



Panel discussion on Open Science and Reproducibility

LATTICE 2024, LIVERPOOL, 2024-08-02

Plan

- ▶ Definitions and motivations
- ▶ Panelist introductions and lightning talks
- ▶ Q&A via Slido

Join at
slido.com
#9989 867

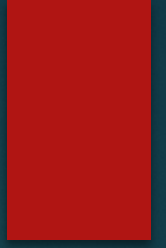


Who am I?

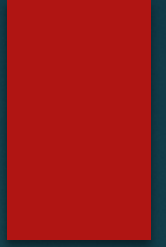
- ▶ STFC Research Software Engineer Fellow
- ▶ Background in BSM lattice quantum field theory
- ▶ Strong interest in reproducibility and openness of data analysis workflows



Definitions



Reproducibility



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Same data + same analysis → Same results

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- ▶ Replicability:

- New data + same analysis → same results

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- ▶ Replicability:

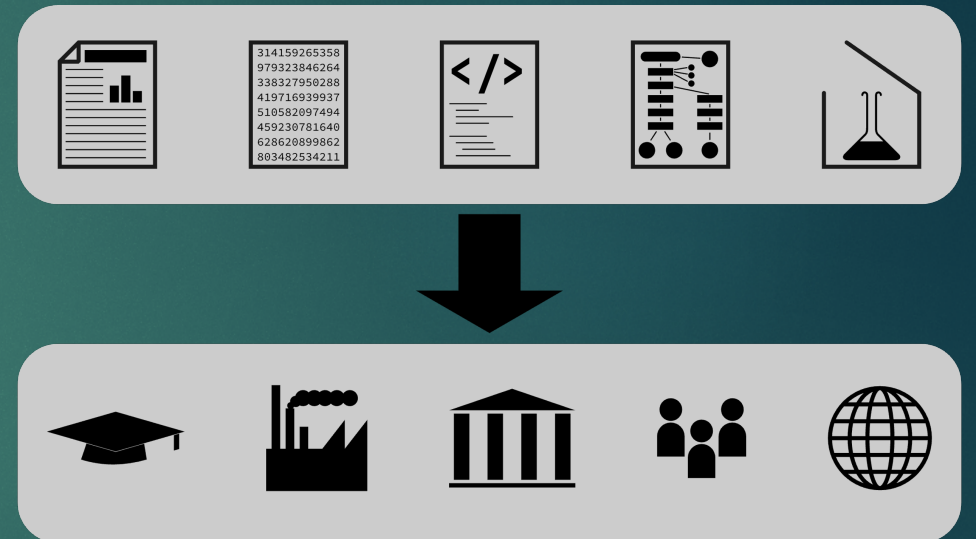
- New data + same analysis → same results

- ▶ Robustness:

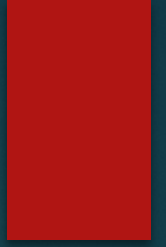
- Same data + new analysis → same results

Open science

- ▶ The movement to make all research accessible to all levels of society.
- ▶ Including, but not limited to:
 - ▶ Publications
 - ▶ Physical samples
 - ▶ Data
 - ▶ Software
- ▶ A direction to be strived in



FAIR



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Research data (and software) should be:

FAIR

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Findable

FAIR

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Findable



Accessible

FAIR

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- ▶ Findable
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- ▶ Interoperable

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Independently of whether the data are open

Motivations

Nullius in verba



THE ROYAL SOCIETY'S HOUSE IN CRANE COURT (see page 104).

Public money \Rightarrow Public results



Our funders are requiring it!



Science and
Technology
Facilities Council

Policy

STFC scientific data policy

Policy providing guidance on data management to the staff and communities of the Science and Technology Facilities Council (STFC)

From: STFC
Published: 1 April 2016

Data resulting from publicly funded research should be made publicly available... unless there are specific reasons (e.g. legislation, ethical, privacy and security) why this should not happen

Introductions

Who am I?

- ▶ Associate Research Scientist at The Cyprus Institute
- ▶ Background in Lattice Gauge Theories
- ▶ Strong interest and involvement in European Commission projects on Open Science and the European Open Science Cloud (EOSC)



More to be done for Open Science!

- ▶ LGT community has launched sharing data
 - ILDG (2002)
- ▶ However, OS has evolved little since then
- ▶ Funding Agencies are imposing OS
 - in Horizon Europe, OS is "modus operandi"
- ▶ LGT community is falling behind
- ▶ Need to catch up...
- ▶ Harmonize with bigger initiatives (EOSC)



Do we need Initiatives?



- ▶ Open Science initiative in LGT?
 - Identifying the needs
 - Creation of tools for RDM
 - Semantic advancements
 - Metadata schemas?
 - Ontological schemas?
 - Use Cases
 - Training agenda
- ▶ Begin with something of a smaller scale
 - Support capacity building
 - Support ILDG?



INFRA-EOSC calls?



www.oscars-project.eu

Who am I?

- ▶ Professor for theoretical physics at University of Bonn
- ▶ Background in Lattice QCD and algorithms
- ▶ ILDG data sharer for 15 years
- ▶ Practical interest in research data management



ILDG is our Asset

- ▶ Lattice community was way ahead of its time
- ▶ First of all, ILDG enables collaborations
 - Within the community
 - Within collaborations
- ▶ In addition,
 - Supports good scientific practice (reproducibility, etc...)
 - Helps with funding agencies

ILDG is our Asset

- ▶ We should try to maintain and develop it further!
 - And we made big progress recently!
- ▶ While keeping in mind
 - Our needs and requirements
 - Open science shouldn't end in itself
- ▶ But it requires a community wide effort!
- ▶ Should build on new national funding schemes for RDM, like PUNCH4NFDI in Germany



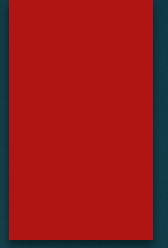
⟨NUMERIQS⟩

Anna Hasenfratz

- ▶ Professor of physics at University of Colorado Boulder, USA
- ▶ Background in lattice QFT: QCD, BSM, new phases (SMG); improved actions, RG on lattice
- ▶ Interested in research data management and sharing



Goal of data sharing:



- ❖ Validate numerical predictions
 - Investigate unconventional systems:
 - Conformal or exotic phases – UV and IR fixed points
 - Emerging UVFP ? Symmetric Mass Generation
 - Calculate "unconventional" quantities:
 - Order parameter of exotic phases
 - Scaling dimensions, RG beta function, hyperscaling, etc
- ❖ When controversies arise, subject all data from different groups to the same analysis
- ❖ Share data, share analysis code ?

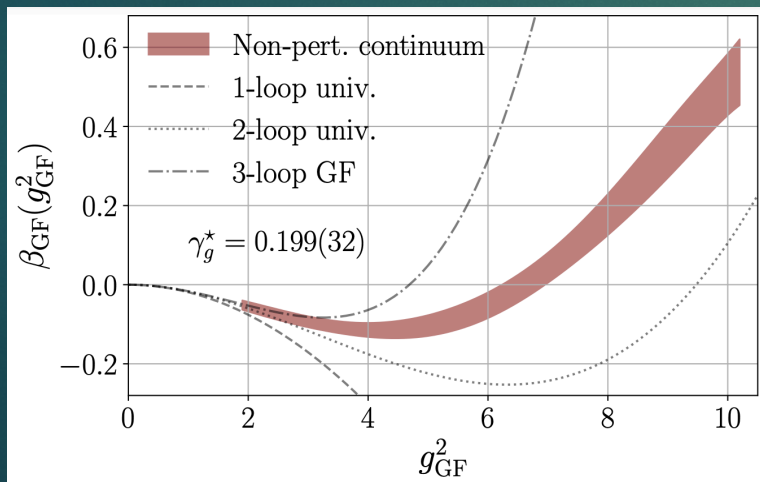
How much do we share?

How much effort is required from both parties?

Example:

AH, Peterson, PRD 109 (2024) 11, 114507
12-flavor beta function
Data uploaded to Zenodo

Re-analyzed and validated by Bennett et al
(poster Lattice 2024)



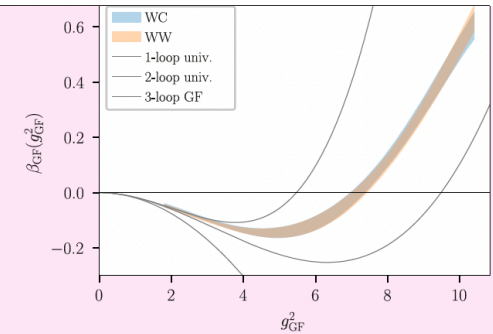
Towards the β function of $SU(2)$ with adjoint matter using Pauli-Villars fields

Ed Bennett, Andreas Athenodorou, Georg Bergner, Pietro Butti, Biagio Lucini

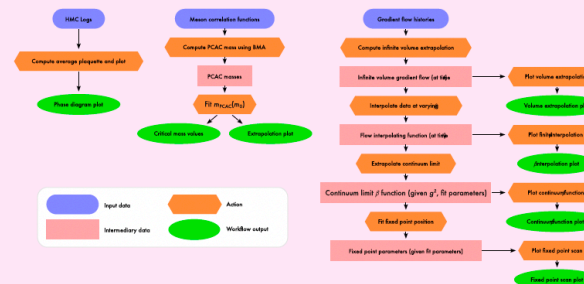
Analysis workflow

The data analysis pipeline is written using Snakemake, connecting individual tools each making use of pyerrors. This allows simple rules (e.g. how to transform one or more input data files to an output containing one or more statistical quantities) to be easily composed, independent steps to be parallelised, and redundant computations to be skipped.

To generate every plot on this poster, excluding the one in this box, starting from the raw output files transferred from HPC, requires a single command (twice: once per N_f), which launches 344 + 81 job steps taking 3 minutes on a 6-core laptop. All required packages are installed automatically; no setup is required beyond installing Snakemake.

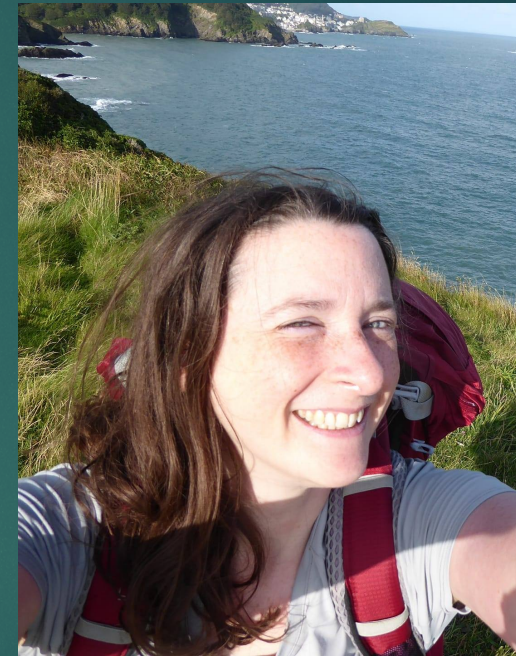


This workflow was tested by adapting it to work with the open data released by Hasenfratz and Peterson [4]. This reproduces their finding of a conformal fixed point in the beta function of the $SU(3)$ theory with 12 fundamental Dirac flavours.. Reproducing every figure of the corresponding paper deriving from the released data requires a single command, which launches 4227 job steps taking 19 minutes on a 6-core laptop.



Louise Chisholm

- ▶ Joint Director UK Square Kilometer Array (SKA) Regional Centre
- ▶ Background: Professional Research & Strategy Manager, launched and led UCL-wide eResearch Community, PhD in Epigenetics
- ▶ Interested in developing digital research infrastructure ecosystems, FAIR Data sharing communities



Square Kilometre Array: next-generation radio astronomy facility



- ▶ Developing an end-to-end system from telescope time proposal to science delivery
- ▶ Enabling FAIR data sharing: metadata standards, data sharing policies, proprietary periods

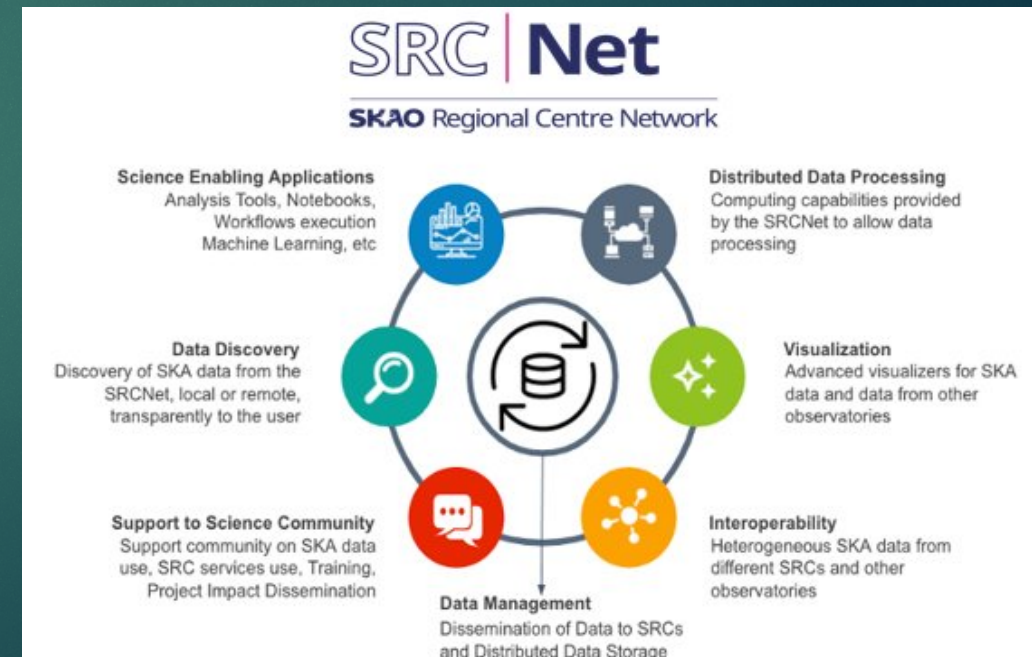


SKA-Mid



SKA-Low

17.01.2024

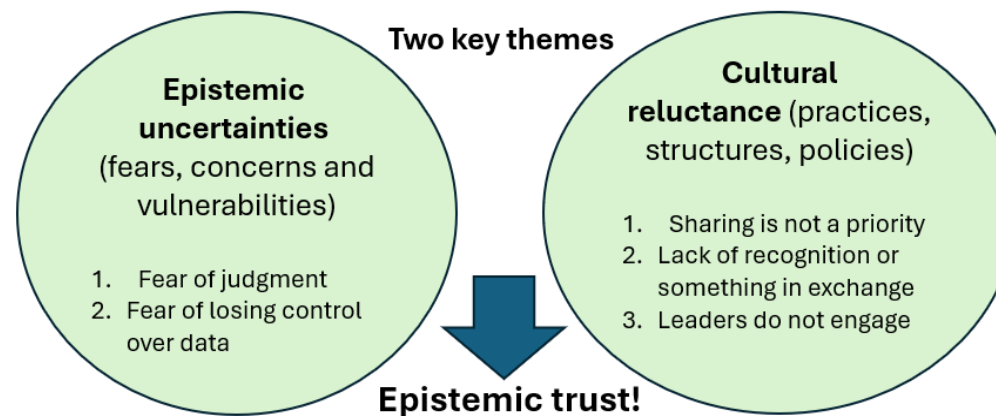


Challenges & opportunities

- ▶ Learning across disciplines
- ▶ Approach to proposing and undertaking research
- ▶ Team Science
 - New professions
- ▶ Funding mechanisms
 - Harness data resources
 - Infrastructure
 - People

FAIR Data Accelerator

Ethnography Study identified social and cultural barriers to implementing the FAIR principles



Identity Negotiation and Professional Development in the Context of the Digital Transformation of Research Communities

Duran del Fierro et al. <https://doi.org/10.5281/zenodo.12806507>

Q&A