NEUTRON SCIENCE
Sustainability in ErUM-Data

July 30th, 2025 | Stefan Häusler | JCNS

Challenges for Neutron Science

- Only one neutron source in Germany (FRM II in Garching)
- Overbooking factor for instruments up to 8
- Continuous operation, 240 days per year (4 reactor cycles), 24/7 (restart 2026)
- We should not sacrifice reliability or limit the number of experiments.

Sustainability challenges

Digital infrastructure

- Software technologies
- Research data management

Technical infrastructure

- Energy efficiency
- Memory / storage consumption
- Method optimization

Software development

Sustainable development

- Professionally developed, well documented
- Open-source, flexible, easily extendable
- Maintained on facility level
- Deployed as a cloud solution

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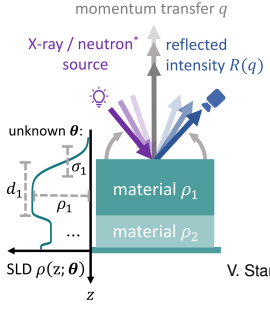
Sustainability through shared use

- Grazing incidence small- and wide-angle scattering with neutrons and x-rays
- Neutron/x-ray reflectivity
- Ptychography, spectroscopy and particle physics

Software development

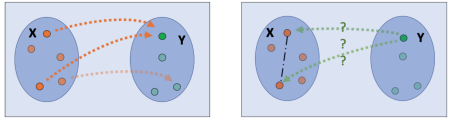
Versatile Inverse Problem fRamework (VIPR), BMBF project, 2023–2026

Data-driven solutions for inverse problems integrated at JCNS data pipelines (MLZ).

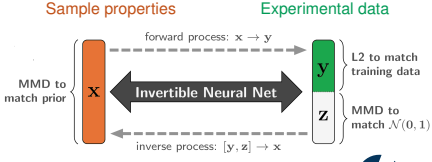


V. Starostin et al. (2024)

Ill-posed inverse problems are key to x-ray/neutron scattering



Invertible Neural Network (INN)



Efficienct use of neutron beam time

Perform more experiments in the same amount of time.

AI-assisted Data Analysis

- **Real-time adjustment:** Statistics and instrument setting (q-range)
- **Real-time inference:** Recommendation system for SANS, VIPR, GISAXS data, ...

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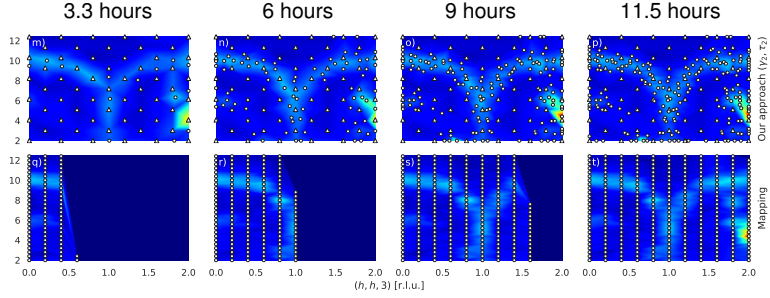
AI-assisted Data Acquisition

Active learning-assisted neutron spectroscopy (ARIANE) M. Teixeira Parente, et. al. Nat. Commun. (2023)



Research data management

Adhere to **FAIR** principles

- **F**indable, **A**ccesible, **I**nteroperable, **R**eusable
- Metadata capture and experiment documentation
- Standardized data formats
- Implementation of metadata catalogues
- Development of a **D**ata **A**nalysis **a**s **a** **S**ervice platform

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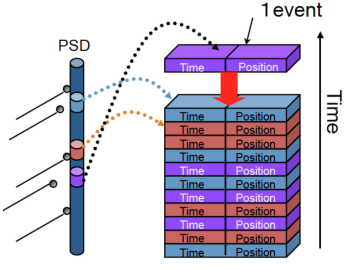
Technical infrastructure

Edge computing	vs.	Federated infrastructures
Servers at MLZ	vs.	JSC, Helmholtz HIFIS
Reduced data transfer		Collaborative research

Filtering event data in real time:

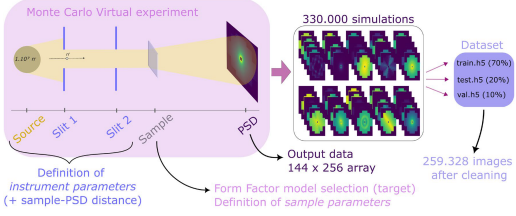


- Individual neutron events must be processed in real time, as the resulting data rates cannot be stored.
- Location and time of each event are recorded.
- Must be running during the experiment
- Must be available 24/7

Model complexity optimization

Small, specialised models that consume few resources.

Recommendation system for SANS beamline KWS-1 at FRM-II (edge computing).



Fast and efficient training on small datasets for reliable predictions.

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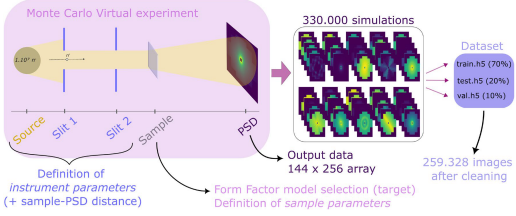

J. Robledo et. al., 2024

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Large, universally applicable models

- **Applicable across scenarios:** Foundation models (HFMI, ELLIPSE)
- **Applicable across instruments:** Reduction of instument specific effects.

Thank you for your attention!