

Discussion about Conclusions and Next Steps



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What is the outcome of this workshop?

- With respect to the outcome of the first workshop in 2023

documented in the paper “Resource-aware Research on Universe and Matter: Call-to-Action in Digital Transformation”

<https://doi.org/10.1140/epjs/s11734-024-01436-4>

- What does ChatGPT say?

Item	Call-to-action
Immediately or on short time scale with little effort these measures can be implemented:	
S1	Raise awareness of the climate challenge at all levels.
S2	Disseminate knowledge of measures to address the challenge.
S3	Monitor and report energy consumption at job level.
S4	Consider carbon footprint for all investments and project plans.
S5	Enhance awareness of the trade-off between research benefit and climate impact.
S6	Use already optimized algorithms in open-source standard libraries or domain-specific libraries.
On a medium time scale of a few years the following measures can be realized:	
M1	Make data FAIR to promote reuse.
M2	Reduce and compress data having the anticipated scientific value of the retained information and the resource requirements in mind.
M3	Optimize the choice of storing intermediate results against re-calculating them.
M4	Optimize job orchestration and scheduling in workflows.
M5	Use workflow management to make processing FAIR.
M6	Make software FAIR and reliable by following good software development practices and ensuring sustainable support.
M7	Design software for optimized energy consumption and provide tools to measure it.
M8	Continue research on potential of AI, in particular generative and pre-trained models, or other new technologies for efficient use of resources, but balance gain of research action against resource consumption of these developments.
M9	Expand detailed monitoring and documentation of energy consumption and CO ₂ e footprint in AI training and inference.
M10	Monitor and report energy consumption at site and project level, provide information of the individual use per scientist/project/publication.
M11	Extend monitoring of resources beyond CO ₂ e (water, material etc.).
M12	Train scientists in good practices.
M13	Strive to become a role model at all levels and help to establish sustainability in everyday life.
M14	Regularly review and update the CO ₂ e reduction plan.
A longer term coordinated planning is required for the following measures:	
L1	Adjust computing in space and time to the availability of renewable energy, e.g. computing centers close to off-shore wind parks with a job scheduling using only or mainly the surplus of renewable energy available at a given time.
L2	Develop software and middleware that can respond dynamically to the availability of renewable energy.
L3	Optimize power usage effectiveness.
L4	Re-use of produced heat.
L5	Adjust hardware lifetime considering emissions due to procurement and operation.
L6	Include the resources needed for continuous IT support into project planning.

Table 2 Call-to-action in digital transformation: portfolio of measures to be taken, ordered in terms of effort and time they take.

S1 Raise awareness of the climate challenge at all levels.

Kurzfassung: Die Teilnehmenden betonen, dass das Thema Klima-Dringlichkeit überall - von einzelnen Forschenden bis zur Politik - präsent sein muss.

- D_S: 'We need a collective narrative of what we as a community are trying to do to energise individual scientists that their impact matters.'

- I_L: 'We should involve people who have the power to make decisions. The action has to be taken by them.'

- T_K: 'Talks about sustainability and creation of a sustainability task force at Belle II.'

S2 Disseminate knowledge of measures to address the challenge.

Kurzfassung: Wissenstransfer geschieht über Vorträge, Konferenzen und publikumswirksame Formate.

- M_E: 'Meanwhile the group of authors received invitations to various conferences.'

- C_W: 'Utilizing students as ambassadors among their community - allows us to reach broad audiences.'

- A_W: 'Proceed with offering training events (Schools, Workshops) for PhDs.'

S3 Monitor and report energy consumption at job level.

Kurzfassung: Erste Rechenzentren erfassen den Energie- und CO₂-Verbrauch pro Job und spiegeln ihn den Nutzenden zurück.

- M_E: 'Monitoring and reporting is being done at various sites - VISPA attempts informing their users as well.'

- M_S: 'WLCG and EGI have ongoing efforts to perform accounting of elapsed compute time, consumed energy and created CO₂ footprint.'

- M_S: 'plans are on the way in PUNCH4NFDI, WLCG, EGI (SUSFECIT).'

S4 Consider carbon footprint for all investments and project plans.

Kurzfassung: Neue Großprojekte sollen CO₂-Bilanzen schon in der Planungsphase einpreisen.

- J_E: 'Planning of ET computing centre. Harder for ongoing large-scale projects.'

- K_L: 'Input into European Strategy of Particle Physics - sustainability also included in more general contributions.'

- HG_S: 'Quantitative metrics should be used whenever possible to estimate life-cycle GHG emissions of computers.'

S5 Enhance awareness of the trade-off between research benefit and climate impact.

Kurzfassung: Der Nutzen einer Analyse soll stets gegen ihren ökologischen Preis abgewogen werden.

- M_E: 'This point is still difficult to include in practice - Easier on PhD level than on Bachelor level.'

- HG_S: 'The CO₂ emissions should be weighed against the impact of the respective research, in terms of its usefulness to the research community and grand challenges.'

- T_E: 'If there are two equally large knowledge gains, but one is cheaper, I should do the cheaper first.'

S6 Use already optimized algorithms in open-source or domain-specific libraries.

Kurzfassung: Viele Arbeitsgruppen setzen inzwischen bewusst auf bestehende, effiziente Bibliotheken statt Eigenentwicklungen.

- M_E: 'Many young researchers actually follow this as it turns out to be much more efficient both in saving development time and in applying the algorithms.'

- V_K: 'Efficient software that runs at scale can reduce emissions - working towards energy certifications for software programs.'

M1 Make data FAIR to promote reuse.

Kurzfassung: Durch FAIR-Prinzipien wird Mehrfachnutzung erleichtert und Doppelarbeit vermieden.

- T_K: 'New reinterpretation method described - application to Belle II data (6, but no quantitative measurement).'
- *M1 entry in list* 'Make data FAIR to promote reuse.'

M2 Reduce and compress data having scientific value in mind.

Kurzfassung: Ziel ist drastische Datenreduktion bei Erhalt wesentlicher Information.

- M_D: 'Lossy data compression promises a factor 100 - the tricky part is to lose only what is scientifically meaningless.'
- K_L: 'First HEPMC files on the ATLAS open data portal - removing the need to rerun these calculations.'

M3 Optimize the choice of storing intermediate results vs. recalculating them.

Kurzfassung: Zwischenergebnisse werden nur dann gespeichert, wenn das günstiger ist als Neuberechnung.

- M_E: 'Here I see a lot of efficient working styles, see e.g. Workflow management below.'
- M_E: 'Extracting modular calculations - may be too specific for this write-up'.

M4 Optimize job orchestration and scheduling in workflows.

Kurzfassung: Bessere Workflow-Steuerung vermeidet Leerlauf und spart Rechenzeit.

- M_S: 'If SUSFECIT will be funded a first attempt will be implemented.'
- Ka_S: 'What about Analysis trains - they run mainly over night.'

M5 Use workflow management to make processing FAIR.

Kurzfassung: Standardisierte Workflow-Tools erzeugen Nachvollziehbarkeit und Effizienz.

- T_K: 'Paper - A workflow management guideline (arXiv:2212.01422).'
- M_E: 'User analysis workflow management system - law - enabling automated re-calculations of only the necessary parts.'

M6 Make software FAIR and reliable by good practices & sustainable support.

Kurzfassung: Sauber dokumentierter, gemeinsam gepflegter Code senkt langfristig Ressourcenbedarf.

- M_E: 'Here we could gain a lot from projects suggested for ErUM-Data funding.'
- K_L: 'Every experiment should provide simple check lists of measures to make code more efficient.'

M7 Design software for optimized energy consumption and provide measurement tools.

Kurzfassung: Energieverbrauch soll bereits im Software-Design minimiert und gemessen werden können.

- M_E: 'Simple energy consumption algorithms exist - awkward-arrays allow sizeable chunks of events to be processed in parallel.'
- T_K: 'Benchmarks show that the RNTuple format in ROOT provides significant efficiency gains over TTree.'

M8 Research on AI & new technologies, balancing gain vs. resource use.

Kurzfassung: KI-gestützte Beschleuniger werden entwickelt, doch ihr Energiebedarf muss sich lohnen.

- T_K: 'Development of various models for speeding up simulations in the KISS project.'

- J_E: 'Fast AI-based calorimeter simulations in HEP well-studied by now - LHCb now also uses it.'

- M_E: 'Low-Rank-Adaptation has been tested using LLMs for classification tasks with remarkable accuracy.'

M9 Expand detailed monitoring of energy & CO₂e in AI training/inference.

Kurzfassung: Spezifische Messungen für KI-Workloads sind in Vorbereitung.

- M_S: 'Plans are on the way in PUNCH4NFDI, WLCG, EGI (SUSFECIT).'

M10 Monitor and report energy at site & project level, incl. per scientist.

Kurzfassung: Verbrauchsdaten sollen bis auf Personen- oder Publikationsebene aufgeschlüsselt werden.

- M_E: 'Giving information of the use per scientist/project/publication is explored in small-scale VISPA computing cluster.'

- V_L: 'Feedback to the computing users on the CO₂ emissions of the job - increases awareness.'

M11 Extend monitoring beyond CO₂e (water, material etc.).

Kurzfassung: Ressourcenerfassung soll weitere Umweltfaktoren umfassen.

- M_S: 'Plans are on the way in WLCG, EGI (SUSFECIT).'

M12 Train scientists in good practices.

Kurzfassung: Schulungen, Mentoring und Botschafter-Programme sollen effiziente Nutzung verbreiten.

- A_W & B_F: 'Code consulting' programme - 'make your code sustainable'.

- P_W: 'A training can help students understand that the resources they use are limited and precious.'

- I_L: 'Tutors should also be trained in teaching such things.'

M13 Strive to become a role model and embed sustainability in everyday life.

Kurzfassung: Die Community möchte Vorbild sein und Nachhaltigkeit als Selbstverständlichkeit etablieren.

- M_E: '- At all levels - I find this a high demand! - the talk by Christopher Schrader gave us excellent input for ways to communicate our intentions.'

- S_K: 'The ErUM community takes a lead in developing strategies and technologies for sustainable computing.'

M14 Regularly review and update the CO₂e reduction plan.

Kurzfassung: Reduktionsziele sollen kontinuierlich überprüft und angepasst werden.

- (Keine explizite Diskussion außer dem Listenpunkt - wurde von den Teilnehmenden als notwendig anerkannt.)

L1 Adjust computing to renewable-energy availability (location & scheduling).

Kurzfassung: Rechenjobs werden räumlich und zeitlich auf Phasen mit viel Ökostrom verlegt.

- M_S: 'Try to calculate only when sun is shining or wind is blowing - transfer jobs from one site with low RE fraction to another with high available RE fraction.'
- D_S: 'Introduce - computing lanes that determine the level of freedom that the datacentre operators have.'
- V_L: 'Use sustainable computing queues as default - limit or penalize immediate queues if overused.'
- Achim Stahl: 'Some tasks can wait for green power, others not.'

L2 Develop software & middleware that reacts to renewable-energy availability.

Kurzfassung: Intelligente Orchestrierung entscheidet automatisch, wann und wo Jobs laufen.

- M_S: 'Requires development - of interlinked ecosystems for forecasting available RE and orchestration of jobs.'

L3 Optimize power usage effectiveness.

Kurzfassung: Rechenzentren arbeiten an noch effizienterem Energie- und Kühlungseinsatz.

- M_E: 'This challenge is actually well accepted by large computing centers.'

L4 Re-use of produced heat.

Kurzfassung: Abwärme aus Rechenzentren soll sinnvoll genutzt werden, z. B. für Fernwärme.

- M_E: 'This challenge seems also well accepted by large computing centers.'

L5 Adjust hardware lifetime considering procurement & operation emissions.

Kurzfassung: Langlebigkeit und Materialwahl der Hardware werden in die CO₂-Bilanz einbezogen.

- V_L: 'The use (and origin) of rare earths - needs to be minimized. This decreases the embedded footprint of the hardware.'
- PCF documents (Eoin Woods): 'detail embedded emissions of servers, provided by vendors.'

L6 Include resources for continuous IT support into project planning.

Kurzfassung: Nachhaltige IT benötigt dauerhafte personelle und finanzielle Ressourcen.

- (Keine spezifischen Einzelzitate; wurde jedoch in der Liste der langfristigen Maßnahmen als notwendig festgehalten.)

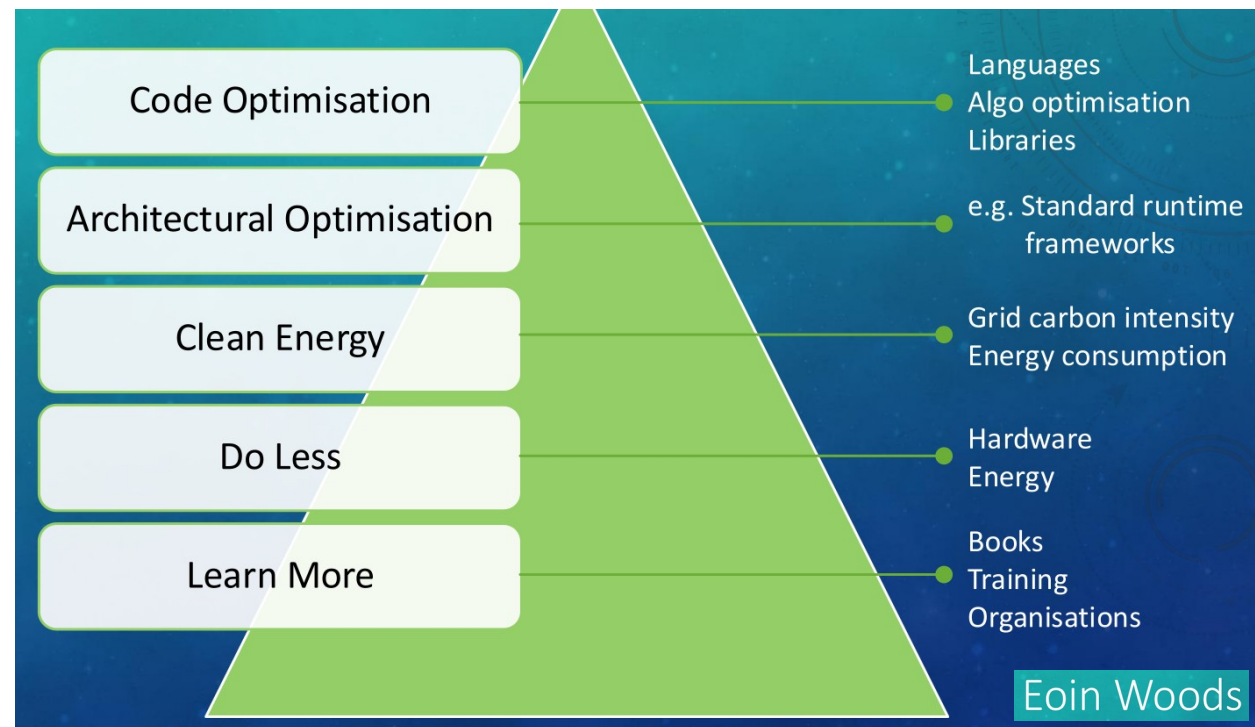
Progress since first workshop?

- Lots of advances in many directions
(see for example many talks at this workshop)
- Maybe not as much and as fast as we were hoping for
- Still some work to be done
- ➔ How can we improve?
- ➔ What new aspects arose in the meantime?
- ➔ Next steps?

How can we improve?

- **Communication!** → from footprint to handprint
 - **What are the right incentives?**
many nudging ideas (e.g. awards, reporting, ...),
CO₂ budget, CO₂ trading/cost, “Klimageld”, ...

- **Focus on the right things?**
- **Interaction with funding agencies?**



EMPFEHLUNGEN ZUR BERÜCKSICHTIGUNG VON NACHHALTIGKEITSASPEKTEN IN DER NATURWISSENSCHAFTLICHEN GRUNDLAGENFORSCHUNG AN GROßGERÄTEN

Ergebnisse des 2. Prisma-Trialogs „Nachhaltigkeit in der Forschung an Großgeräten:
Ressourceneffizienz und Zukunftssicherung“ am 15.05.2024

Die Transformation zu mehr Nachhaltigkeit in der Wissenschaft benötigt Ressourcen,
die bereitgestellt werden müssen. Dies gilt gleichermaßen für alle Bereiche.

Ein aktiver und strukturierter Dialog zwischen Vertretern aus der Forschung, der Politik
(inkl. Fördermittelgeber), der Zivilgesellschaft und der Industrie kann eine
ressourceneffiziente und nachhaltige Forschung an und Entwicklung von Großgeräten
wesentlich unterstützen.

1 Nachhaltige Forschungsplanung und -organisation ermöglichen

Anreize für die nachhaltige Planung und Organisation der Forschung und Anerkennung
von Engagement sind essenziell, um die Attraktivität – insbesondere für den
wissenschaftlichen Nachwuchs – zu erhöhen. Dazu gehört auch die Finanzierung von
Maßnahmen mit Bezug zu mehr Nachhaltigkeit (s. z. B. Softwareentwicklung oder
energieeffiziente Weiterentwicklung von Geräten).

Wissenschaftlerinnen und Wissenschaftler müssen selbst Verantwortung übernehmen,
einen Beitrag zur Reduktion von CO₂e-Emissionen zu leisten – ohne dabei ihr
Forschungsziel zu gefährden. Diese Selbstverpflichtung der Wissenschaft zu einem
nachhaltigem Forschungsprozess sollte mit einem Leitfragenkatalog unterstützt
werden, der das Bewusstsein dafür schärft, wie eine Reduktion der CO₂e-Emissionen
erreicht werden kann.

New aspects?

- (Communication)
 - Ethical aspects of our work (with AI) and their relation to sustainability (in a more general sense)
 - Risk of deskilling, teaching
 - Responsibility
- Machines cannot relieve humans of their responsibility
- Explainability, trust
 - ...
 - New contacts
 - Many (small) exchanged/new idea

Ethical aspects

- Dealing with Deskillling and AI-Dependency
- AI impact on teaching ($\approx$ testing). What can we lose?
- Responsibility: Do we have to worry about this? In bad published results? In instrument control? In biases?
- Is being able to blame X ("make accountable for") something we even want? Need? Accountability counterbalances benefit?
- Is there a vaccination against the plausibility bias?
- Provenance in LLM-Land: is there a threshold for AI declarations? Best practices for epistemic qualifiers?
- What does authorship mean in the age LLMs? And what if there is AGI?
- How can we improve trust in the presence of largely opaque systems?
- What "unfair" (or unwise?) biases could *our* AI applications exhibit? What could we do to mitigate them?
- Does AI replace human creativity in ErUM research?
- How to tie in all this with our sustainability narrative?
- Sustainable use of resources from an ethical perspective? Sorts of sustainability: ecological/social/economical
- Weighing openness with inclusivity (given open tech in general requires more skills)
- Assuming we could build a machine that is smarter, more loving, emphatic, whatever than humans: Would that even mean we ought to go?

Metaphysics (beyond ErUM-Data)

- Humans vs. machines, consciousness

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Metaphysics (beyond ErUM-Data)

- Humans vs. machines, consciousness



Next steps

- Workshop report
- Editorial team?
- Timescale?
- Journal?
- Further workshops?

Further conclusions

- Format of the workshop much appreciated, sufficient time for discussions, also during coffee breaks and meals
- Excellent organization
- Many thanks to Angela, Jan, and Benjamin!