



Programming & Sustainability

Our Professional Footprint as Scientists

Pardis Niknejadi

On behalf of the yHEP Know your footprint team: Valerie Lang, Naman Kumar Bhalla, Simran Gurdasani

August 21st, 2024
Python Programming School in Aachen



universitätfreiburg

Impact you and your work can have

As part of the Python Programming School this week, you are learning:

- Efficient Python Programming
- Accelerator Optimised Programming
- GPU Programming





Impact you and your work can have

As part of the Python Programming School this week, you are learning:

- Efficient Python Programming
- Accelerator Optimised Programming
- GPU Programming

Why and when they are important!





CO₂ and Ground Temperature (128 years ago)

First publication on relationship of atmospheric CO₂ and ground temperature

• Prof. Svante Arrhenius, On the Influence of Carbonic Acid in the Air upon the Temperature of the Ground Philosophical Magazine and Journal of Science Series 5, Volume 41, April **1896**, pages 237-276. Link

	Je.	Carbonic Acid=067.					Carbonic Acid=1.5.				Carbonic Acid=2·0.						Carbonie Acid=2.5.					Carbonic Acid=3·0.				
	Latitude.	Dec Feb.	March- May.	June- Aug.	Sept Nov.	Mean of the year.	Dec Feb.	March- May.	June-	Sept Nov.	Mean of	Dec Feb.	March- May.	June-	Sept Nov.	Mean of the year,	Feb.	March-	June-	Sept Nov.	Mean of the year.	Dec Feb.	March- May.	June-	Sept Nov.	Mean of the year.
urope _	70	_2-0	_30	_3.4	_3:1	_3:1	3:3	3.4	3:8	3:6	3:2	60	6:1	6:0	6:1	6:05	-9	8:0	7.9	80	7:95	9-1	9.3	9-4	94	9.3
	60	-3.0	-3:2	-3.4	-3.3	-3.22	3.4	3.7	3.6	38	3.6	6.1	6-1	5.8	6.1	6.02	90	8.0	7.6	7.9	7:87	9:3	9.5	8-9	9.5	9-3
	50 40	-3.2	-3:3	-3.3	-34	-3:3	37	3.8	3.4	3.7	3.(6.1	6-1	5.5	6.0	5-92	8-0	7.9	7.0	7.9	7:7	9.5	9.4	8.6	9.2	9-17
	30	-51	-54	-02	50	-002	01	50	00	00		00	Ü	01	00	01	0	10	00		1 12		0.0		7.0	0.1
	20	-3.3	-32	-3.1	-3.1	-3.17						56				5.3	'.2	7.0		6.7					7.9	
	10	-3.1	-3.1	-3.0	-3.1							5 52		4.9		5.02					6.52		- 1		7.5	7.52
	0	-3.1	-3.0	-3.0	-30	-3.02	3.2	3.2	3.1	3.1	3.	50	5-0	4.9	4.9	4.95					6.42				7.3	
	-10	-3.0	-3.0	-3.1	-3.0	-3.02	3.1	3.1	3.2	3.2	8.	4.0	4-0	5-0	5.0	4*95	3-4	6.4	6.6			7.3	7.3	7.4		7:35
	-20	-3.1	-3.1	-3.2	-3.1	-3.12	3.2	3.2	3.2	3.2	3:	5.0	5-0	5.2	5.1	5.07	3.6	6.6	6.7	6.7	6.65	7.4	7.5	8.0	7.6	7.62
	-30	-3.1	-3.2	-3.3	-3.2	-3.2	3.2	3.2	3.4	3.3	3:	5.2	5.3	5.5	5.4	5.35	3.7	6.8	7.0	7.0	6.87	7.9	8.1	86	8.3	8.22
	-40	-3.3	-3:3	-3.4	-34	-3:35	3.4	3.5	37	3.5	3:	2 5.5	5*6	5.8	5-6	5-62	7-0	7.2	7.7	7.4	7.32	8.6	8-7	9.1	8.8	8.8
		-3.4	-3.4	-3.3	-34	-3:37	3.6	3.7	3.8	3.7	3.	5.8	6-0	60	6.0	5.95	7:7	7.9	7.9	7.9	7.85	9.1	9.2	9.4	9.3	9-25
	-50 -60	-3.2	- 3.3	_	_	_	3.8	3.7	_	_	-	6.0	6.1	-	-	-	7.9	8.0	-	-	-	9.4	9.5	-		



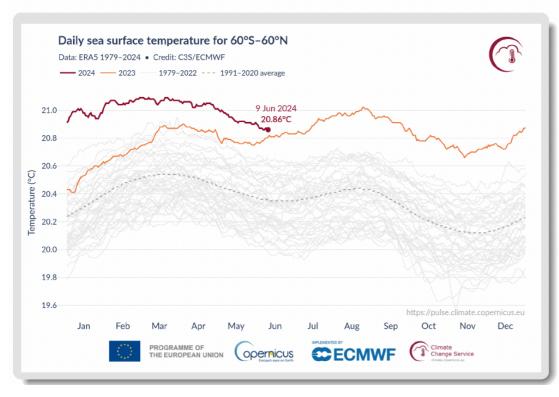
- → CO₂ increase by a factor 2: Temperature increase of ~6°C
- → Surprisingly accurate given coarse understanding >100 years ago
- Confirmed and refined since then in many studies (e.g. Nobel prize 2021)





CO₂ and Ground Temperature (now)

- ightharpoonup Data from Copernicus Satellite ightharpoonup daily sea surface temperature since 1979
 - ullet Strongest anomaly observed in January 2024 \Rightarrow March 2024 hottest month



- ➤ Comparing last 12 months with 1850–1900 average:
 - Global average 1.63°C higher
 - Europe average 1.76°C higher

Already reached and surpassing the ideal target of $1.5^{\circ}\mathrm{C}$ set by Paris climate agreement 2015!

<u>Link</u>

https://climate.copernicus.eu/surface-air-temperature-may-2024





Atmospheric CO₂.Concentration

https://keelingcurve.ucsd.edu/

The Keeling Curve

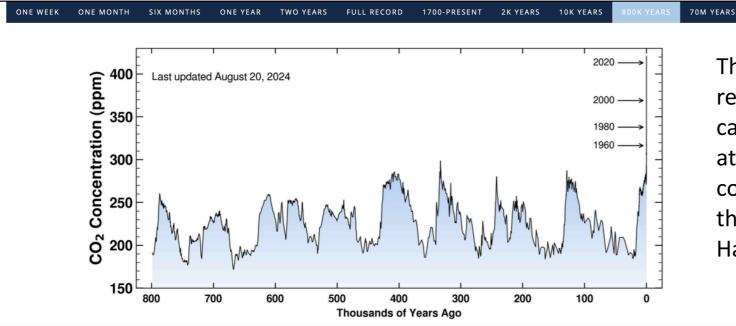
HISTORY MEASUREMENT NOTES

VIDEOS

OTHER CLIMATE INDICATORS

Q

*Latest CO₂ reading: 422.63 ppm



The Keeling Curve is a graph that represents the concentration of carbon dioxide (CO2) in Earth's atmosphere over time, based on continuous measurements taken at the Mauna Loa Observatory in Hawaii





Atmospheric CO₂.Concentration

https://keelingcurve.ucsd.edu/

The Keeling Curve

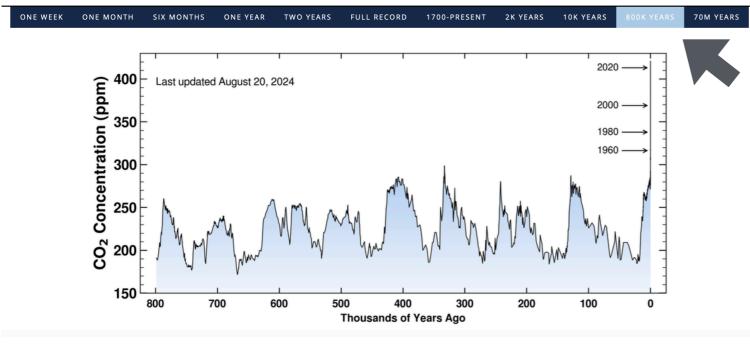
HISTORY MEASUREMENT NOTES

VIDEOS

OTHER CLIMATE INDICATORS

Q

*Latest CO₂ reading: 422.63 ppm



Combined with data from ice cores over the last 800k years, the Composition of air trapped in ice from Antarctica





Atmospheric CO₂.Concentration

https://keelingcurve.ucsd.edu/

The Keeling Curve

HISTORY MEASUREMENT NOTES

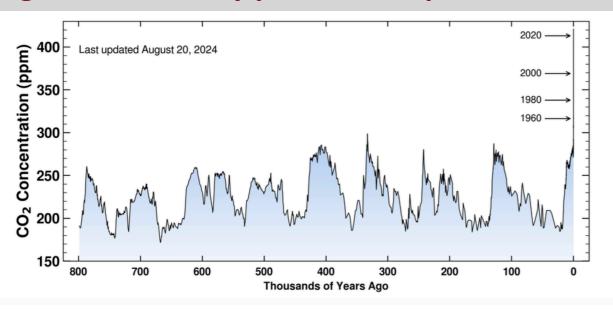
VIDEOS

OTHER CLIMATE INDICATORS

Q

*Latest CO₂ reading: 422.63 ppm

40% higher than at any point in the past 800,000 years



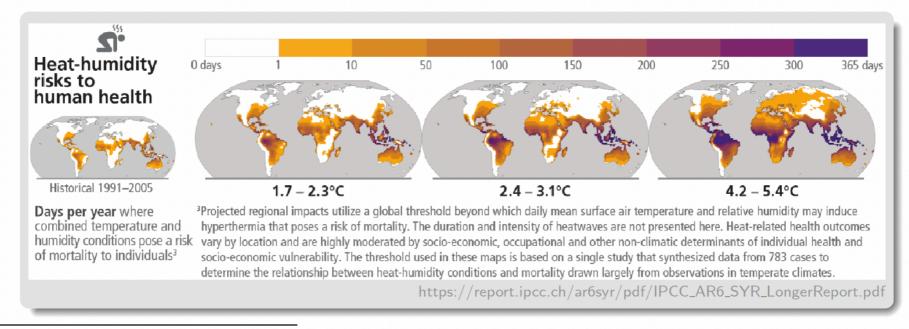
Combined with data from ice cores over the last 800k years, the Composition of air trapped in ice from Antarctica





Consequences

- ▶ Projections for impact of climate change on natural and human systems:
 - With $> 2^{\circ}\mathrm{C}$ rise in temperature, risks posed in regions around the equator:
 - \Rightarrow Risk of losing 100% of animal species
 - ⇒ Risk of Hyperthermia* due to heat-humidity conditions throughout the year



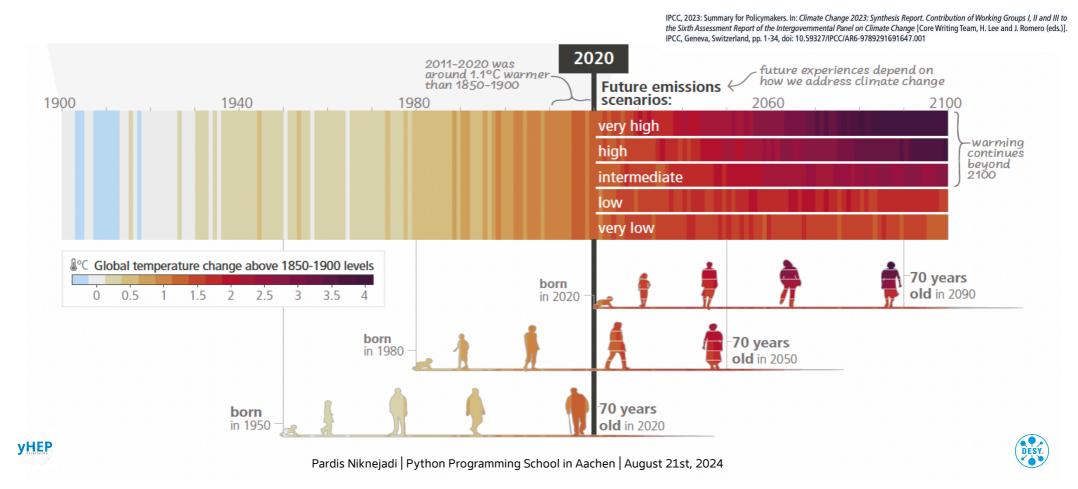
^{*}Hyperthermia: Failure of heat-regulating mechanisms of the body due to extreme external heat





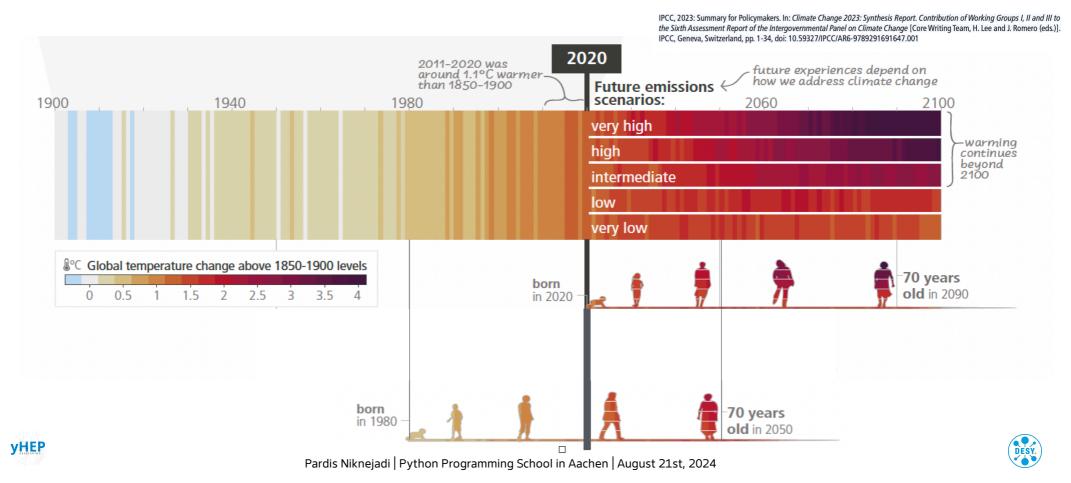
How Different The World Will Be

The extent to which current and future generations will experience a hotter and different world depends on choices now and in the near term



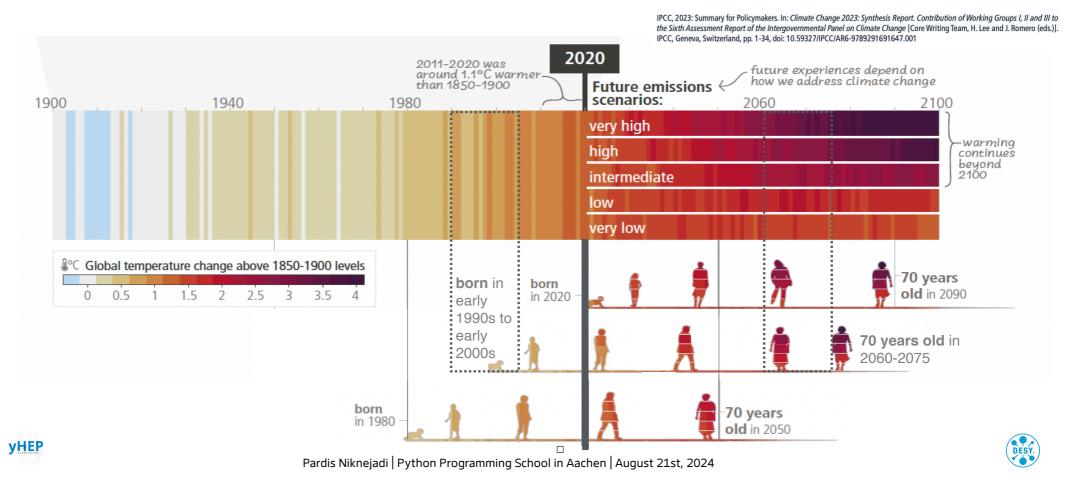
How Different Your World Will Be?

The extent to which current and future generations will experience a hotter and different world depends on choices now and in the near term.



How Different Your World Will Be

The extent to which current and future generations will experience a hotter and different world depends on choices now and in the near term



Our remaining carbon budget:

► Excerpt from the Paris Agreement 2015

Holding the increase in the global average temperature to well below 2°C above pre-industrial levels and pursuing efforts to limit the temperature increase to 1.5°C above pre-industrial levels, recognizing that this would significantly reduce the risks and impacts of climate change;

 $https://treaties.un.org/doc/Treaties/2016/02/20160215\%2006-03\%20PM/Ch_XXVII-7-d.pdf$

- ▶ Temperature targets set to 1.5° C (2.0° C) above pre-industrial levels (1850–1900)
 - \Rightarrow Translates to global carbon budget* of $400\,\mathrm{GtCO}_2$ (1150 GtCO₂)
- Naively assuming equal yearly emissions from 2020–2050 for a static population of 8 billion people:

Annual per person carbon budget =
$$\frac{400 \times 10^9 \, tCO_2}{30 \, years \times 8 \times 10^9 \, people}$$

$$\left(\frac{1150 \times 10^{3} \text{ tCO}_{2}}{30 \text{ years} \times 8 \times 10^{9} \text{ peop}}\right)$$

 $1.7\,\mathrm{tCO}_2$

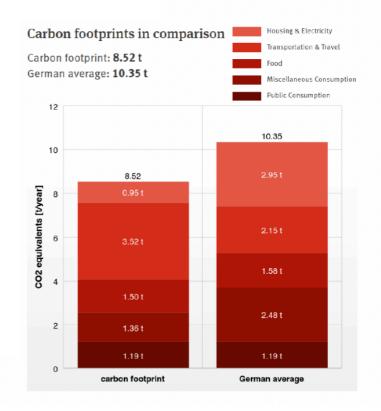
^{*}Carbon budget defined from the beginning of 2020 until global carbon neutrality is achieved





Know Your Footprint Calculator (personal)

- \blacktriangleright Know your footprint (Kyf) calculator \rightarrow tool to estimate carbon emissions for researchers
 - Private emissions in Germany: Carbon Calculator by German Federal Environment Ministry (UBA)*

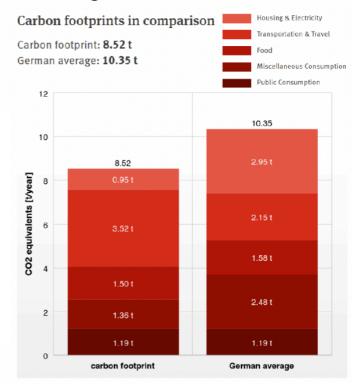


^{*}Permission duly granted by UBA





- \blacktriangleright Know your footprint (Kyf) calculator \rightarrow tool to estimate carbon emissions for researchers
 - Private emissions in Germany: Carbon Calculator by German Federal Environment Ministry (UBA)*
 - ullet Professional emissions in HEP and related fields o split into 4 categories:
 - ⇒ Experiment
 - ⇒ Institute
 - \Rightarrow Computing
 - \Rightarrow Travel



^{*}Permission duly granted by UBA





Impact you and your work can have

As part of the Python Programming School this week, you are learning:

- Efficient Python Programming
- Accelerator Optimised Programming
- GPU Programming

Why and when they are essential?



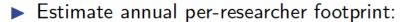


Our Professional Footprint as Scientists: Experiment, Collaboration or Project

- ► Possible choices offered:
 - Large LHC experiment

CERN environmental report(s)

- Small LHC experiment
- and LHCb technical design report
- Small HEP experiment
- $^* o \mathsf{DESY}$ electricity consumption
- Astrophysics experiment
- \rightarrow ESO annual report



- (Total annual experiment footrint)/(Total experiment members)
- ullet Experiment member o collaboration members or users (and operators) as per applicability
- ullet Do not consider indirect benefits to society o too vague and diffuses responsibility
- We researchers designing, building and operating detectors, and analysing data must take responsibility

^{*}Choice between green and conventional electricity





Institute or Research Center

- Possible choices offered:
 - Research centre → CERN environmental report(s)
 - University $^* \rightarrow$ University of Freiburg environmental report (Cross check with Leibniz University Hannover)

Category	Emissions [tCO ₂ e]
Electricity	3158
Heating (gas+fuel) + Other	11 250
Water purification	176
Waste	1875
Procurement	104 974
Total	121 433
Total without Procurement	16 459

CERN (Research Centre)

- Estimate annual per-researcher footprint:
 - (Total annual institute footrint)/(Effective number of institute members)
 - One year outside COVID-19 pandemic considered representative
 - ⇒ 2019 for University of Freiburg, 2022 for CERN
 - University of Freiburg preferred over Leibniz University Hannover as default university footprint:
 - ⇒ Procurement information omitted by Leibniz University Hannover
 - ⇒ Decent agreement in overlapping categories



^{*}Choice between green and conventional electricity

Institute or Research Center

- Possible choices offered:
 - Research centre \rightarrow CERN environmental report(s)
 - University * → University of Freiburg environmental report
 (Cross check with Leibniz University Hannover)

Category	Emissions [tCO ₂ e]
Electricity	2431 (19 224)
Heating/Cooling	13 584
Water	14
Waste	577
Procurement	14 486
Total	31 092 (47 885)

University of Freiburg

- Estimate annual per-researcher footprint:
 - (Total annual institute footrint)/(Effective number of institute members)
 - One year outside COVID-19 pandemic considered representative
 - ⇒ 2019 for University of Freiburg, 2022 for CERN
 - University of Freiburg preferred over Leibniz University Hannover as default university footprint:
 - ⇒ Procurement information omitted by Leibniz University Hannover
 - ⇒ Decent agreement in overlapping categories



^{*}Choice between green and conventional electricity

Our Professional Footprint as Scientists: Business Travel

- Only considering business travel
 - ⇒ Private travel included in private footprint
- ▶ International research environment
 - ⇒ Travel important for personal connections
 - Most notably missed during COVID-19 pandemic
- ▶ But travel leads to CO₂ emissions
 - ⇒ Need to reconsider which trips are essential
 - Avoid air travel if possible
 - Consider extending business trips to combine with vacations
- Possibility for detailed calculations for business trips in Kyf calculator
- Alternatively, also possible to configure with benchmark trips



thetrainline.co



- ► Focus on high-performance computing (HPC)
 - Specify researcher's individual computing workload in core hours
 - ullet Distinguish between CPU and GPU o based on computational task
 - ⇒ Several possibilities to tune configuration
 - ⇒ Assume optimal core utilisation



JUPITER - Exascale in Europa

Copyright:

— Forschungszentrum Jülich

- ▶ Potential to add footprint for large external data storage resources
- ▶ Personal computers, small institute clusters, etc.
 - \Rightarrow Assumed to be covered personal or institute electricity and procurement
- ▶ Benchmark scenarios provided for user-friendliness





Computing

Calculation of computing footprint

 $Total[tCO_2e] = f_{PUE} \cdot f_{overh} \cdot n_{WPC} \cdot f_{conv}$

- · With:
 - f_{PUE} = HPC's Power Usage Effectiveness (PUE)
 → Default: 1.5 (Global average) → New CERN computing centre target: 1.1
 - f_{overh} = Overhead factor for power consumption when computing cores are idle
 → Default: 1.17 (Hawk supercomputer idle time at the HPC Stuttgart)
 - n_{WPC} = Workload Power Consumption (WPC)

$$n_{WPC} = p_{CPU-core} \cdot l_{core-h,CPU} + p_{GPU} \cdot l_{h,GPU}$$

 $p_{\mathit{CPU-core}/\mathit{GPU}}$ = Power consumption in kW for each CPU core/GPU

→ Default: 7.25W (CPU - from the DESY Maxwell cluster with AMD EPYC 75F3 CPU cores), 250W (GPU - median of range, reported on a forum of NVIDIA GPU users)
l_{core-h CPU/h GPU} = CPU workload measured in core hours/ GPU usage hours → User input

• f_{conv} = Conversion factor from kWh to gCO₂e \rightarrow Both, green and conventional (default) electricity possible



JUPITER - Exascale in Europa

Copyright:

— Forschungszentrum Jülich



Computing

Four benchmark scenarios available in Kyf calculator

- Low usage
 - PhD student with several jobs per week → Average of 4000 CPU core-h/month
- · Medium usage
 - Doctoral student or post-doctoral researcher, strongly involved in data analysis → Based on top five ranked users at the Uni-Freiburg HPC: Black-Forest Grid (BFG)
 - → Average of 30 000 CPU core-h/month
- · High usage
 - Accelerator scientist, studying accelerator performance with particle tracking codes and semi particle in-cell (PIC) codes → With code optimized for GPUs: 2500 GPU h/month (≈ 80 000 CPU core-h/month)
- · Extremely high usage
 - Researcher running PIC simulations or high-resolution imaging analysis → 8000 GPU h/month (≈ 300 000 CPU core-h/month)



JUPITER - Exascale in Europa

Copyright:

— Forschungszentrum Jülich

Scenario	Annual footprint [tCO ₂ e]						
Low	0.25						
Medium	1.91						
High	5.48						
Extremely high	17.52						

With conventional electricity





Computing

Four benchmark scenarios available in Kyf calculator

- Low usage
 - PhD student with several jobs per week → Average of 4000 CPU core-h/month
- · Medium usage

 Doctoral student or post-doctoral researcher, strongly involved in data analysis → Based on top five ranked users at the Uni-Freiburg HPC: Black-Forest Grid (BFG)

→ Average of 30 000 CPU core-h/month

High usage
 My Motivation

- Accelerator scientist, studying accelerator performance with particle tracking codes and semi particle in-cell (PIC) codes → With code optimized for GPUs: 2500 GPU h/month (≈ 80 000 CPU core-h/month)
- · Extremely high usage
 - Researcher running PIC simulations or high-resolution imaging analysis → 8000 GPU h/month (≈ 300 000 CPU core-h/month)



JUPITER - Exascale in Europa

Copyright:

— Forschungszentrum Jülich

Scenario	Annual footprint [tCO ₂ e]
Low	0.25
Medium	1.91
High	5.48
Extremely high	17.52

With conventional electricity





Computing: Area's we still like to work on



JUPITER - Exascale in Europa

Copyright:

— Forschungszentrum Jülich

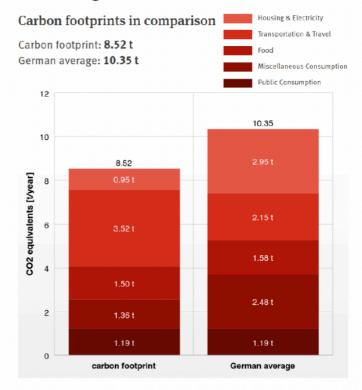
f_{overh} = Overhead factor for power consumption when computing cores are idle
 → Default: 1.17 (Hawk supercomputer idle time at the HPC Stuttgart)

Potential to add footprint for large external data storage resources





- \blacktriangleright Know your footprint (Kyf) calculator \rightarrow tool to estimate carbon emissions for researchers
 - Private emissions in Germany: Carbon Calculator by German Federal Environment Ministry (UBA)*
 - Professional emissions in HEP and related fields → split into 4 categories:
 - \Rightarrow Experiment
 - \Rightarrow Institute
 - ⇒ Computing
 - \Rightarrow Travel
 - Each category configurable for an individual, i.e. for your individual research situation
 - Investigate the impact of each category
- ► Know your footprint calculator now live: Kyf Calculator
- ► Paper discussing the basis of Kyf calculator available online on arXiv: arXiv:2403.03308v1



^{*}Permission duly granted by UBA





yHEP: Know your footprint (Kyf-2024)

We, in the **young High Energy Physicists** (yHEP) association, want to encourage you to evaluate your carbon footprint for both private and professional life. Mitigating climate change and reducing carbon footprints can only occur when we understand the biggest contributors to our emissions, and can thus address them one by one. This tool is meant to help you gain a first understanding.

- For the private footprint, we refer to the carbon calculator by the German Federal Environment Agency (UBA). You will find a link later.
- For the professional footprint in High Energy Physics (HEP) and related research areas, we have developed the calculator ourselves. A description of the calculations, the sources and the assumptions that went into it can be found here: arXiv:2403.03308
- If you want, you can anonymously submit your result to yHEP at the end, so that we can gather some statistics regarding researchers in and related to Germany. But this is not mandatory. If you want to send us feedback on the survey, you will get a chance at the end as well.

We wish you interesting insights!

This survey is anonymous.

The record of your survey responses does not contain any identifying information about you, unless a specific survey question explicitly asked for it.

If you used an identifying token to access this survey, please rest assured that this token will not be stored together with your responses. It is managed in a separate database and will only be updated to indicate whether you did (or did not) complete this survey. There is no way of matching identification tokens with survey responses.

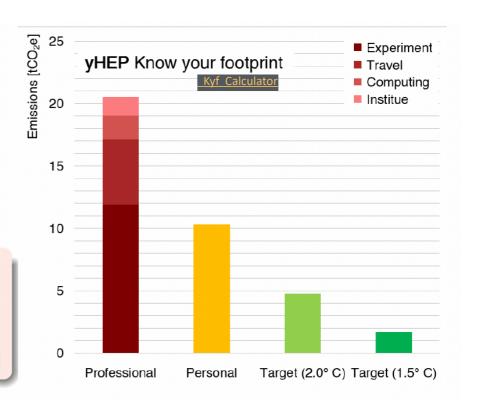
Next

Kyf Calculator



Benchmark Researcher

- Doctoral researcher as a benchmark case:
 - Working on a large LHC experiment
 - Employed by a university (conventional electricity)
 - Medium computing level (conventional electricity)
 - Annual travel:
 - ⇒ Two 1-week trips by train in Germany
 - ⇒ One 1-week flight travel in Europe
 - ⇒ One 2-week transcontinental travel
- Professional footprint double of private footprint
- ▶ Both far above the targets set in Paris agreement
- ► HEP researchers urgently need to address this
 - ⇒ Become part of the solution to the climate crisis!









Please consider submitting your results ⇒ provides us better statistics to understand trends

- The climate crisis is progressing and intensifying each year.
- •HEP and related fields contribute to global emissions. In the benchmark case, the total footprint 6 (18) times was more than what is needed for the 2.0 degree C (1.5 degree C) target





The goal of the Kyf Campaign

Understanding our professional footprint and identifying the impact of different categories



Please consider submitting your results ⇒ provides us better statistics to understand trends

- The climate crisis is progressing and intensifying each year.
- •HEP and related fields contribute to global emissions. In the benchmark case, the total footprint 6 (18) times was more than what is needed for the 2.0 degree C (1.5 degree C) target





Aiming to Go Beyond Carbon Neutrality with Responsible Research Practices and Innovation



- Institute
- Computing
 - Optimizing data centers
 - Adopting energy-efficient algorithms
 - Leveraging renewable energy sources
 - Improving hardware efficiencies
- Travel
- Experiment
 - Innovations such as carbon capture technologies

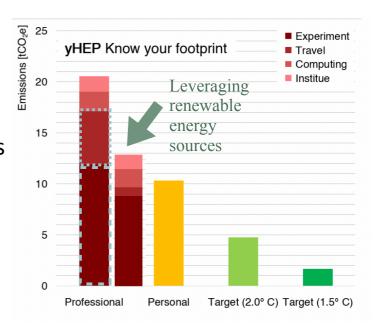




Aiming to Go Beyond Carbon Neutrality with Responsible Research Practices and Innovation



- Institute
- Computing
 - Optimizing data centers
 - Adopting energy-efficient algorithms
 - Leveraging renewable energy sources
 - Improving hardware efficiencies
- Travel
- Experiment
 - Innovations such as carbon capture technologies



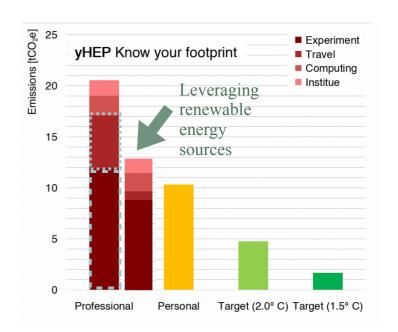




Aiming to Go Beyond Carbon Neutrality with Responsible Research Practices and Innovation



- Convert to tCO₂e → 2 options:
 - Green electricity → Assume 100% photo-voltaic (PV) based production: → 35 gCO₂e/kWh
 - German electricity mix in 2023
 → Includes already >40% from wind, solar and water power
 → 416 gCO₂e/kWh
 (for comparison: gas: 572 gCO₂e/kWh, coal: 1167 gCO₂e/kWh)



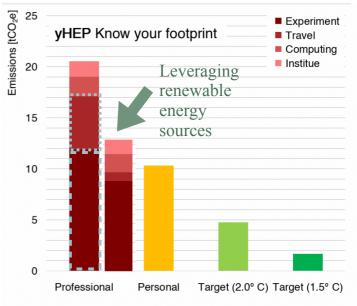




Aiming to Go Beyond Carbon Neutrality with Responsible Research Practices and Innovation











Impact you and your work can have

As part of the Python Programming School this week, you are learning:

- Efficient Python Programming
- Accelerator Optimised Programming
- GPU Programming

Why and when they are critical!





Your Role:

You are better programmers than graduate students ten years ago You are here to learn how to be more efficient Keep up the good work

- ◆ Continue the culture of sharing and learning from each other
- ◆ Follow FAIR guidelines: make reusable/accessible software and data
- ♦ Where you can start the dialogue and advocate for more sustainable programming and data analysis practices





Aiming to Go Beyond Carbon Neutrality with Responsible Research Practices and Innovation



Please consider submitting your results ⇒ provides us better statistics to understand trends

Making every gram of CO₂ not emitted count:

By strategically focusing on negative emission opportunities, we can tip the scale toward a more sustainable and environmentally positive future in HEP.



