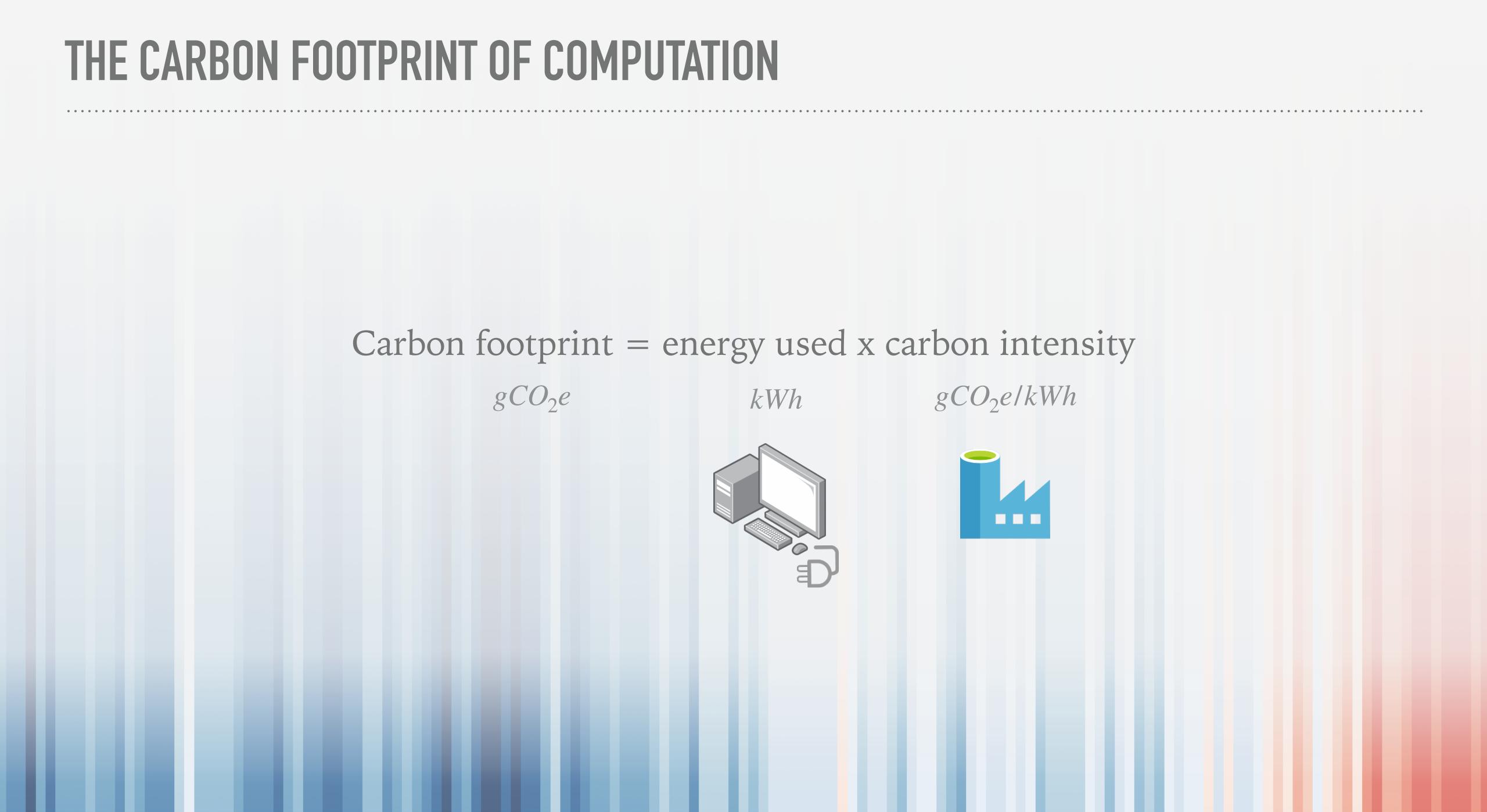


kWh

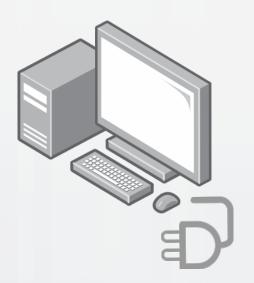
 gCO_2e/kWh







THE CARBON FOOTPRINT OF COMPUTATION: ENERGY NEEDED



Running time (h)

> Power draw of processing cores(W)

ADVANCED SCIENCE

Research Article 🛛 🔂 Open Access 🛛 😨 🚺

Green Algorithms: Quantifying the Carbon Footprint of Computation

Loïc Lannelongue 🔀, Jason Grealey, Michael Inouye 🔀

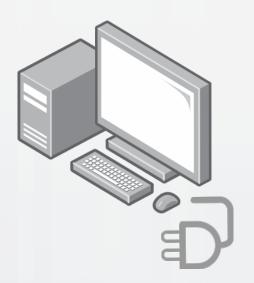
First published: 02 May 2021 | https://doi.org/10.1002/advs.202100707

 $E = t \times (P_c + P_m) \times PUE$ $f \qquad f \qquad (P_c + P_m) \times PUE$

Power draw from memory (W) Efficiency of the data centre



THE CARBON FOOTPRINT OF COMPUTATION: ENERGY NEEDED



Running time (h)

> Power draw of processing cores(W)

ADVANCED SCIENCE

Research Article 🛛 🔂 Open Access 🛛 😨 👔

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First published: 02 May 2021 | https://doi.org/10.1002/advs.202100707

PUE =

Total Facility Power

 $E = t \times (P_c + P_m) \times PUE$

Efficiency of the data centre

Power draw from memory (W)

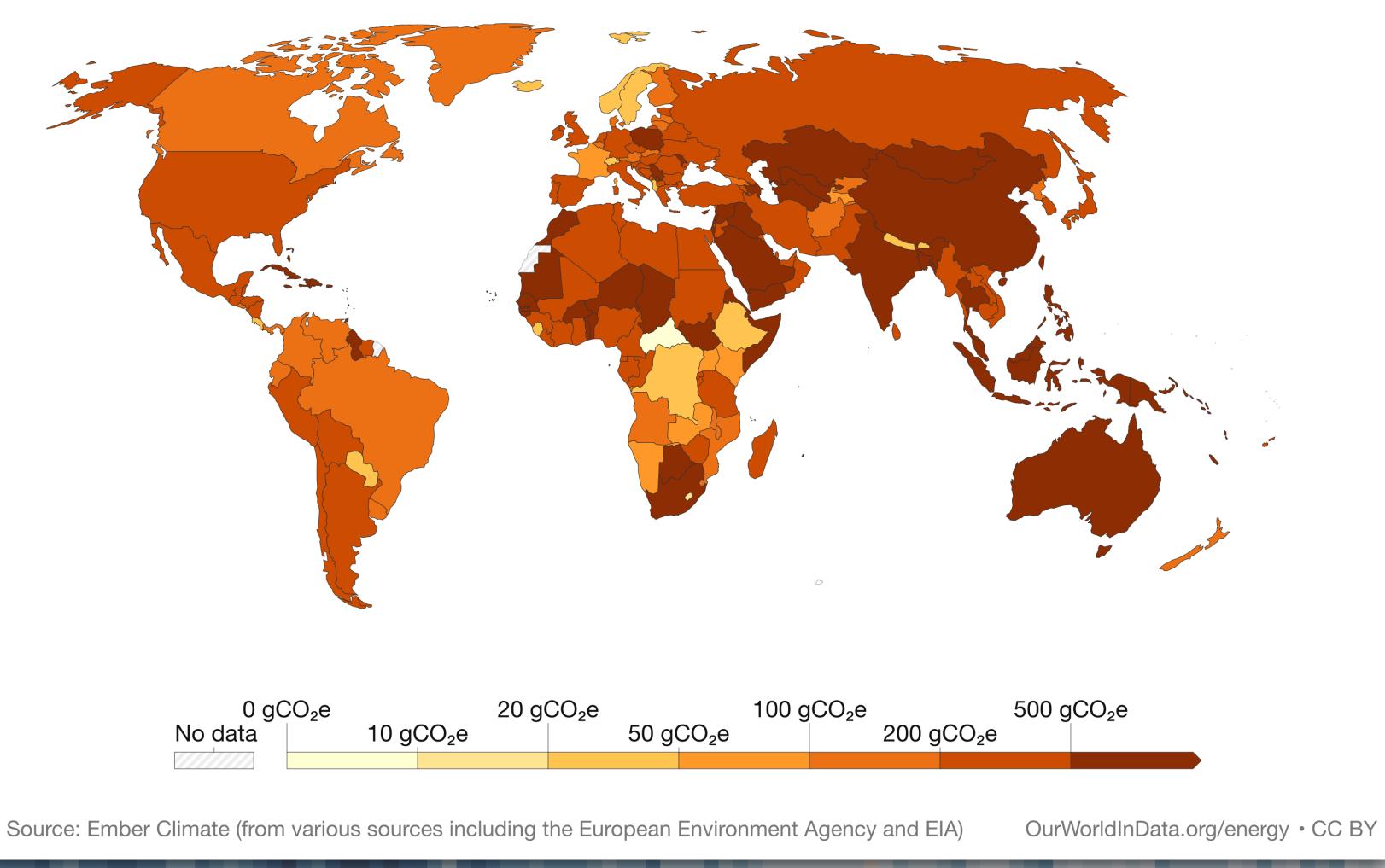
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Carbon intensity of electricity, 2022

Carbon intensity is measured in grams of carbon dioxide-equivalents¹ emitted per kilowatt-hour of electricity.

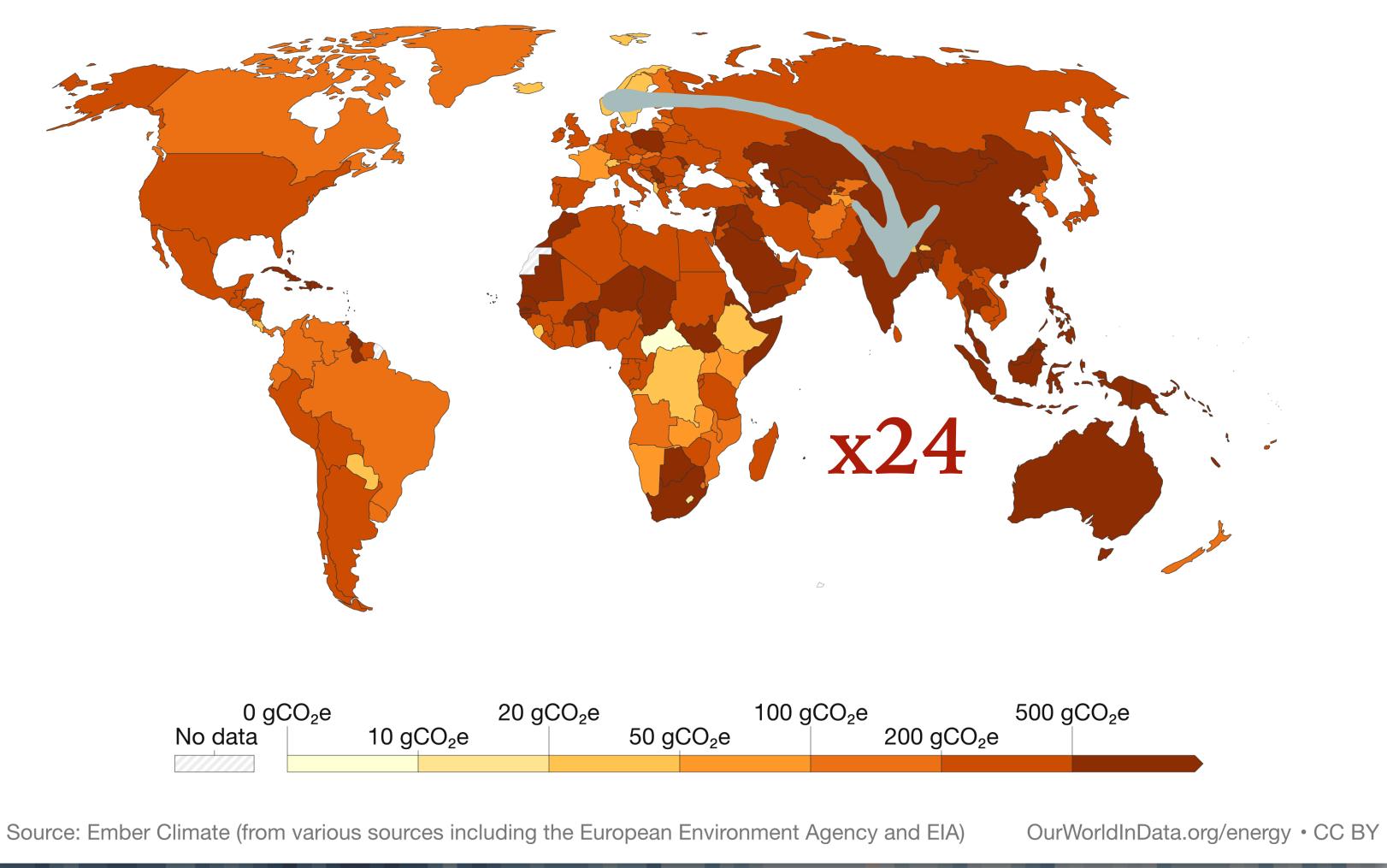


Our World in Data



Carbon intensity of electricity, 2022

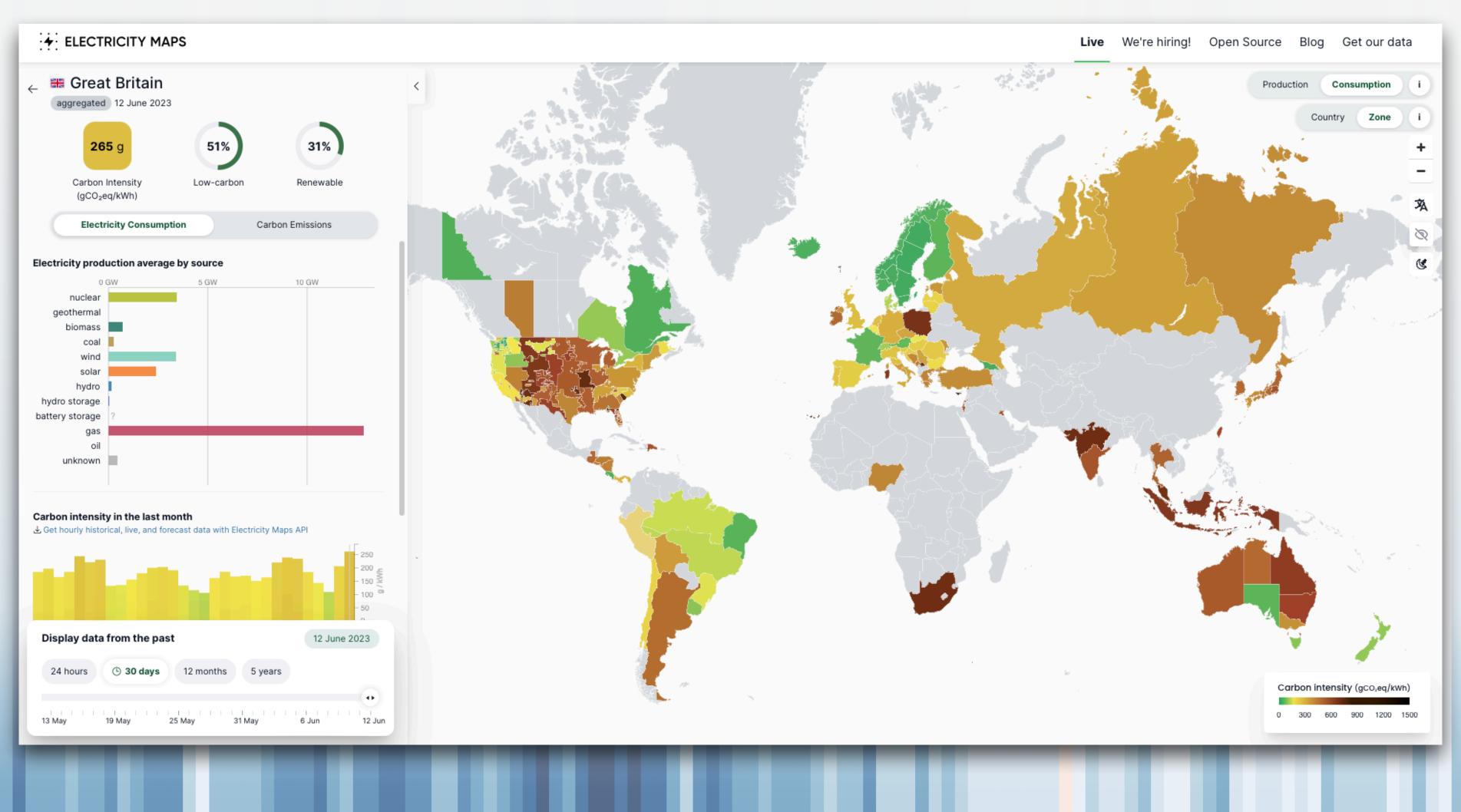
Carbon intensity is measured in grams of carbon dioxide-equivalents¹ emitted per kilowatt-hour of electricity.

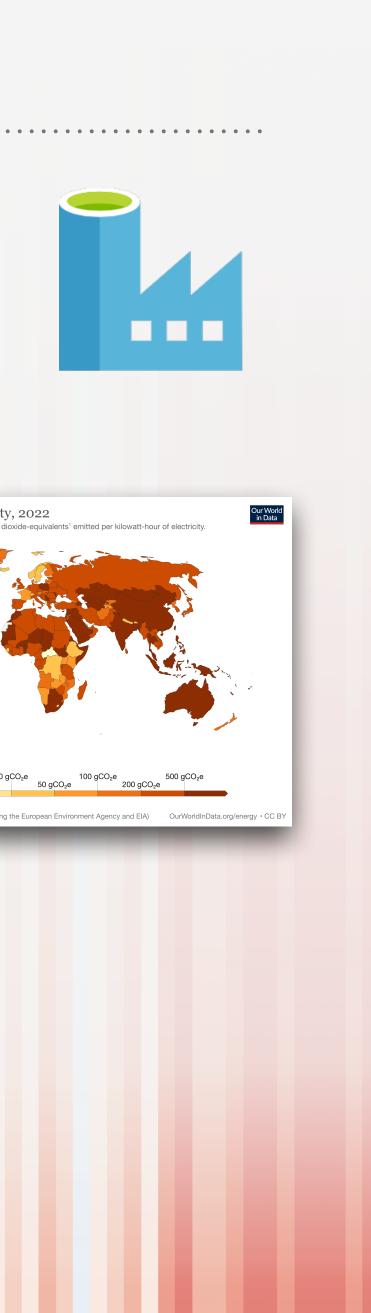




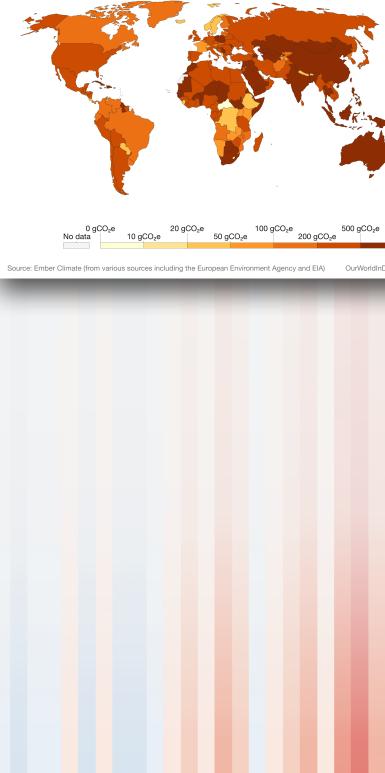


www.electricitymap.org

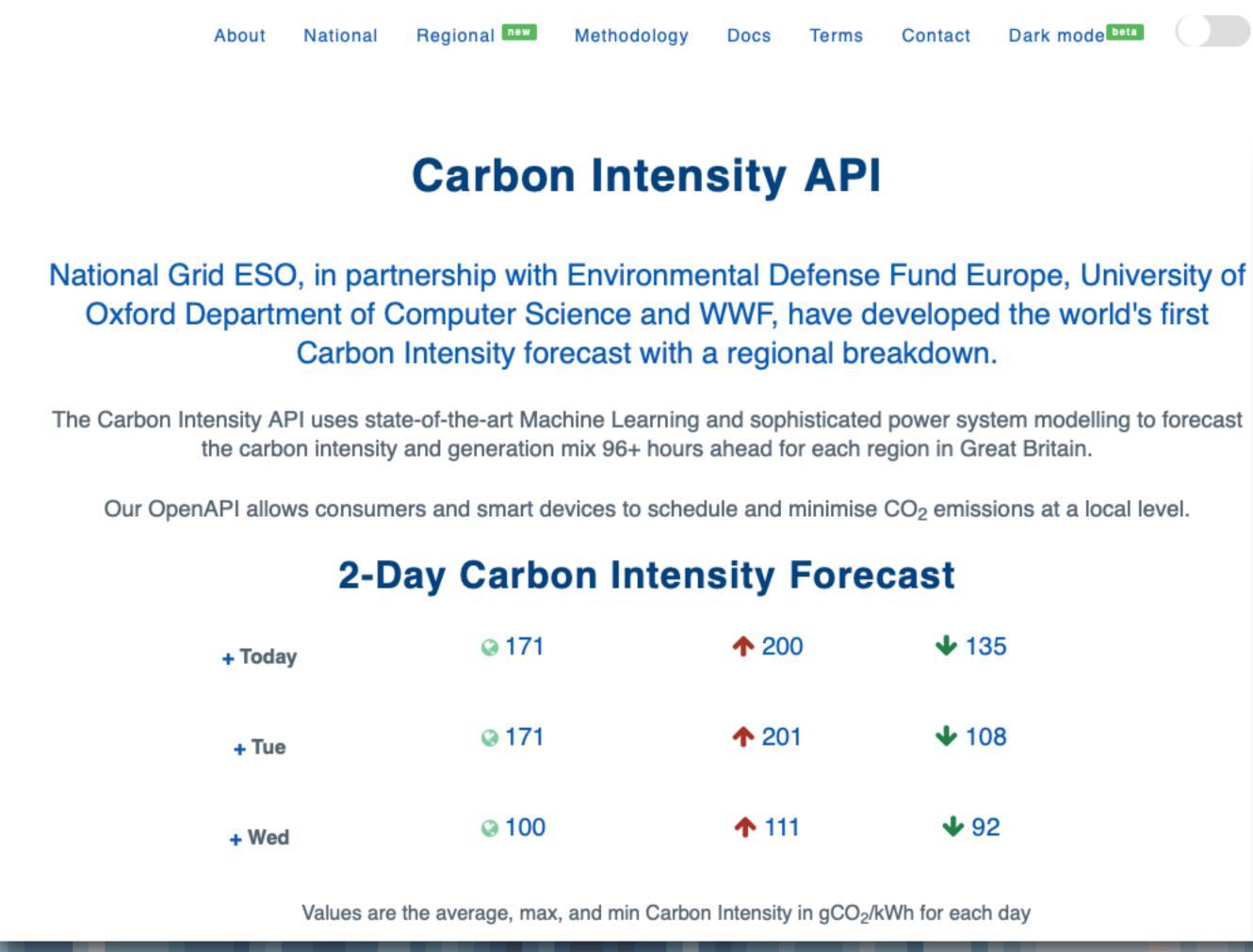




Carbon intensity of electricity, 2022



https://carbonintensity.org.uk/



Dark mode beta



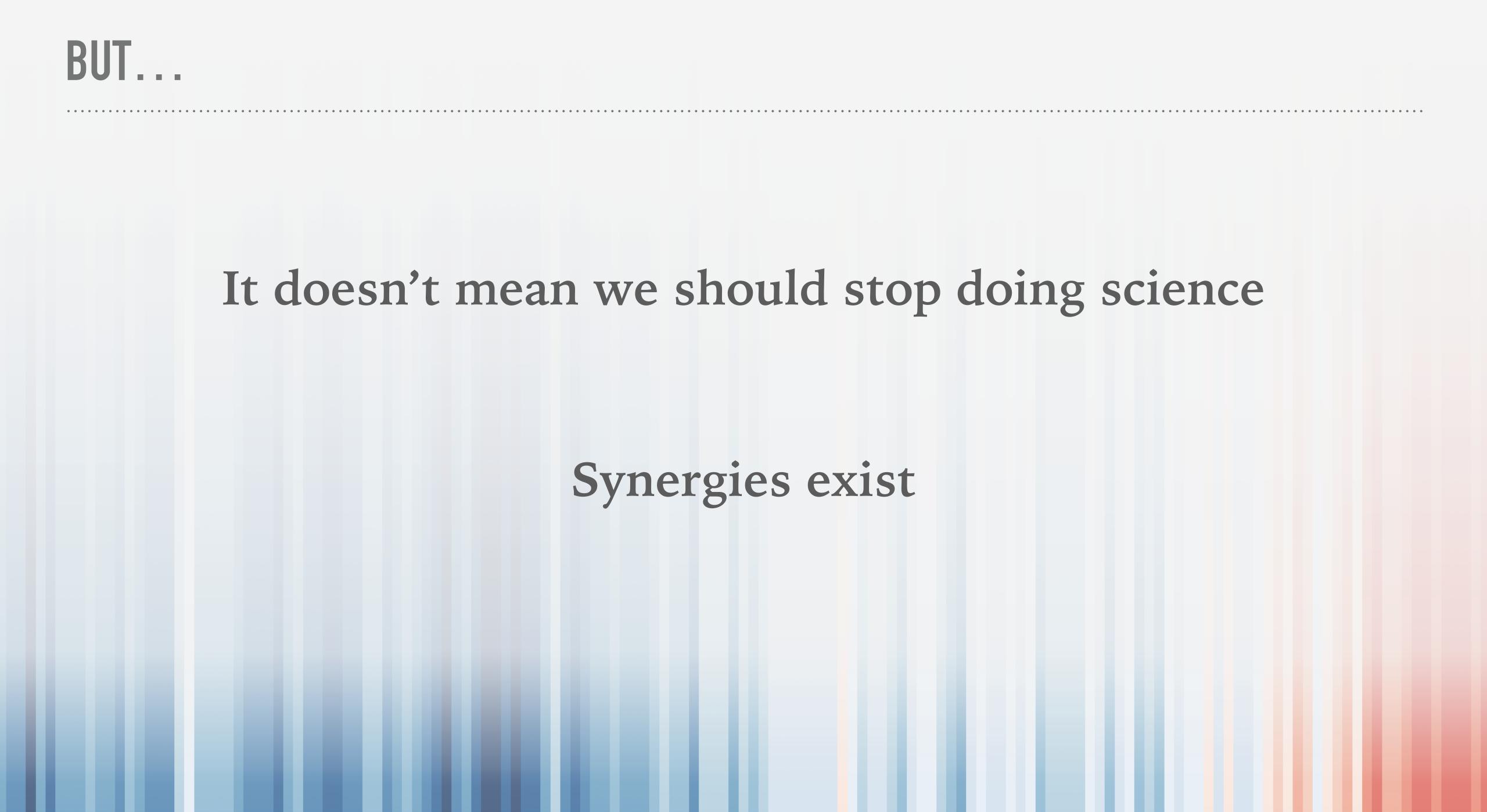
Key: Very High - High - Moderate - Low - Very Low





It doesn't mean we should stop doing science

Synergies exist



GREENER PRINCIPLES FOR SUSTAINABLE COMPUTATIONAL SCIENCE

nature computational science

Explore content \checkmark About the journal \checkmark Publish with us \checkmark

<u>nature</u> > <u>nature computational science</u> > <u>perspectives</u> > article

Perspective Published: 26 June 2023

GREENER principles for environmentally sustainable computational science

Loïc Lannelongue ⊡, Hans-Erik G. Aronson, Alex Bateman, Ewan Birney, Talia Caplan, Martin Juckes, Johanna McEntyre, Andrew D. Morris, Gerry Reilly & Michael Inouye

Nature Computational Science 3, 514–521 (2023) Cite this article

515 Accesses | 69 Altmetric | Metrics

Abstract

The carbon footprint of scientific computing is substantial, but environmentally sustainable computational science (ESCS) is a nascent field with many opportunities to thrive. To realize the immense green opportunities and continued, yet sustainable, growth of computer science, we must take a coordinated approach to our current challenges, including greater awareness and transparency, improved estimation and wider reporting of environmental impacts. Here, we present a snapshot of where ESCS stands today and introduce the GREENER set of principles, as well as guidance for best practices moving forward.

Collaboration with UK stakeholders



EMBL-EB



Department of Public Health and Primary Care



Health Data Research UK







GREENER PRINCIPLES FOR SUSTAINABLE COMPUTATIONAL SCIENCE

Governance

Responsibility

Estimation

Energy and embodied impacts

New collaborations

Education

Research

All actors in computational research have a key role to play and can lead the efforts towards sustainable computing.

Embracing both individual and institutional responsibility regarding the environmental impacts of research. This involves being transparent about these and initiating bold initiatives to reduce them.

Monitoring environmental impacts to identify inefficiencies and opportunities for improvement.

Minimising energy needs of computations and favouring low-carbon energy sources, while also considering the broader environmental impacts (e.g. water usage, mining of raw materials etc.).

Cooperating to leverage low-carbon infrastructures, facilitate equitable access to lowcarbon computation and limit wasted resources.

Training all stakeholders to be aware of the sustainability challenges of HPC and to be equipped with the skills to tackle them.

Dedicate research efforts to green computing to improve our understanding of power usage, support sustainable software engineering and enable energy-efficient research. Cultural change: make environmental sustainability a core element of research



FROM THEORY TO PRACTICE

Estimating and reporting the carbon footprint of algorithms

ESTIMATING CARBON FOOTPRINTS IN PRACTICE

nature reviews methods primers

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nature > nature reviews methods primers > comment > article

Comment Published: 16 February 2023

Carbon footprint estimation for computational research

Loïc Lannelongue 🖂 & Michael Inouye

<u>Nature Reviews Methods Primers</u> **3**, Article number: 9 (2023) Cite this article

187 Accesses **23** Altmetric <u>Metrics</u>

Data analysis relies heavily on computation, and algorithms have grown more demanding in terms of hardware and energy. Monitoring their environmental impacts is and will continue to be an essential part of sustainable research. Here, we provide guidance on how to do so accurately and with limited overheads.

Publish with us \checkmark



EXISTING TOOLS

carbontracker

pypi v1.1.6 💮 python 3.8 | 3.9 | 3.10 💭 build passing License MIT

About

carbontracker is a tool for tracking and predicting the energy consumption and carbon footprint of training deep learning models as described in <u>Anthony et al. (2020)</u>.



What it is



A lightweight and easy-to-use Python pip package



Emissions tracked based on your power consumption & locationdependent carbon intensity



experiment-impact-tracker

The experiment-impact-tracker is meant to be a simple drop-in method to track energy usage, carbon emissions, and compute utilization of your system. Currently, on Linux systems with Intel chips (that support the RAPL or powergadget interfaces) and NVIDIA GPUs, we record: power draw from CPU and GPU, hardware information, python package versions, estimated carbon emissions information, etc. In California we even support realtime carbon emission information by querying caiso.com!

Once all this information is logged, you can generate an online appendix which shows off this information like seen here:

https://breakend.github.io/RL-Energy-Leaderboard/reinforcement_learning_energy_leaderboard/pongnoframeskipv4_experiments/ppo2_stable_baselines,_default_settings/0.html

Cloud Carbon Footprint

Cloud Carbon Emissions Measurement and Analysis Tool

Understand how your cloud usage impacts our environment and what you can do about it

CUMULATOR — a tool to quantify and report the carbon footprint of machine learning computations and communication in academia and healthcare

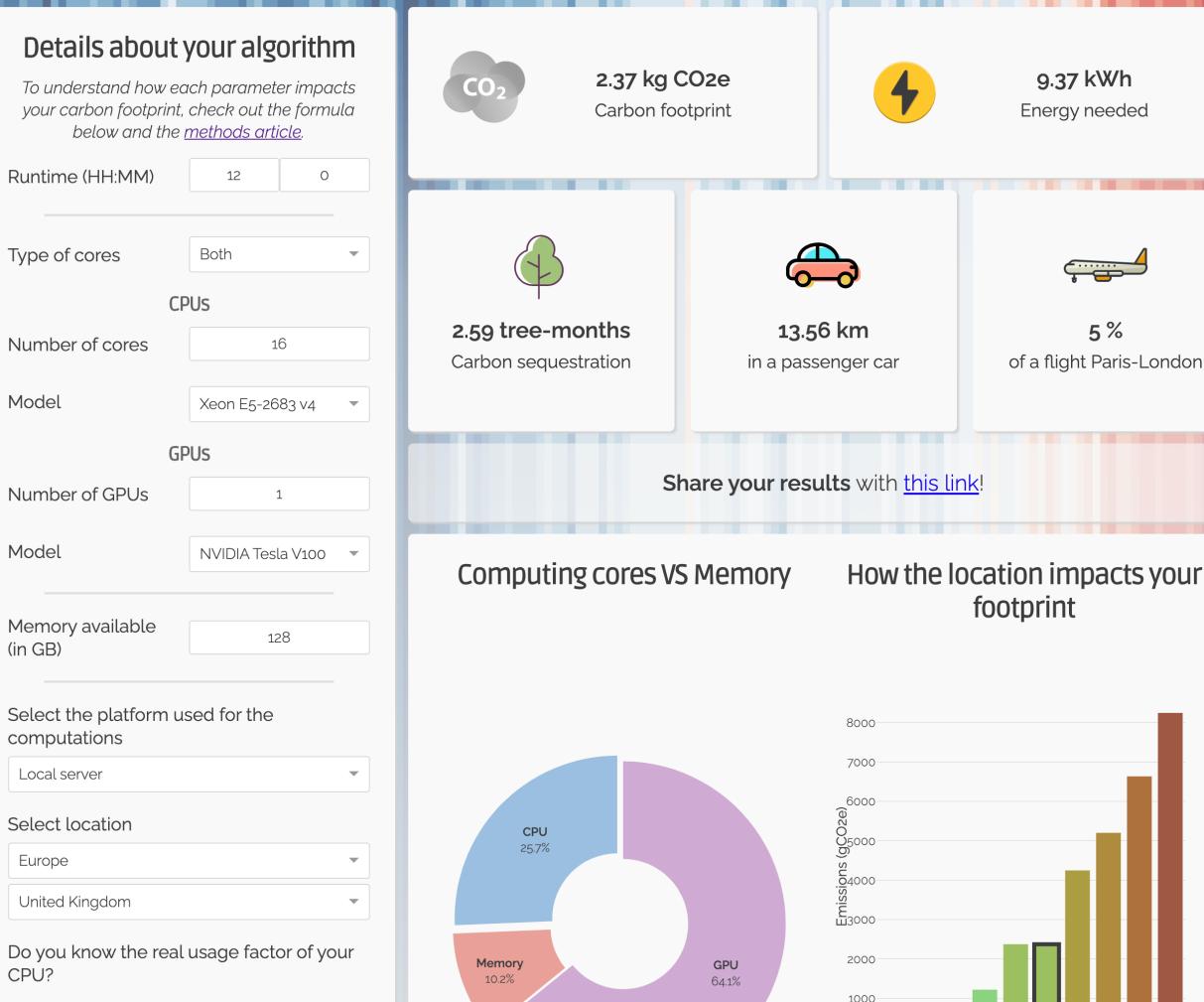
💄 Trébaol, Tristan

2020



Green Algorithms

How green are your computations?



○ Yes 🔘 No

Do you know the real usage factor of your GPU?

○ Yes 🔘 No

Do you know the Power Usage Efficiency (PUE) of your local data centre?

ADVANCED SCIENCE

Open Access

Research Article 🔂 Open Access 😨 💽

Green Algorithms: Quantifying the Carbon Footprint of Computation

Loïc Lannelongue 🔀, Jason Grealey, Michael Inouye 🔀

First published: 02 May 2021 | https://doi.org/10.1002/advs.202100707

THE GREEN ALGORITHMS CALCULATOR

calculator.green-algorithms.org



Jason Grealey

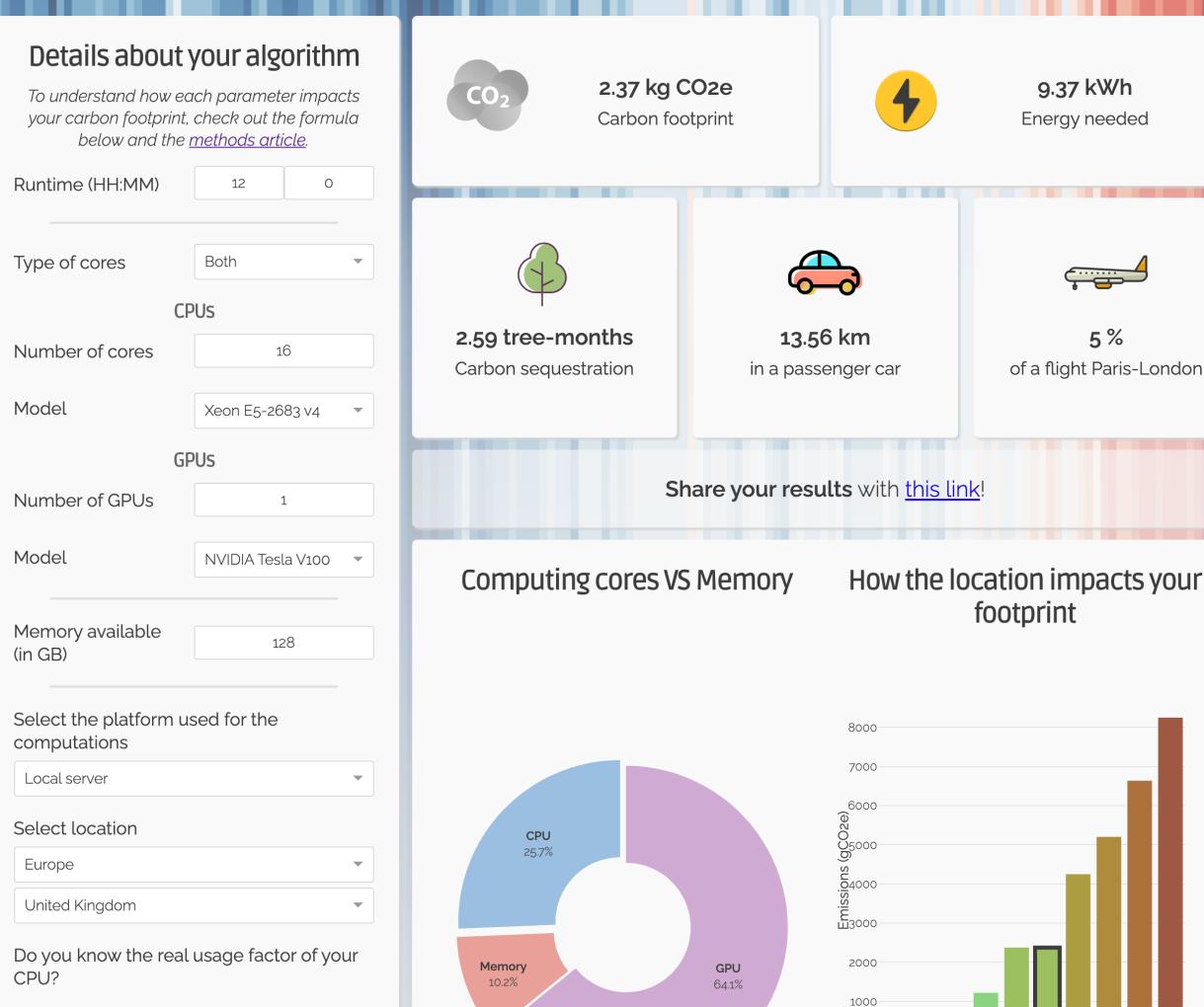


Michael Inouye



Green Algorithms

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Do you know the Power Usage Efficiency (PUE) of your local data centre?

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ਿੰ master → ਿੰ 6 branches	◊ 3 tags	Go to file
Liannelongue Updated data	i for v2.0	a73d2de on 21 May 🕥 177 commits
assets	Updated text	2 months ago
🖿 data	Updated data for v2.0	2 months ago
images	Update file	12 months ago
old	clean folder	16 months ago
🗋 .gitignore	initial commit	17 months ago

https://github.com/GreenAlgorithms/green-algorithms-tool

THE GREEN ALGORITHMS CALCULATOR

calculator.green-algorithms.org



Jason Grealey



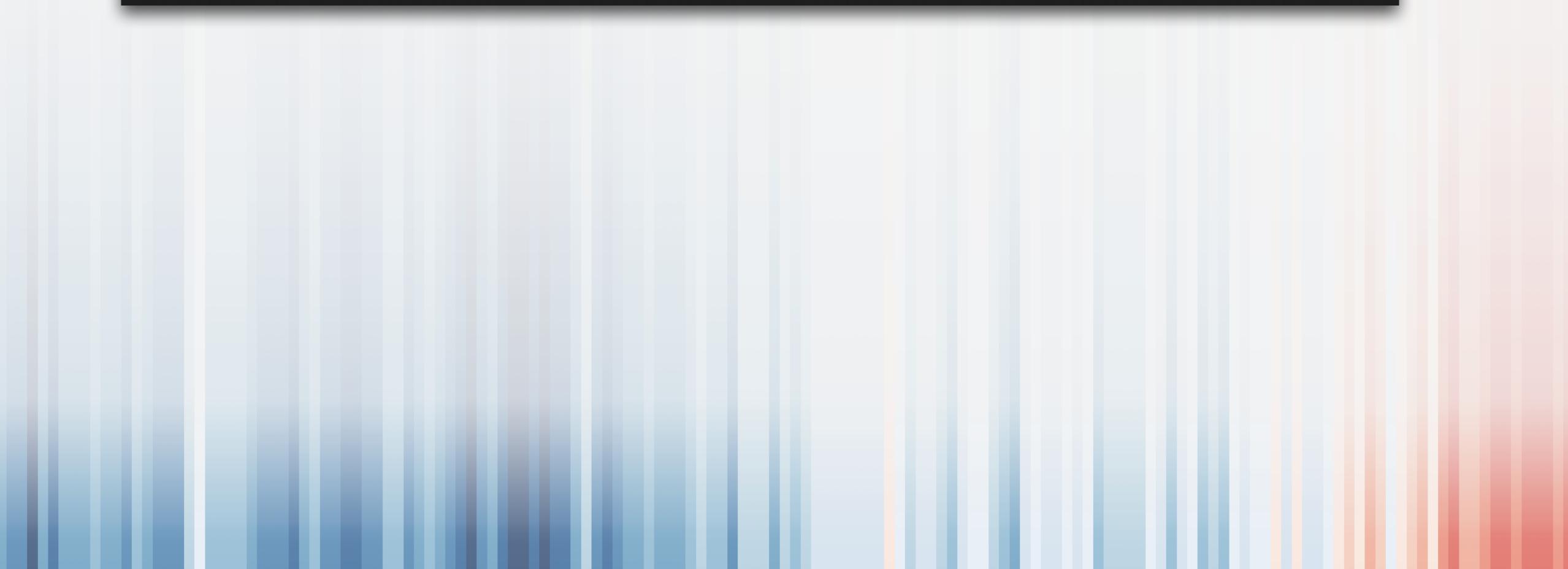
Michael Inouye





GREEN ALGORITHMS 4 HPC

GreenAlgorithms4HPC]\$ myCarbonFootprint.sh --STARTDAY 2020-01-01 --ENDDAY 2020-06-01





GREEN ALGORITHMS 4 HPC

GreenAlgorithms4HPC]\$ myCarbonFootprint.sh --STARTDAY 2020-01-01 --ENDDAY 2020-06-01

#######################################	
# #	
# Your carbon footprint on CSD3 #	
# (2021-01-01 / 2021-12-31) #	
# #	
#######################################	
222 kgCO2e	
This is equivalent to:	
– 20 tree-years	
- driving 1,268 km	
- 4.44 flights between Paris and London	
26.0% of your jobs failed, which represents a waste of	of 51 k
On average, you request at least 1.0 times the memory	
Energy used: 960.17 kWh	
– CPUs: 88.91 kWh (9%)	
- GPUs: 713.81 kWh (74%)	
- Memory: 32.22 kWh (3%)	
- Data centre overheads: 125.24 kWh (13%)	
Carbon intensity used for the calculations: 231.12 gCO2e	/kWh
Summary of your usage:	
 First/last job recorded on that period: 2021-01-0 	1/2021
 Number of jobs: 1,490 (1,102 completed) 	1,2021
- Core hours used/charged: 1,302.1 (CPU), 2,852.0 (GPU)
- Total usage time (i.e. when cores were performing	
- CPU: 430 days 03:58:39	Compe
- GPU: 118 days 20:01:30	
– Total wallclock time: 132 days 10:49:44	
 Total memory requested: 40,981 GB 	
Limitations to keep in mind:	
- The workload manager doesn't alway log the exact	
- For now, we assume that GPU jobs only use 1 GPU a	
(both of these may lead to slightly overestimated o	
 Conversely, the wasted energy due to memory overa 	illocat
Any bugs, questions, suggestions? Email LL582@medschl.ca	m.ac.u
Calculated using the Green Algorithms framework: www.gre	
Please cite https://onlinelibrary.wiley.com/doi/10.1002/	

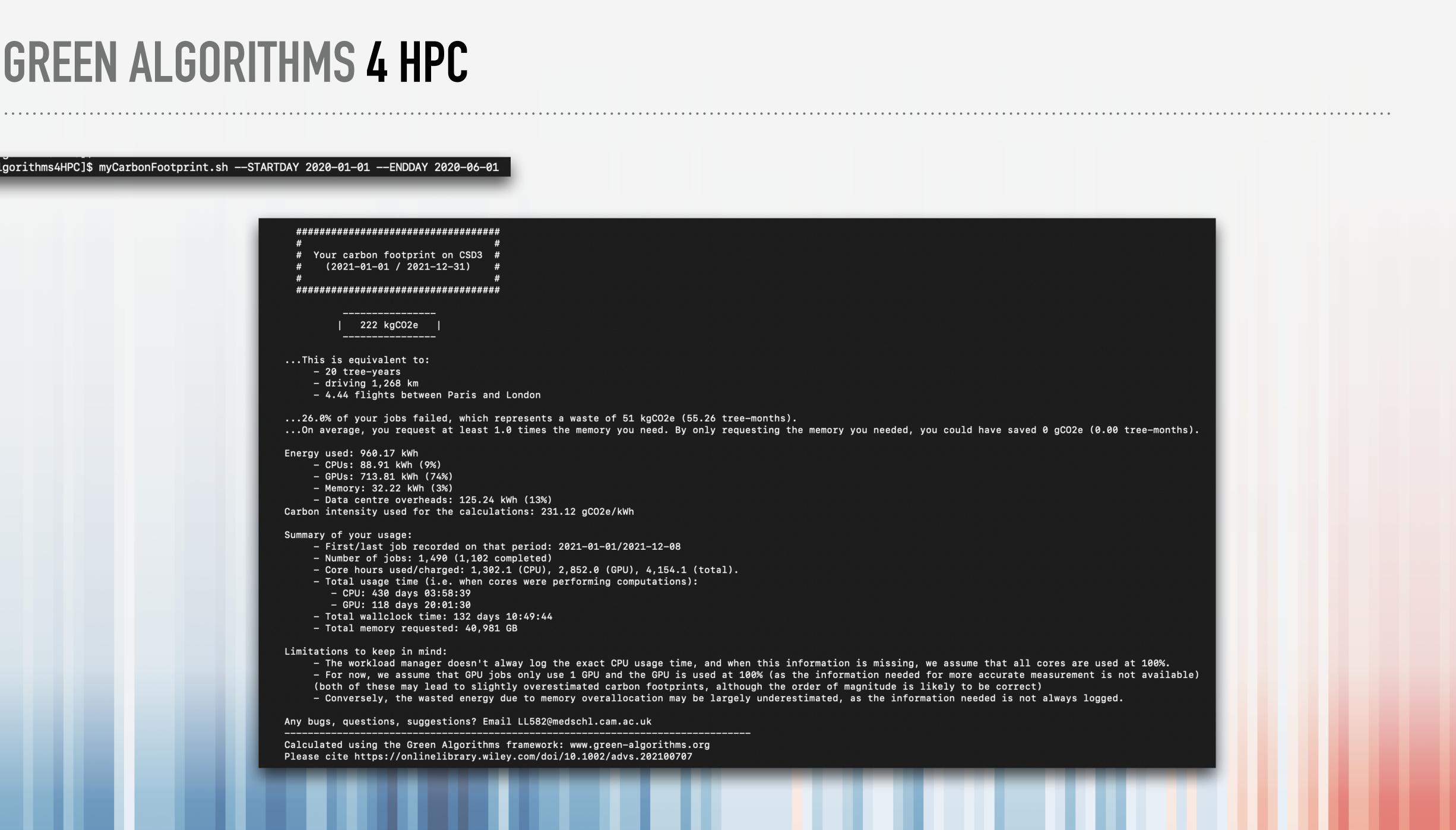
kgCO2e (55.26 tree-months). need. By only requesting the memory you needed, you could have saved 0 gCO2e (0.00 tree-months).

-12-08

4,154.1 (total). itations):

sage time, and when this information is missing, we assume that all cores are used at 100%. e GPU is used at 100% (as the information needed for more accurate measurement is not available) footprints, although the order of magnitude is likely to be correct) tion may be largely underestimated, as the information needed is not always logged.

gorithms.org 202100707



GREEN ALGORITHMS 4 HPC

GreenAlgorithms4HPC]\$ myCarbonFootprint.sh --STARTDAY 2020-01-01 --ENDDAY 2020-06-01

Green/	Algorithms / GreenAlgorithms4HPC	Public	থি Pin
<> Code	⊙ Issues 1 ដి Pull requests ⊙ Acti	ions 🖽 Projects 🖽 Wiki 😲 Security 🗠 Insights 🕸 S	ettings
	ੋਟ main → ਟੈਟ 1 branch ा 🛇 4 tags	Go to file Add file -	<> Code -
	Llannelongue minor edit	a5e35a6 17 days ago	🕑 52 commits
	example_files	Fix example files	17 days ago
	🗋 .gitignore	Calculate core hours charged (mainly for sanity checks)	6 months ago
	GreenAlgorithms_global.py	minor edit	17 days ago
	GreenAlgorithms_workloadManage	AdduseCustomLogs option (formerlyuseLoggedOutput) and op	17 days ago



... This is equivalent to: - 20 tree-years - driving 1,268 km - 4.44 flights between Paris and London

Energy used: 960.17 kWh - CPUs: 88.91 kWh (9%)

https://github.com/GreenAlgorithms/GreenAlgorithms4HPC

Your carbon footprint on CSD3 # (2021-01-01 / 2021-12-31)

222 kgC02e

...26.0% of your jobs failed, which represents a waste of 51 kgCO2e (55.26 tree-months). ... On average, you request at least 1.0 times the memory you need. By only requesting the memory you

- GPUs: 713.81 kWh (74%)
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Summary of your usage:

- First/last job recorded on that period: 2021-01-01/2021-12-08
- Number of jobs: 1,490 (1,102 completed)
- Core hours used/charged: 1,302.1 (CPU), 2,852.0 (GPU), 4,154.1 (total).
- Total usage time (i.e. when cores were performing computations):
- CPU: 430 days 03:58:39
- GPU: 118 days 20:01:30
- Total wallclock time: 132 days 10:49:44
- Total memory requested: 40,981 GB



IT ENABLES DEEP DIVES INTO PARTICULAR FIELDS



MOLECULAR BIOLOGY AND EVOLUTION MOLECULAR BIOLOGY AND EVOLUTION Smbe ssues More content 🔻 Submit 💌 Alerts About 💌 **Article Navigation** Embracing Green Computing in Molecular Phylogenetics 👌 **Article Navigation** Sudhir Kumar 🖂 Molecular Biology and Evolution, Volume 39, Issue 3, March 2022, msac043, https://doi.org/10.1093/molbev/msac043 Published: 04 March 2022 The Carbon Footprint of Bioinformatics **3** Jason Grealey 🖾, Loïc Lannelongue, Woei-Yuh Saw, Jonathan Marten, Guillaume Méric, Sergio Ruiz-Carmona, Michael Inouye 🐱 🛛 Author Notes Molecular Biology and Evolution, Volume 39, Issue 3, March 2022, msac034, https://doi.org/10.1093/molbev/msac034 Published: 10 February 2022 Woei Yuh Guillaume Michael Sergio



Jason Grealey



Saw



Jonathan Marten

Ruiz-Carmona

Méric

Inouye



IT ENABLES ENVIRONMENTAL IMPACT STATEMENTS



Ministère de la Transition écologique et de la Cohésion des territoires Ministère de la Transition énergétique



Actualités Politiques publiques Démarches Ministères onstrateurs d'IA pour les transitions écologique et énergétique → Appel à projets Démonstrateurs d'intelligence artificielle

Du 13 juillet au 07 novembre 2022

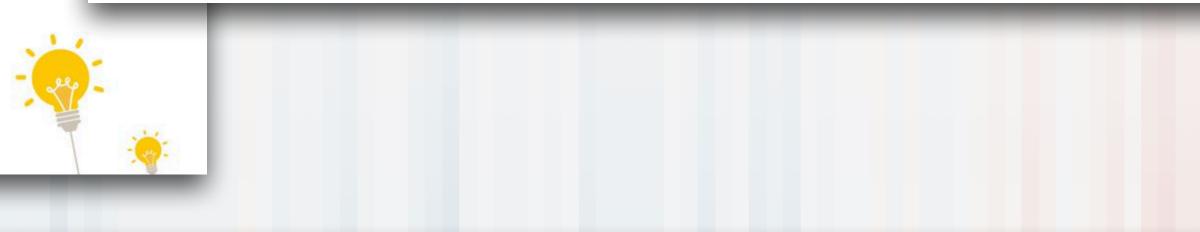
Appel à projets Démonstrateurs d'IA pour les transitions écologique et énergétique

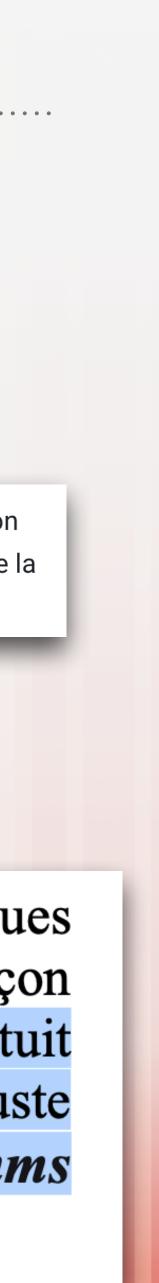
> Estimer la consommation énergétique des services ou des produits numériques Ο développés dans le cadre du projet (algorithmes et composants) exprimée de façon crédible et mesurable. Le porteur de projet s'appuiera sur l'outil en ligne et gratuit ci-dessous. Son code est ouvert et sa méthodologie est considérée comme robuste vis-à-vis de la littérature existante^{3 4}. Il s'agit de Green Algorithms (GT), Lannelongue et al, <u>https://www.green-algorithms.org/</u>



Q

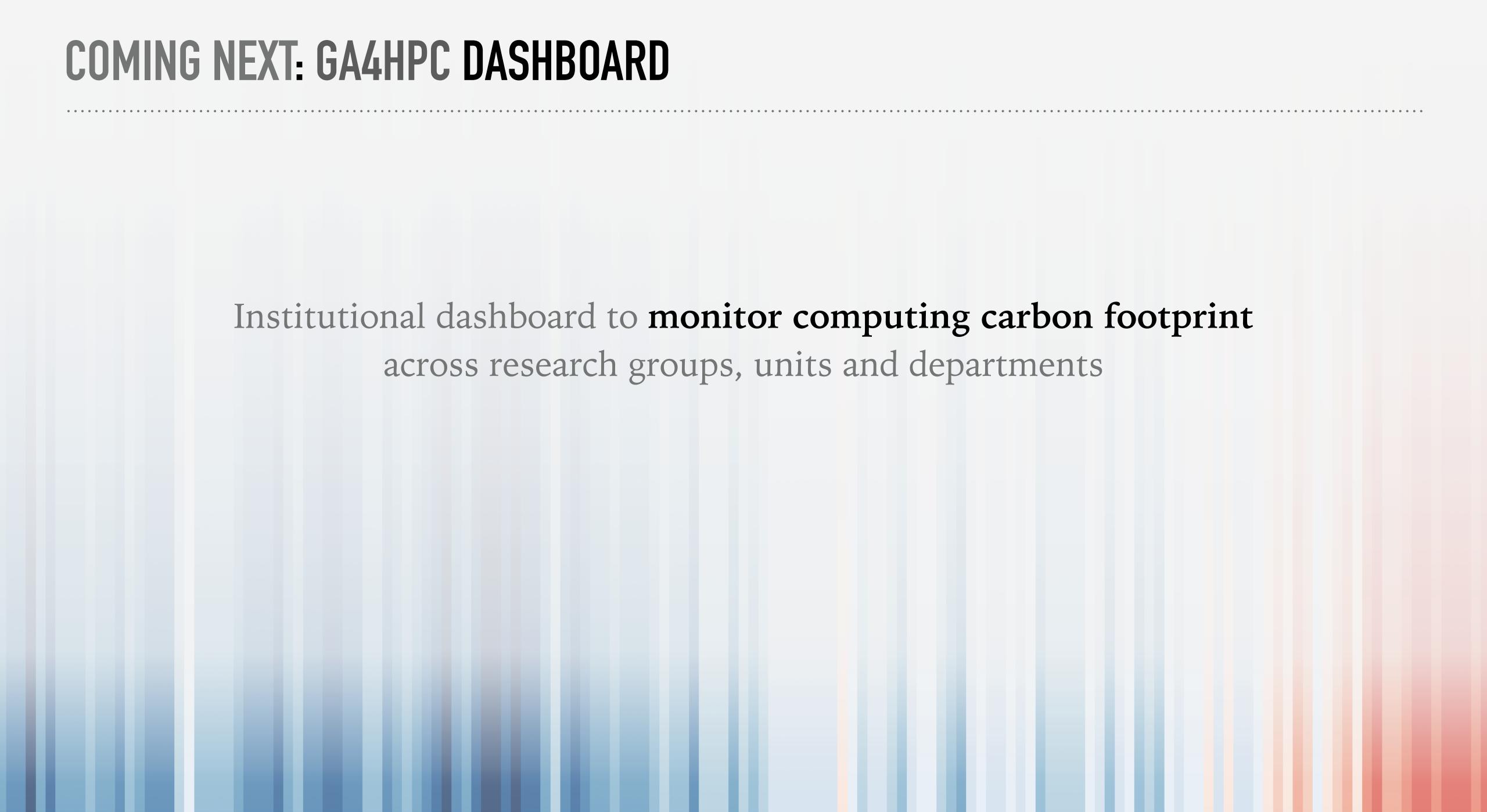
Elle appuie l'appel à projet « démonstrateurs d'IA frugale dans les territoires pour la transition écologique », doté de 40 millions d'euros sur cinq ans, dans le cadre de la seconde phase de la stratégie nationale pour l'intelligence artificielle (SNIA).





COMING NEXT: GA4HPC DASHBOARD

Institutional dashboard to monitor computing carbon footprint across research groups, units and departments



COMING NEXT: GA4HPC DASHBOARD

Concept pioneered by EMBL-EBI (and others!)

Y EMBL-EBI – Carbon footprint

Last updated: Thursday, 22 Jun 2023, 18:00

Introduction

Activity Groups Memory CPU Runtime Status Details Activity Memory Status Groups Reports Contact FAQ

Computing is a major contributor to energy consumption, and thus is one of the main sources of carbon emission. In the context of the global climate crisis, it is imperative that individuals and organizations find ways to assess then reduce the carbon footprint of their work.

This page aims to represent the carbon footprint that we are, collectively and individually, responsible for at EMBL-EBI. LSF jobs submitted to the Codon High Performance Cluster were monitored, information such as resource requested, run time, memory efficiency, etc. were collected, and the carbon footprint was calculated using the formula proposed by Green Algorithms and the following assumptions:

CPU	Intel Xeon Gold 6252, 6.3 W/core		
GPU	NVIDIA Tesla V100, 300 W/core		
Memory power	0.3725 W/GB		
Power usage effectiveness	1.2 (https://kaodata.com/sustainability)		
Carbon intensity	231.12 gCO ₂ e/kWh		
Energy cost	£0.34/kWh		

We built this tool in the hope to raise awareness of computing usage, highlight resources waste, and foster good computing practices. This is intended to be a lightweight carbon footprint calculator, not a cluster monitoring system.

Activity

Overall activity over the past 14 days.

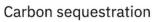






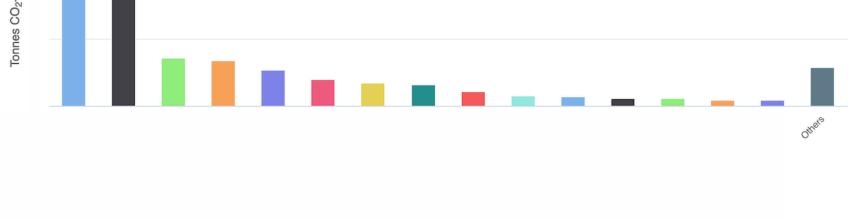


London – Tokyo

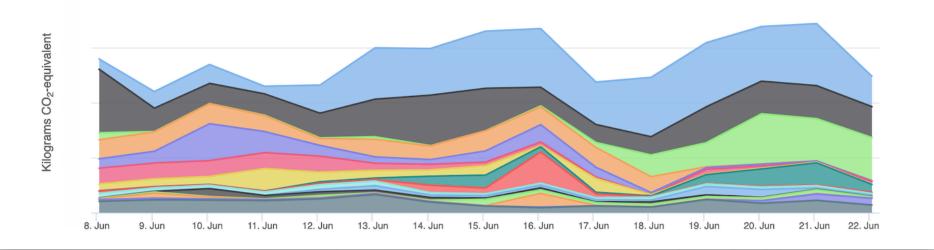


EMBL-EB

Research & service groups Carbon footprint of research and service groups in the past 14 days. Main contributors to EMBL-EBI's carbon footprint



Daily carbon footprint







Alex Bateman

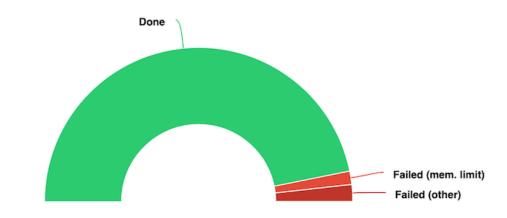


COMING NEXT: GA4HPC DASHBOARD

Concept pioneered by EMBL-EBI (and others!)

Status

Because any resource spent on a job is wasted if the job fails, it is important to test scripts and pipelines on small datasets. The chart below shows the success rate of jobs that completed in the past 14 days.



Failed jobs represent They are responsible for 24.1% of the overall carbon footprint. kg of CO₂e and a cost of £ 6.1% of failed jobs ran for at least an hour before failing, and are reponsible for 23.0% of the overall carbon footprint.

EMBL-EB





Alex Bateman

Memory efficiency of recent successful jobs





GREEN ALGORITHMS 4 HPC: THE DASHBOARD

Next step: an open source, easy to deploy, reliable and transparent SLURM-based dashboard implementing GA4HPC in computing facilities



Green Algorithms dashboard

Your organisation

Last updated: Monday 17 Jul 2023, 10:44

Introduction Activity All departments Groups (DPHPC) Users (Inouve) Credits Contact FAQ

Computing is a major contributor to energy consumption, and thus is one of the main sources of the carbon emission of our research. In the context of the global climate crisis, it is imperative that individuals and organizations find ways to assess the reduce the carbon footprint of their work

This page aims to represent the carbon footprint that we are, collectively and individually, responsible for. SLURM jobs submitted to the High Performance Cluster are logged automatically (including information such as resource requested, run time, memory efficiency, etc.), and the corresponding carbon footprint was calculated using the framework proposed by Green Algorithms and the following assumptions

СРИ	5.9 - 9.4 W/core (see here for models)
GPU	NVIDIA A100 (300 W) and NVIDIA Tesla P100 (250 W)
Memory power	0.3725 W/GB
Power usage effectiveness	1.15
Carbon intensity	231.12 gCO ₂ e/kWh
Energy cost	£0.34/kWh
MARKE IN THE REPORT OF A REPORT OF	

We built this tool in the hope to raise awareness of computing usage, highlight resources waste, and foster good computing practices. This is intended to be a lightweight carbon footprint calculator, not a cluster monitoring system

Activity

Overall activity between 2023-06-15 and 2023-06-16.

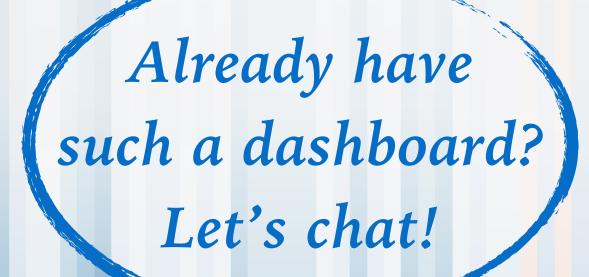






SLURM does not track activity on the login nodes, so the number above only measure the impact of compute nodes.

Interested in piloting it in your organisation? Let's chat!







Alex Bateman



Michael Inouye





COMING NEXT (PART 2): NEXTFLOW PLUGIN

nf-co2footprint උ

nf-co2footprint

Home

nf-co2footprint

CO2footprint-measures

Usage

Parameters

Contributing

Contribution instructions

nf-co2footprint

A Nextflow plugin to estimate the CO₂ footprint of

Introduction

The nf-co2footprint plugin estimates the energy consu on the Nextflow resource usage metrics and information the underlying compute system. The carbon intensity of the energy production is then used to estimate the respective CO₂ emission.

The calculation is based on the carbon footprint computation method developed in the Green Algorithms project: www.green-algorithms.org

Green Algorithms: Quantifying the Carbon Footprint of Computation.

Lannelongue, L., Grealey, J., Inouye, M.,

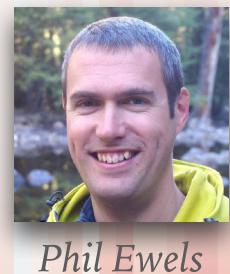
Adv. Sci. 2021, 2100707. https://doi.org/10.1002/advs.202100707

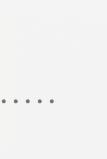
The nf-co2footprint plugin generates a detailed TXT carbon footprint report containing the energy consumption, the estimated CO₂ emission and other relevant metrics for each task. Additionally, an HTML report is generated with information about the carbon footprint of the whole pipeline run and containing plots showing, for instance, an overview of the CO₂ emissions for the different processes.

iội Q Search	Ç nextflow-io/nf-co2footprint ☆₂ ೪₃
D	Table of contents
	Introduction
	Quick Start
pipeline runs.	Credits
mption for each pipeline task based	
in about the power consumption of	







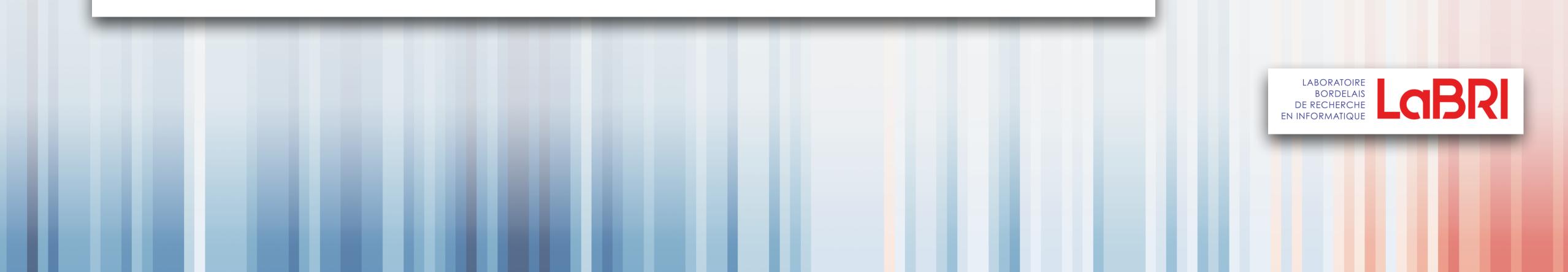


A DETAILED GUIDE FOR DEEP LEARNING

ENVIRONMENTAL RESEARCH COMMUNICATIONS

ACCEPTED MANUSCRIPT • OPEN ACCESS How to estimate carbon footprint when training deep learning models? A guide and review

Lucia Bouza Heguerte¹, Aurélie Bugeau² (D) and Loïc Lannelongue³ Accepted Manuscript online 8 September 2023 • © 2023 The Author(s). Published by IOP Publishing Ltd





Lucia Souza

Aurélie Bureau



TRANSPARENCY, FROM ALL OF US

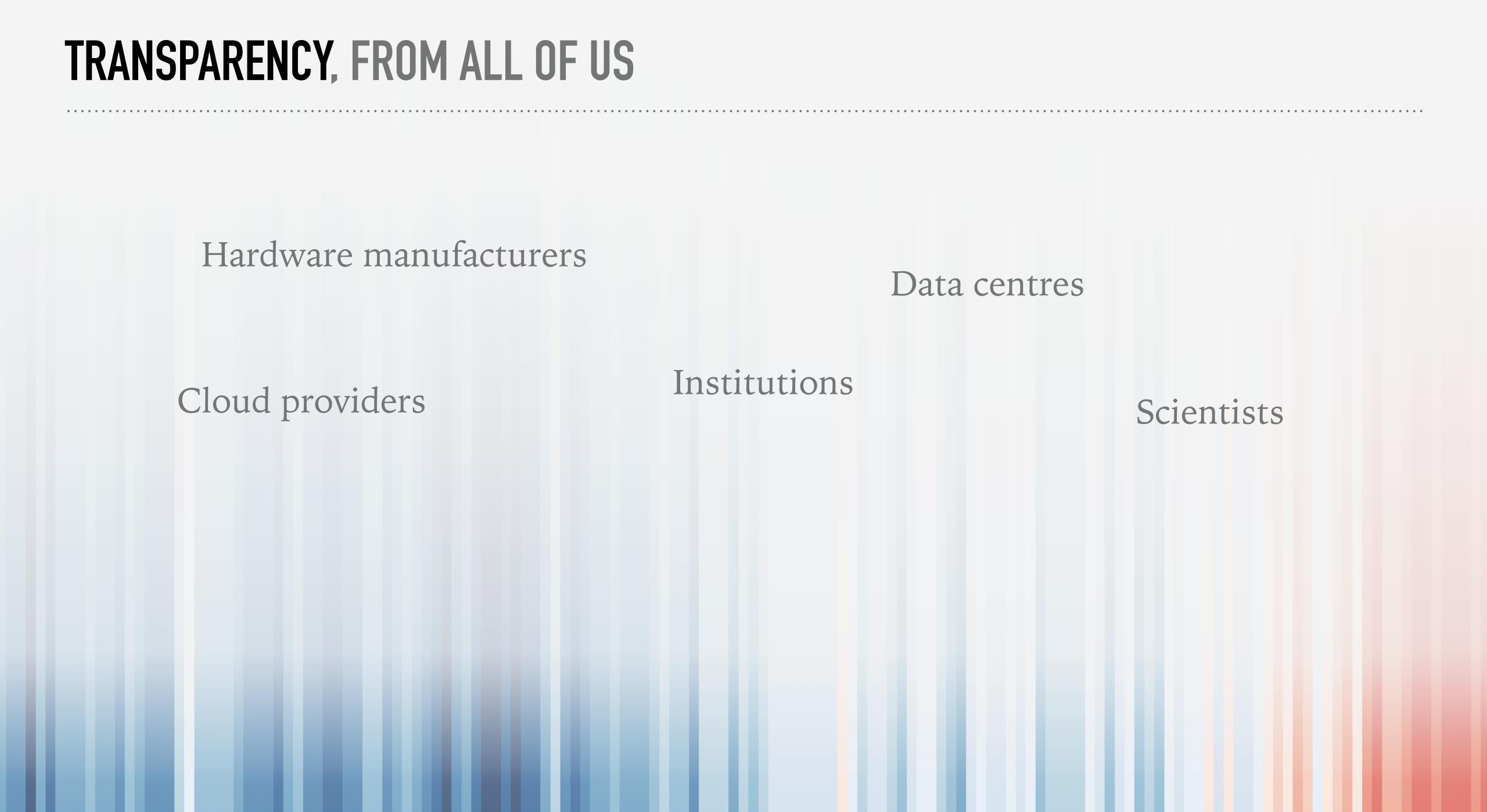
Hardware manufacturers

Cloud providers

Data centres

Institutions

Scientists



TRANSPARENCY, FROM ALL OF US

Carbon impact and offsetting

We used GreenAlgorithms v.1.0 (ref. $\frac{121}{2}$) to estimate that the main computational work in this study had a carbon impact of at least 2,660 kg of CO₂ emissions (CO₂e), corresponding to 233 tree-years. As a commitment to the reduction of carbon emissions associated with computation in research, we consequently funded planting of 30 trees through a local Australian charity, which across their lifetime will sequester a combined estimated 8,040 kg of CO₂e, or three times the amount of CO₂e generated by this study.

Youwen Qin et al., Combined effects of host genetics and diet on human gut microbiota and incident disease in a single population cohort, Nature Genetics, 2022

Carbon impact and offsetting

We used GreenAlgorithms v.1.0 (ref. $\frac{84}{}$) to estimate that the main computational work in this study had a carbon impact of at least 1,004 kg of CO₂ emissions (CO₂e), corresponding to 94 tree-years. As a commitment to the reduction of carbon emissions associated with computation in research, we consequently funded the planting of 45 trees through a local Australian charity, which across their lifetime will sequester a combined estimated 12,000 kg of CO₂e, or 12 times the amount of CO₂e generated by this study.

Yu Xu et al., An atlas of genetic scores to predict multi-omic traits, Nature, 2023

Carbon footprint of this project

We did our best to minimise greenhouse gas emissions related to this project and, using the Green Algorithms calculator (v2.1) [35], we estimated that the carbon footprint of this project was 51 kgCO₂e, which corresponds to 4.7 tree-years.

Lannelongue & Inouye, Inference mechanisms and prediction of protein-protein interactions, bioRxiv, 2022



TRANSPARENCY, FROM ALL OF US

Research Open Access Published: 19 August 2022

A comprehensive evaluation of microbial differential abundance analysis methods: current status and potential solutions

Lu Yang & Jun Chen

Microbiome **10**, Article number: 130 (2022) Cite this article

others (146.1s vs 1.2–57.8 s). For large sample sizes, ZicoSeq can complete the analysis at an average of 5 and 25 min for n = 1000 and 5000, respectively (Fig. S22). Based on the Green Algorithms (green-algorithms.org v2.1 [62]) and the geographic location of Minnesota, USA, ZicoSeq has a carbon footprint of 0.06 g CO2e, 0.59 g CO2e, and 3.16 g CO2e for n = 100, 1000, and 5000, respectively.

Equivariant and Modular DeepSets with Applications in Cluster Cosmology

Leander Thiele* Department of Physics Princeton University Princeton, NJ 08544

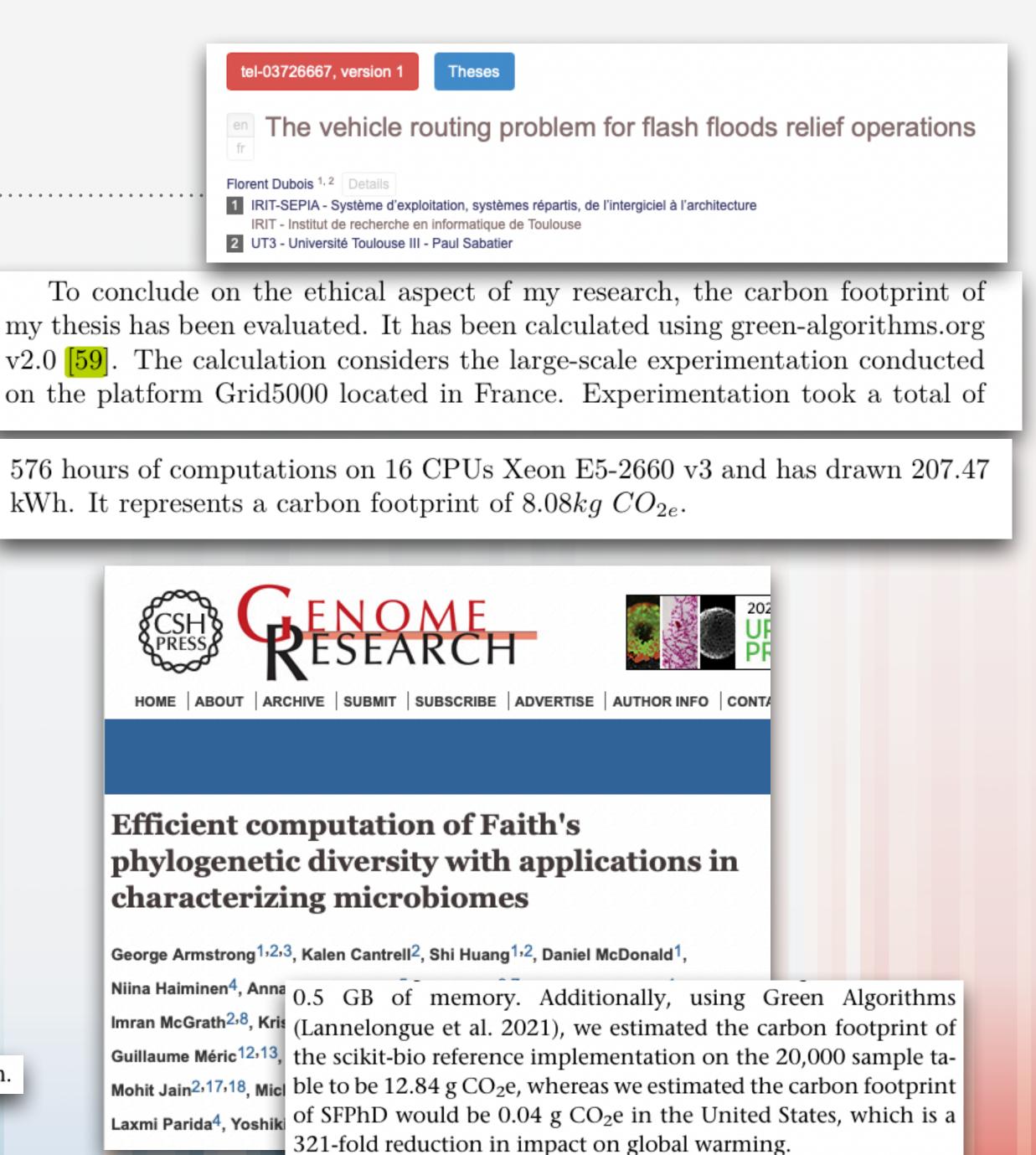
Miles Cranmer Department of Astrophysical Sciences Princeton University Princeton, NJ 08544

William Coulton, Shirley Ho, David N. Spergel Center for Computational Astrophysics

⁶Total compute cost is 13.4 (Tesla P100+9CPU) khr (1.09t CO₂e [26]) with a PyTorch [27] implementation.



kWh. It represents a carbon footprint of $8.08kg \ CO_{2e}$.



FROM ACKNOWLEDGING TO **REDUCING IMPACTS**

Tackling Energy and embodied impact through New Collaborations



WHAT CAN WE DO NOW?

Keep, Repair, Reuse

Promote efficient data centres

Estimate and report your own footprint for your projects

Carefully choose your computing facility

...and include it in your cost-benefit analysis

OPEN ACCESS

EDITORIAL

Ten simple rules to make your computing more environmentally sustainable

Loïc Lannelongue, Jason Grealey, Alex Bateman , Michael Inouye

Published: September 20, 2021 • https://doi.org/10.1371/journal.pcbi.1009324

PLOS COMPUTATIONAL BIOLOGY

Sustainability should be accounted for in renewing policies

Optimise (or use optimised) code







A SUSTAINABILITY STANDARD FOR DRY LAB

Pilot phase underway

Want to be kept updated? Email me! <u>LL582@medschl.cam.ac.uk</u>

Coming soon



FIELD-SPECIFIC GUIDANCE: NEUROSCIENCE

Ten recommendations for reducing the carbon footprint of research computing in human neuroimaging

AUTHORS

Nicholas Edward Souter, Loïc Lannelongue, Gabby Samuel, Chris Racey, Lincoln Colling, Nikhil Bhagwat, Raghavendra Selvan, Charlotte Rae



Nick Souter



Charlotte Rae

Suggested Action: Regularly remove files that you do not need.

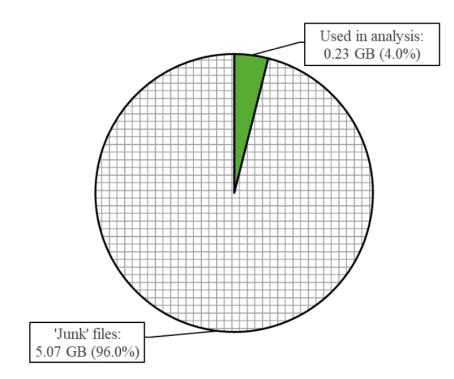
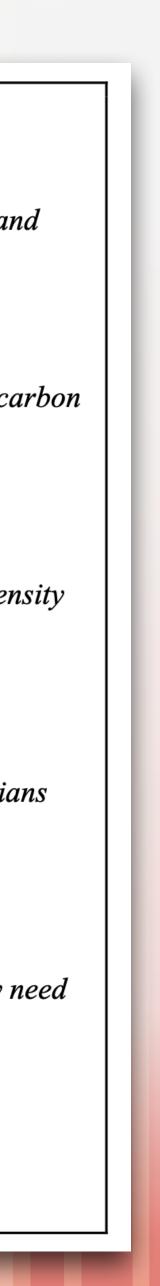


Figure 3. The mean percentage of total data generated by fMRIPrep that is actively used in data analysis (solid green) versus files that can be safely deleted after the completion of

Box 1. Summary of ten recommendations for reducing the carbon footprint of neuroimaging computing

- **1.** Make use of existing preprocessed data when possible, instead of acquiring and processing new data
- 2. Preregister a study analysis plan in order to avoid repetitions
- Quantify and report the carbon footprint of your computing using available carbon tracking tools
- 4. Only run the preprocessing and analysis steps that you need
- 5. Run your computing at lower carbon intensity times and in lower carbon intensity locations
- Regularly remove files that you do not need
- 7. Plan where, and for how long, you will store files, aided by research technicians
- 8. Advocate for non-commercial and centralised data storage solutions
- Publicly share sufficient data to ensure it is FAIR (Findable, Accessible, Interoperable, Reusable), but consider the extent of what others will actually need or use
- **10.** Discuss the importance of greener computing with other neuroimagers and advocate for systemic change



MINIMISING CARBON INTENSITY THROUGH SMART SCHEDULING

CATS

Climate-Aware Task Scheduler

CATS is a Climate-Aware Task Scheduler. It schedules cluster jobs to minimize predicted carbon intensity of running the process. It was created as part of the 2023 Collaborations Workshop.

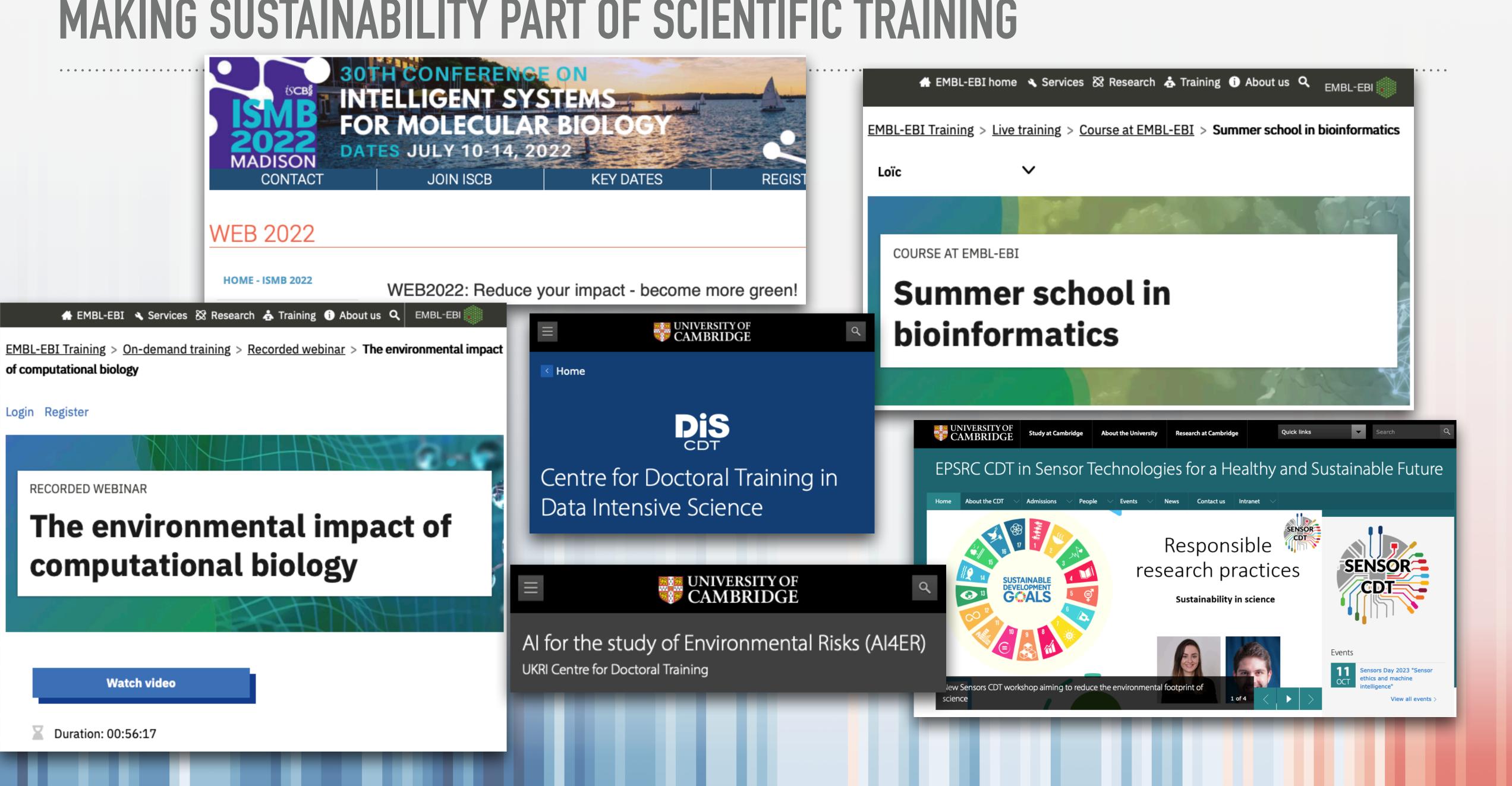
Currently CATS only works in the UK, if you are aware of APIs for realtime grid carbon intensity data in other countries please open an issue and let us know.





MOVING FORWARD: **EDUCATION AND RESEARCH**

MAKING SUSTAINABILITY PART OF SCIENTIFIC TRAINING



IDENTIFY FURTHER OPPORTUNITIES FOR MORE SUSTAINABLE COMPUTING

We believe this resolves all remaining questions on this topic. No further research is needed.

References

- we are, the market, a norme and (~) ~ . "
- Manna, mann, man (m) ma
- wm, m mm. v a (w) n n

JUST ONCE, I WANT TO SEE A RESEARCH PAPER WITH THE GUTS TO END THIS WAY.

Sadly not yet

So dedicated research efforts are needed



IDENTIFY FURTHER OPPORTUNITIES FOR MORE SUSTAINABLE COMPUTING

Table 3

Results for binary-trees, fannkuch-redux, and fasta.

binary-trees					ELSEVIER www.elsevier.com/locate/scico
	Energy (J)	Time (ms)	Ratio (J/ms)	Mb	
(c) C	39.80	1125	0.035	131	
(c) C++	41.23	1129	0.037	132	
(c) Rust \Downarrow_2	49.07	1263	0.039	180	Ranking programming languages by energy efficiency
(c) Fortran 介1	69.82	2112	0.033	133	Check for
(c) Ada \Downarrow_1	95.02	2822	0.034	197	Rui Pereira ", ^b , [*] , Marco Couto ^c , ^b , Francisco Ribeiro ^c , ^b , Rui Rua ^c , ^b ,
(c) Ocaml $\downarrow_1 \Uparrow_2$	100.74	3525	0.029	148	Jácome Cunha ^{c, b} , João Paulo Fernandes ^d , João Saraiva ^{c, b}
(v) Java $\uparrow_1 \Downarrow_{16}$	111.84	3306	0.034	1120	^a C4 — Centro de Competências em Cloud Computing (C4-UBI), Universidade da Beira Interior, Rua Marquês d'Ávila e Bolama, 6201-001,
(v) Lisp $\downarrow_3 \Downarrow_3$	149.55	10570	0.014	373	Covilhã, Portugal ^b HASLab/INESC Tec, Portugal
(v) Racket $\downarrow_4 \Downarrow_6$	155.81	11261	0.014	467	^c Universidade do Minho, Portugal
(i) Hack $\uparrow_2 \Downarrow_9$	156.71	4497	0.035	502	^d Departamento de Engenharia Informática, Faculdade de Engenharia da Universidade do Porto & CISUC, Portugal
(v) C# $\downarrow_1 \Downarrow_1$	189.74	10797	0.018	427	
(v) F# $\downarrow_3 \Downarrow_1$	207.13	15637	0.013	432	
(c) Pascal $\downarrow_3 \Uparrow_5$	214.64	16079	0.013	256	
(c) Chapel $\uparrow_5 \Uparrow_4$	237.29	7265	0.033	335	
(v) Erlang \uparrow_5 \Uparrow_1	266.14	7327	0.036	433	
(c) Haskell $\uparrow_2 \Downarrow_2$	270.15	11582	0.023	494	
(i) Dart $\downarrow_1 \Uparrow_1$	290.27	17197	0.017	475	We need more trained
(i) JavaScript $\downarrow_2 \Downarrow_4$	312.14	21349	0.015	916	
(i) TypeScript $\downarrow_2 \Downarrow_2$	315.10	21686	0.015	915	
(c) Go \uparrow_3 \Uparrow_{13}	636.71	16292	0.039	228	
(i) Jruby $\uparrow_2 \Downarrow_3$	720.53	19276	0.037	1671	
(i) Ruby ↑5	855.12	26634	0.032	482	Recearch Sottware Findinger
(i) PHP 介3	1,397.51	42316	0.033	786	Research Softwares Engineer
	1,793.46	45003	0.040	275	
(i) Python ↑ ₁₅		209217	0.012	1961	
(i) Lua \downarrow_1	2,452.04		0.00-	0 4 4 6	
	2,452.04 3,542.20	96097 n.e.	0.037	2148	

Contents lists available at ScienceDirect Science of Computer Programming www.elsevier.com/locate/scico Ranking programming languages by energy efficiency

We need more trained **Research Softwares Engineers**

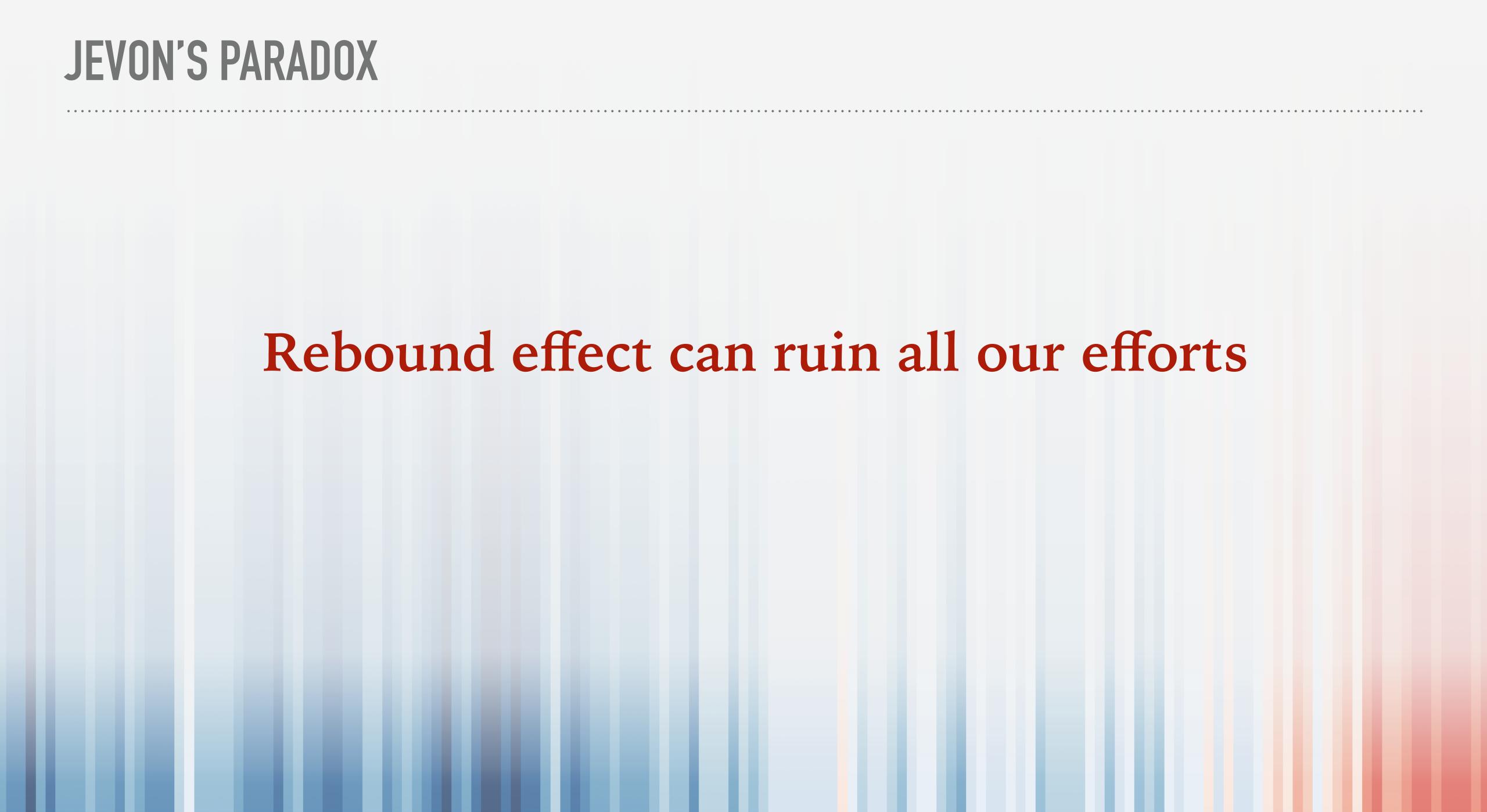






ALL THIS LEADING TO CULTURAL CHANGE

Rebound effect can ruin all our efforts



BUILDING A COMMUNITY

Environmental impacts of computing in health & life sciences research

Are you a health or life sciences researcher who uses computing in your work? Are you concerned about the carbon footprint of your research?

Join us for a free workshop on Greener Research Computing for Health & Life Sciences at the Wellcome **Trust in London**

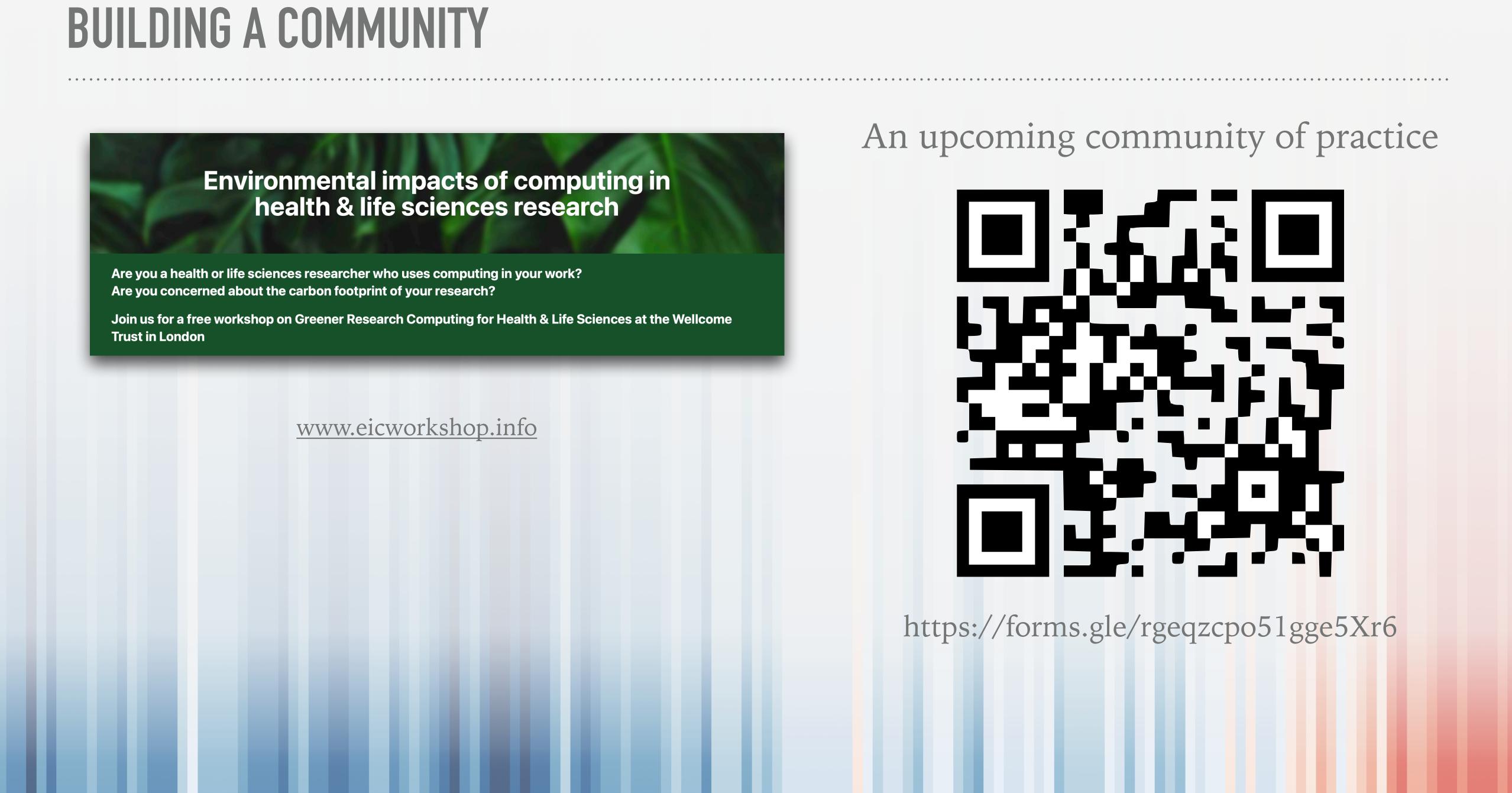
www.eicworkshop.info





https://forms.gle/rgeqzcpo51gge5Xr6





The Green Algorithms website with all resources

At <u>www.green-algorithms.org</u>

Talks

About

Green Algorithms

Towards environmentally sustainable computational science

Carbon footprint calculator

New publication! "Carbon footprint estimation for computational research". We have just released a Comment in Nature Reviews Methods Primers that summarises the different ways you can estimate the environmental impacts of your algorithms. [link] [pdf]

The Green Algorithms project aims at promoting more environmentally sustainable computational science. It regroups calculators that researchers can use to estimate the carbon footprint of their projects, tips on how to be more environmentally friendly, training material, past talks etc.

Green Algorithms Howgreen are your computations?						
Details about your algorithm To understand have each parameter impacts your contexts (polyters), check with the formula below and the <u>methods acticits</u> Runtime (HH:MM) 22 0	Co. 2.37 kg C Carbon foo		9.37 kWh Energy needed			
Duits # CPUs Number of cores 35 Model xeon 55+073 val *	2.59 tree-months Carbon sequestration	13.56 km h a passenger car	5% of a flight Paris-London			
GPUs Number of GPUs s	Sł	are your results with <u>this li</u>	nk			

The online calculator

A tool to easily estimate the carbon footprint of a computation.

Learn more

Green Algorithms 4 HPC

A tool that calculates the carbon footprint of all computations run on an HPC platform.

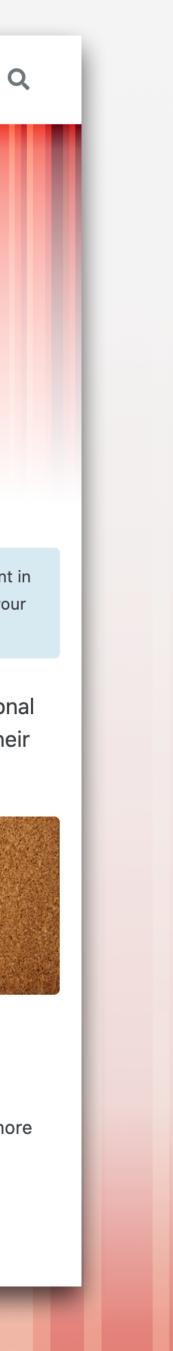
Learn more

30 kgC02e

Tips for green computing

Resources to move towards more sustainable computing.





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> LaBRI Aurélie Bureau Lucia Souza

How to follow the project and reach out www.green-algorithms.org @Loic Lnlg LL582@medschl.cam.ac.uk



KCL

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Wellcome Talia Caplan

UKRI

Martin Juckes

LEAF Martin Farley

The CATS team

Foundation

Cambridge Biomedical NIHR **Research Centre**

Baker

HDRUK Health Data Research UK



Software Sustainability Institute



Medical Council













An upcoming community of practice



https://forms.gle/rgeqzcpo51gge5Xr6