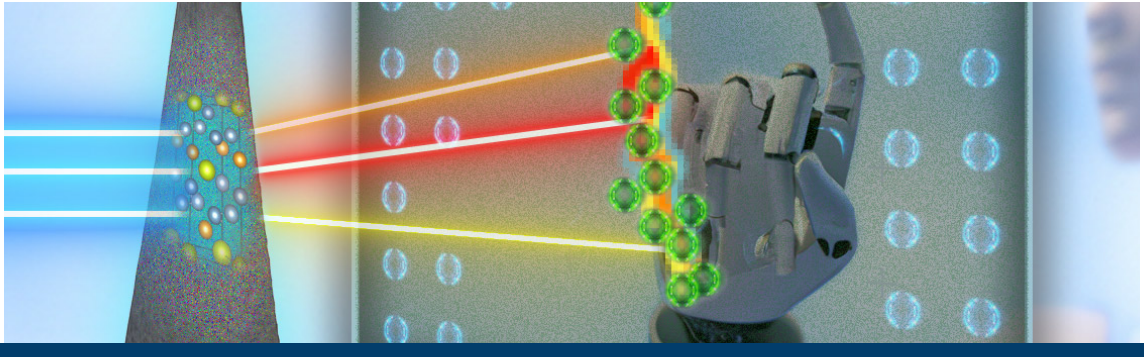


AI ACTIVITIES AT JCNS

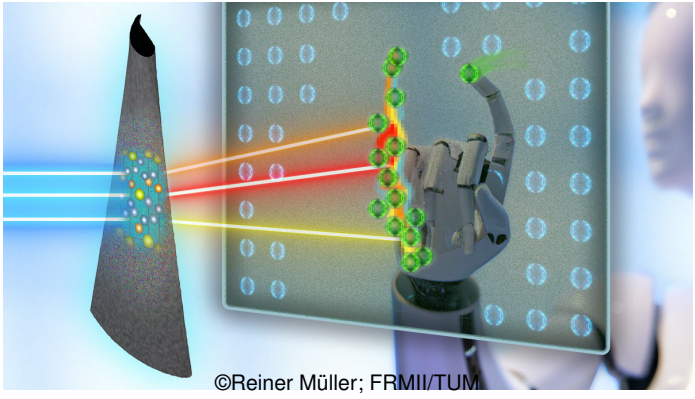
October 8th, 2026 | Ahmad Z. Ihsan, Stefan Häusler, Marina Ganeva | JCNS

Active-learning-assisted experiment steering

Article: *Nat. Commun.* **14**, 2246. doi: `10.1038/s41467-023-37418-8`

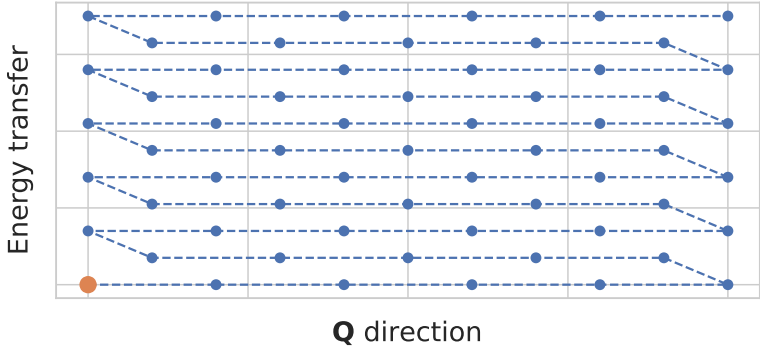
Software: `jugit.fz-juelich.de/ainx/ariane`

Documentation: `ariane.readthedocs.io`



Data requirements: Initialization

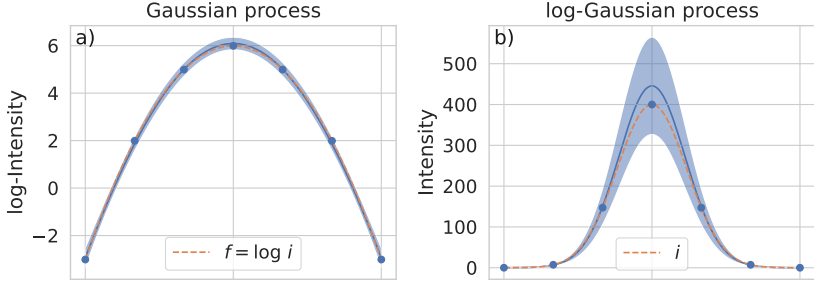
- Our approach is initialized with a sparse grid of measurement points.



- **Note:** Counting times stay constant throughout the whole experiment.

Log-Gaussian processes

- Since intensity functions i are non-negative, we regard log-Gaussian processes.
- Therefore, we fit a GP to **logarithmic** intensities and exponentiate.

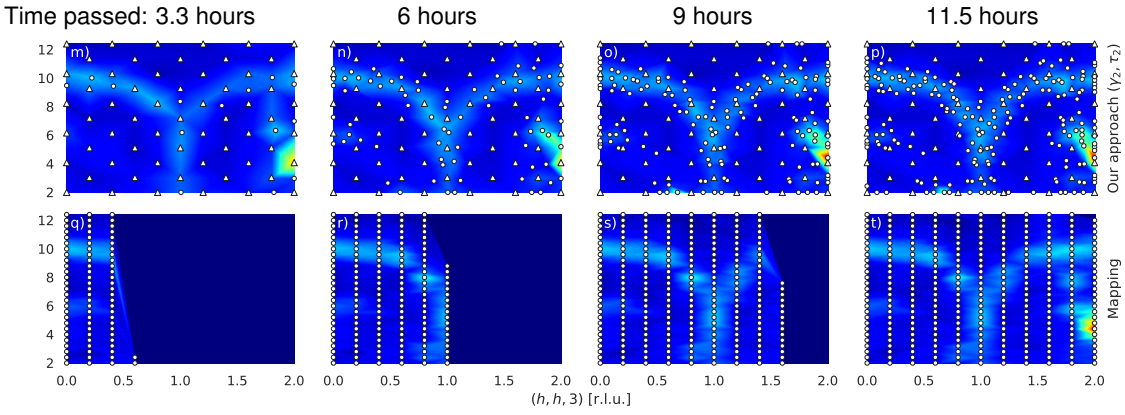


- The posterior log-GP has large uncertainties in regions of signal.

Next measurement point defined by location of maximum uncertainty

Autonomous neutron spectroscopy in action

Experiment at EIGER at PSI



See *Nat. Commun.* **14**, 2246. doi: 10.1038/s41467-023-37418-8 for more information

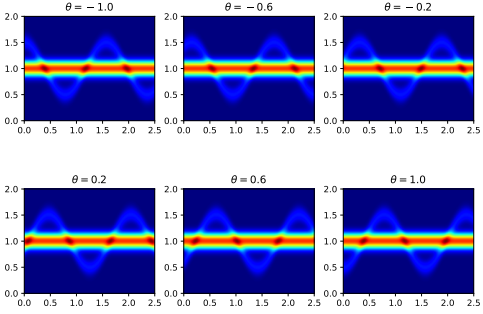
Approach summary

- Universal approach for cases where each additional measurement point is expensive
- Probabilistic: uncertainty is considered
- Does not require a lot of training data: sparse initialization grid is sufficient to start
- Active learning: learns from each measured point
- Physics-agnostic: does not require a theoretical model
- Limitation: not suitable for high-dimensional problems

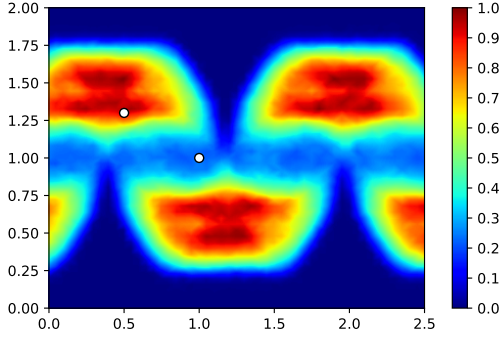
Possible extension: physics-aware approach

Proof-of-concept by Simon Keil

Toy intensity function $f(d_1, d_2, \theta)$



Expected information gain (EIG)

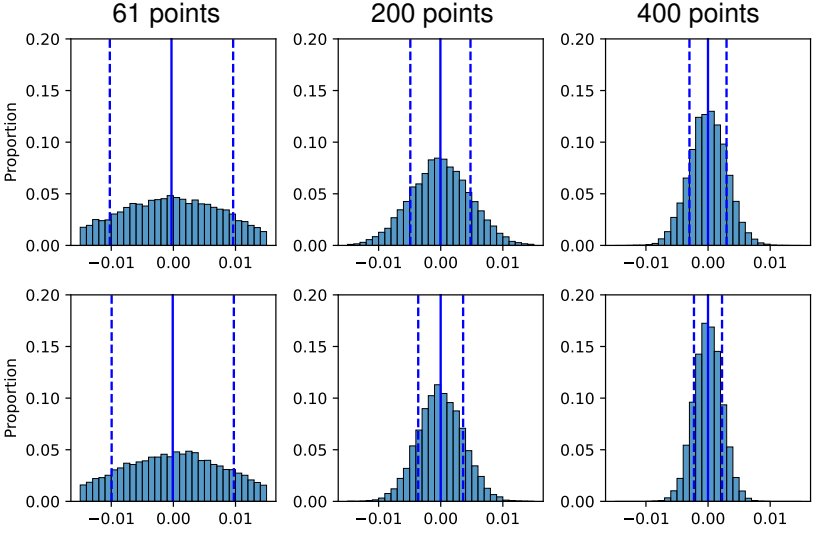


Objective function is weighted by EIG

JÜLICH Forschungszentrum

Possible extension: physics-aware approach

Proof-of-concept by Simon Keil: parameter estimation results

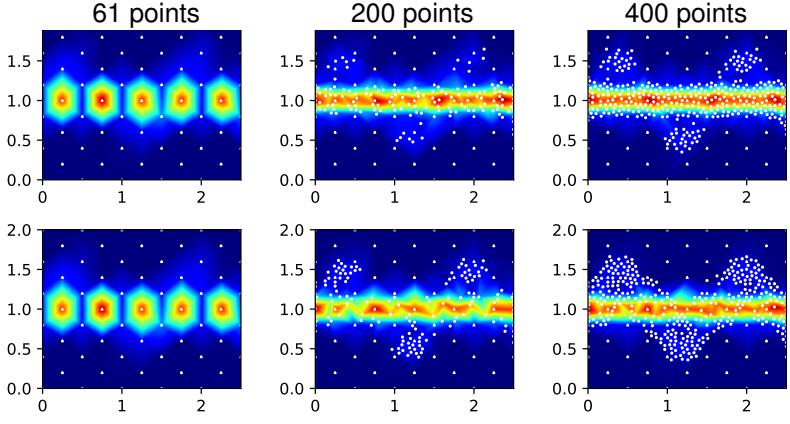


ARIANE
physics-agnostic

ARIANE with EIG
approach

Possible extension: physics-aware approach

Proof-of-concept by Simon Keil: placement of measurement points



Physics-informed approach places points in a different way

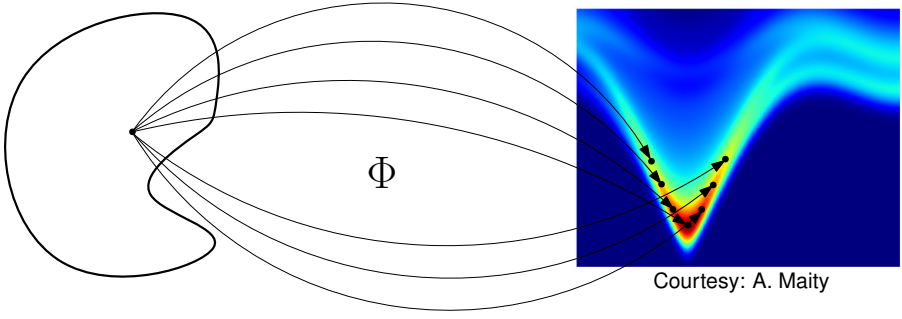
Possible extension: multi-detector option

Parameter space

$\mathcal{P} \subseteq \mathbf{R}^d$

$\mathbf{Q}$-E space

$\mathcal{X} \subseteq \mathbf{R}^n$



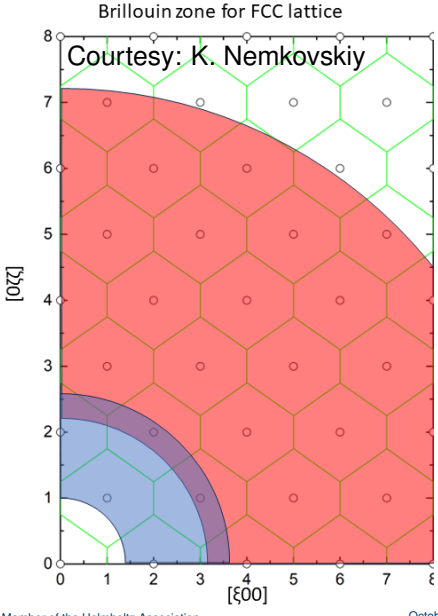
Courtesy: A. Maity

$$\Phi : \mathcal{P} \to \mathcal{X}^m$$

Optimize in $\mathcal{P}$ for multiple points instead of in $\mathcal{X}$ for a single point.

JÜLICH Forschungszentrum

Possible further developments



Thermal TAS: new challenges for the algorithm

- Choice of the Brillouin zone: best signal-to-noise ratio for a desired (magnetic/phonon) signal.
- Identify “Spurions”— may have a high signal, but no scientific information.

Further challenges:

- Automated adjustment of counting time.

Adjustment for other techniques

- TOF experiments / data analysis
- SANS, reflectivity, etc
- Sample environment: temperature, magnetic field

Jülich Neutron AI Agent (JüNA)

Ahmad Z. Ihsan

- JCNS has built a **vast collection** of scientific knowledge, instrument manuals, software, and experiment metadata.
- These resources are distributed across documents, databases, and specialized applications.
- Effectively **accessing and using** them remains challenging.

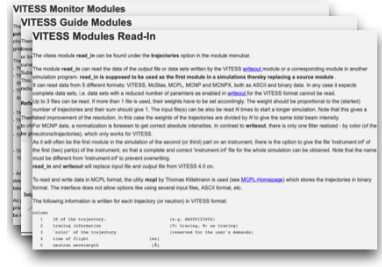
JüNA makes these resources available through task-oriented AI agents.



Knowledge Agent

- Neutron-science and experimentation knowledge
- Instrument and scientific-software manuals
- Experiment and radiation-safety handbooks
- Internal and administrative documents

From scattered documents to traceable, contextual answers.









Experiment Agent

- Helps scientists plan neutron experiments
- Captures sample and measurement metadata
- Configures and runs neutron simulations
- Connects conversational assistance to laboratory tools

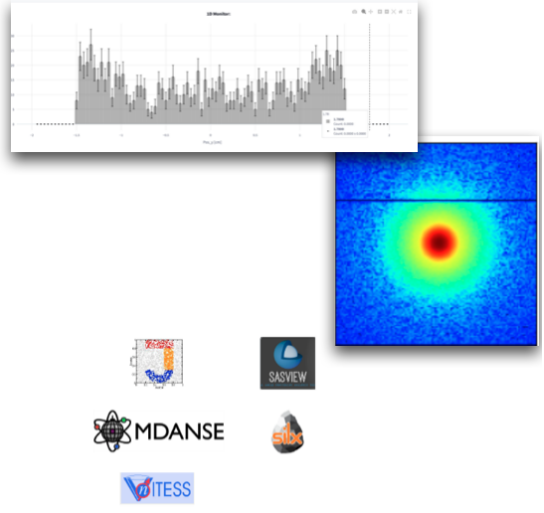
Current directions: user-interface agents and an Electronic Lab Notebook agent.



Data Agent

- Assists scientists in processing and analyzing neutron experiment data
- Connects data workflows to indexed neutron-science software repositories
- Provides repository-aware Q&A, code search, and multi-step analysis

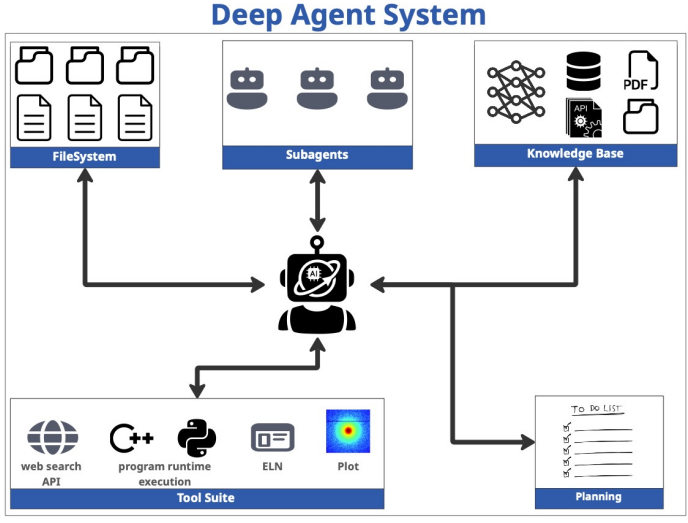
One implementation is the JüNA Code Chat agent.



JüNA Core: The Agentic Foundation

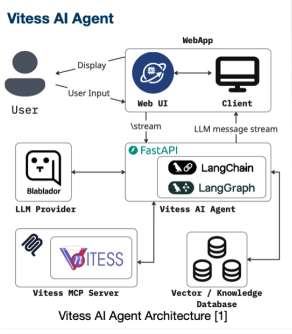
- Provides the shared agentic foundation for JüNA applications
- Manages context, tools, memory, and intermediate results
- Coordinates specialized subagents, knowledge retrieval, planning, and execution

One core, multiple neutron-science assistants.

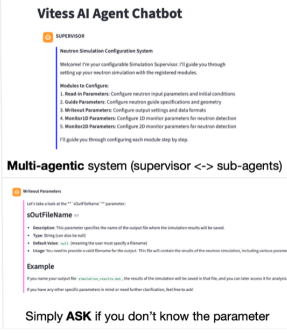


Use Case: VITESS AI Agent

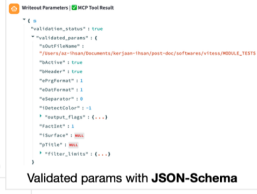
Nicolo Violini and Suparna Das



Vitess AI Agent Architecture [1]



Multi-agentic system (supervisor <-> sub-agents)

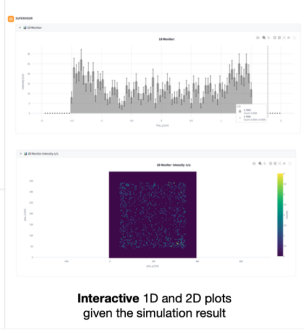


Validated params with **JSON-Schema**

Simply **ASK** if you don't know the parameter



Intelligent simulation execution



Interactive 1D and 2D plots given the simulation result

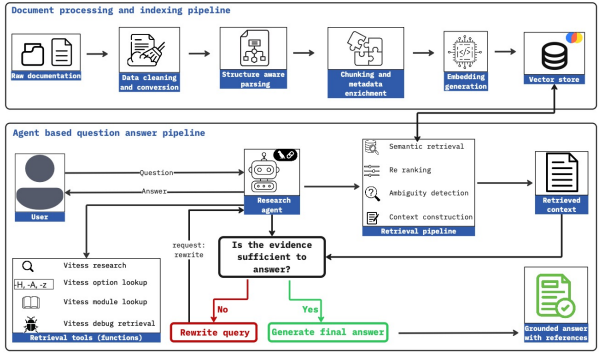
Natural-language guidance from simulation setup to validated execution and interactive results.

JÜLICH Forschungszentrum

VITESS-RAG: Grounded Manual Answers

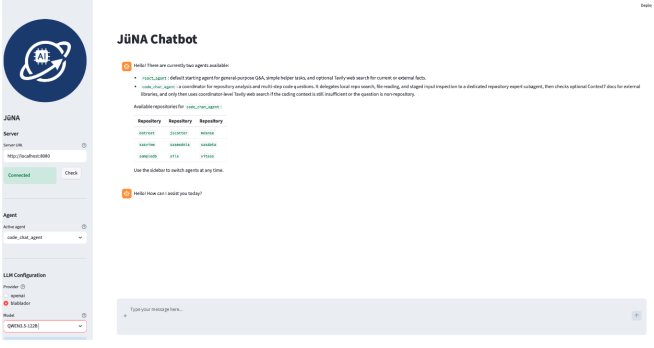
Suparna Das

- **Prepare the manual:** clean, structure-aware parsing, chunking, metadata enrichment, and embedding.
- **Answer questions:** tool-assisted retrieval, evidence checking, query rewriting when needed, and answers with references.



Use Case: JüNA Code Chat

GitHub: `github.com/neutron-simlab/juena-chatbot`



Agentic code assistant

- Indexed neutron-science and experiment-software repositories
- Repository-aware Q&A, code search, and multi-step analysis
- Simulation, data-reduction, and analysis workflows

Community software

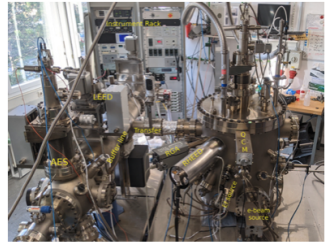
Outlook: JüNA ELN Agent

For NMR and OMBE labs











Conversational access to sample, measurement, and laboratory information.

AI for data analysis

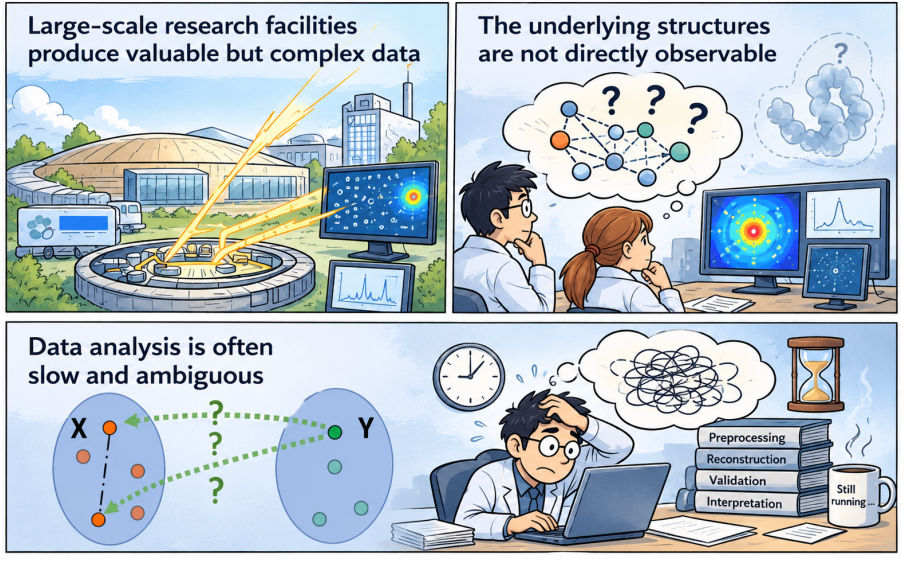


Image generated by ChatGPT

JÜLICH Forschungszentrum

Challenges of AI-assisted data analysis

Data challenges

- Not enough **annotated** experimental data
- Simulated data come from different distribution
- X-ray and neutron data come from different distributions

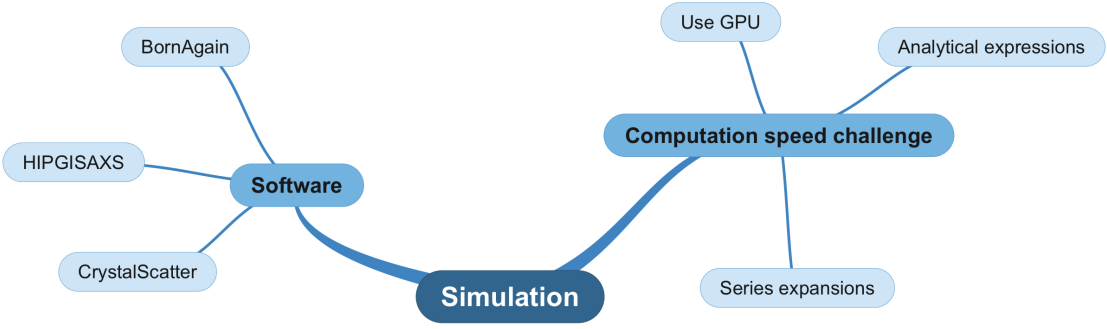
Training challenges

- Choice of loss/objective function, minimizer, NN architecture
- Overfitting/underfitting, exploding/vanishing gradients,...

Evaluation challenges

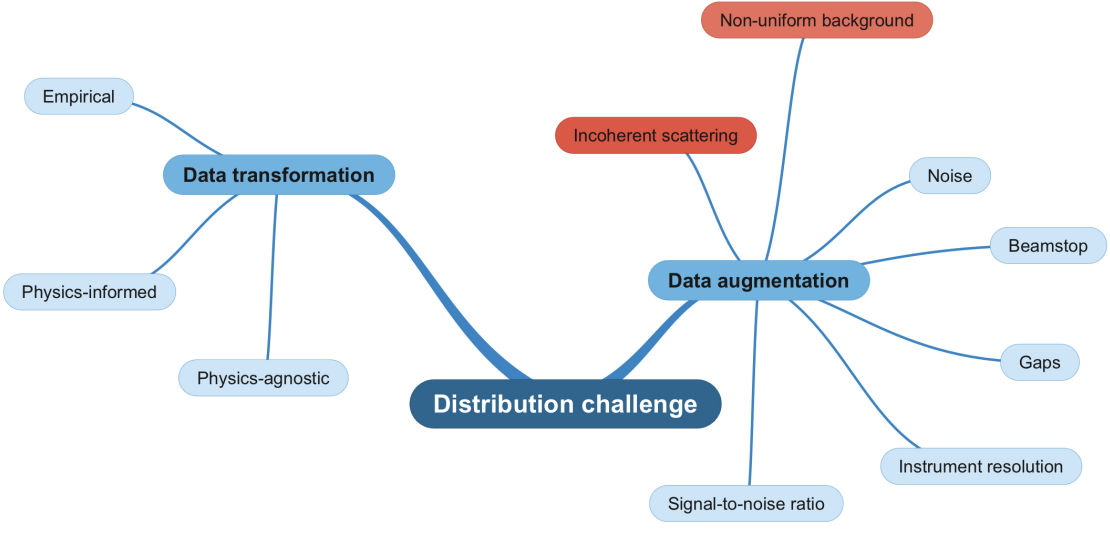
- How much can we trust the prediction made by NN?
- Ill-posed inverse problem $\Rightarrow$ multiple solutions
- Uncertainty evaluation (both, aleatoric and epistemic)

Addressing data challenges: simulation



- ! Simulation speed is affected by multiple numerical integrations
- ! Theoretical formalisms have limitations

Addressing data challenges: distribution

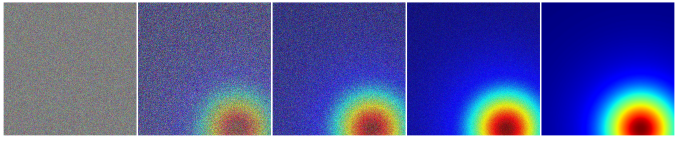


AI solutions for instrument-specific denoising



Siddhartha Nathan

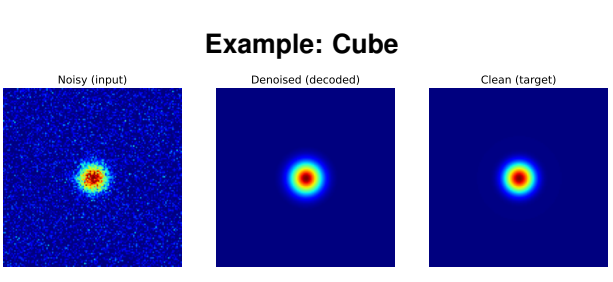
Noisy images, instrument settings provided

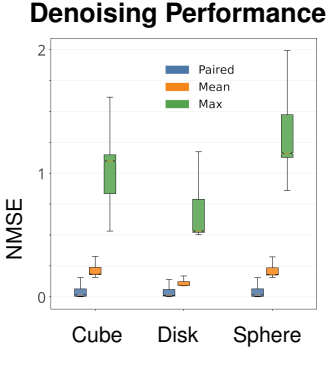


- Model implicitly learns noise-removal mapping
- Potential generalization to different instrument settings
- The goal is to improve the performance of AI when applied downstream

Application to SANS

Synthetic datasets



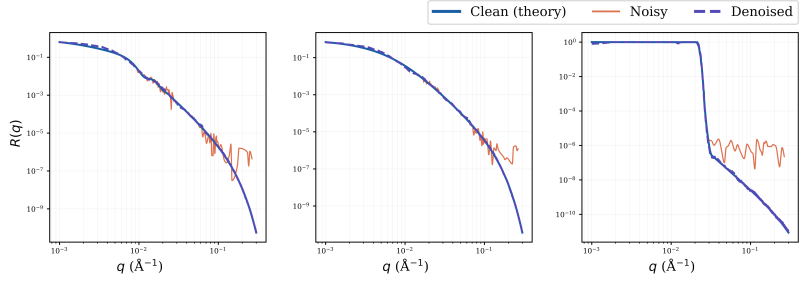


Use case: Analysis of synthetic data generated with the KWS-1 digital twin

Contact: Artem Feoktystov

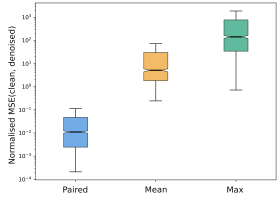
Application to neutron reflectometry

Synthetic datasets



Use case: Analysis of synthetic data generated with the MARIA digital twin

Contact: Alexandros Koutsioumpas



Versatile Inverse Problem Framework

Presently deployed at MARIA reflectometer



Dr. Marina Ganeva
VIPR-Projektkoordination
S. Häusler, M. Levytskyi



Prof. Dr. Christian Gutt
O. Öztürk, F. Unger



Dr. Jeffrey Kelling
R. Aguilar, V. Pandit,
J. Rustamov



Dr. Jens Bornschein
S. Creutzburg, B. Helm,
N. Mothes



Prof. Dr.
Stephan V. Roth
O.E. Asirim, Y. Zhai



Prof. Dr.
Peter
Müller-Buschbaum
J.E. Heger



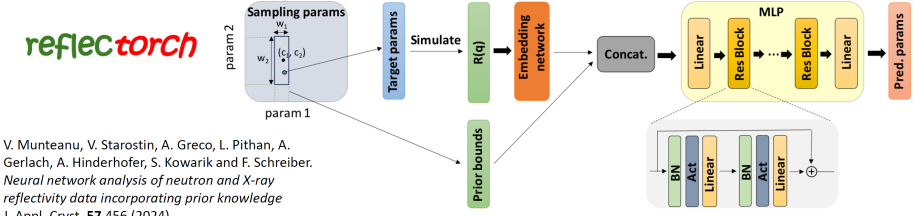
Prof. Dr. Frank Schreiber
A. Gerlach, A. Hinderhofer
V. Munteanu, V. Starostin

Associated partners:

LBL, HZB/BESSY II,
DESY/CMS, FZJ/ER-C,
Rostock University

AI for neutron reflectivity

Current implementations



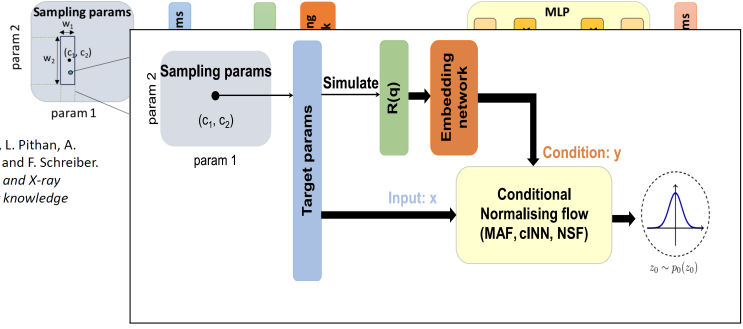
V. Munteanu, V. Starostin, A. Greco, L. Pithan, A. Gerlach, A. Hinderhofer, S. Kowarik and F. Schreiber. *Neural network analysis of neutron and X-ray reflectivity data incorporating prior knowledge* J. Appl. Cryst. **57** 456 (2024)

- Rapid, AI-driven generation of single and multiple candidate solutions
- Downstream parameter optimization via conventional iterative fitting
- Direct integration of physical domain knowledge via parameter prior distributions

AI for neutron reflectivity

Current implementations

reflectorch



V. Munteanu, V. Starostin, A. Greco, L. Pithan, A. Gerlach, A. Hinderhofer, S. Kowarik and F. Schreiber. *Neural network analysis of neutron and X-ray reflectivity data incorporating prior knowledge* J. Appl. Cryst. **57** 456 (2024)

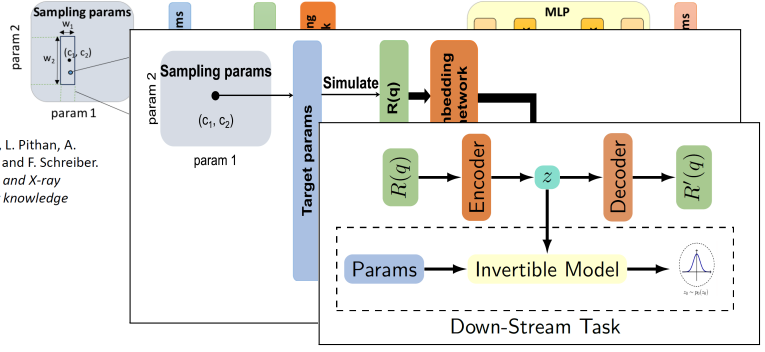
- Rapid, AI-driven generation of single and multiple candidate solutions
- Downstream parameter optimization via conventional iterative fitting
- Direct integration of physical domain knowledge via parameter prior distributions

AI for neutron reflectivity

Current implementations

reflectorch

V. Munteanu, V. Starostin, A. Greco, L. Pithan, A. Gerlach, A. Hinderhofer, S. Kowarik and F. Schreiber. *Neural network analysis of neutron and X-ray reflectivity data incorporating prior knowledge* J. Appl. Cryst. **57** 456 (2024)



- Rapid, AI-driven generation of single and multiple candidate solutions
- Downstream parameter optimization via conventional iterative fitting
- Direct integration of physical domain knowledge via parameter prior distributions

VIPR user interface

Developed by Helm & Walter IT-solutions GmbH

Command Line Interface (VIPR Core)

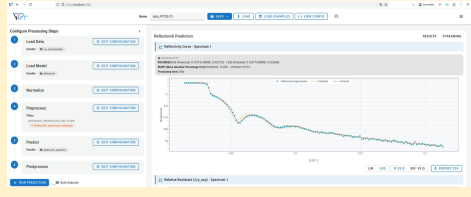
- Configuration via YAML files
- Run from terminal

  `vipr --config config.yaml inference run`
- For automated workflows & scripting



Web Application

- Browser-based interface
- Configuration via GUI
- Parameter testing & visualization
- Uses VIPR Core under the hood



codebase

AI solutions for SANS pattern classification

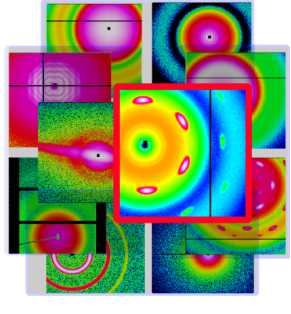
S. Häusler, S. Förster, M. Wagener, M. Ganeva

Nano structures



?

SANS patterns

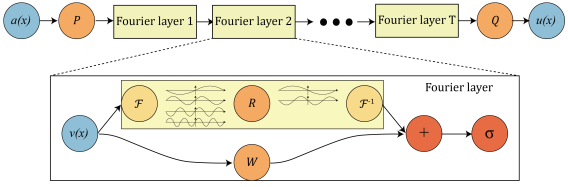


JÜLICH Forschungszentrum

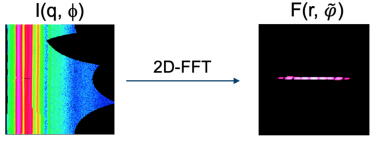
Fast and data-efficient pattern classification

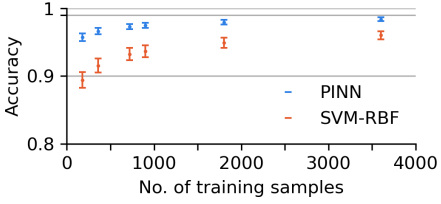
S. Häusler, S. Förster, M. Wagener, M. Ganeva

Physics-informed AI models and input representations:
(FFT + analytic form-factor constraints like Guinier, power-law, Lorentzian, Bessel, . . .)



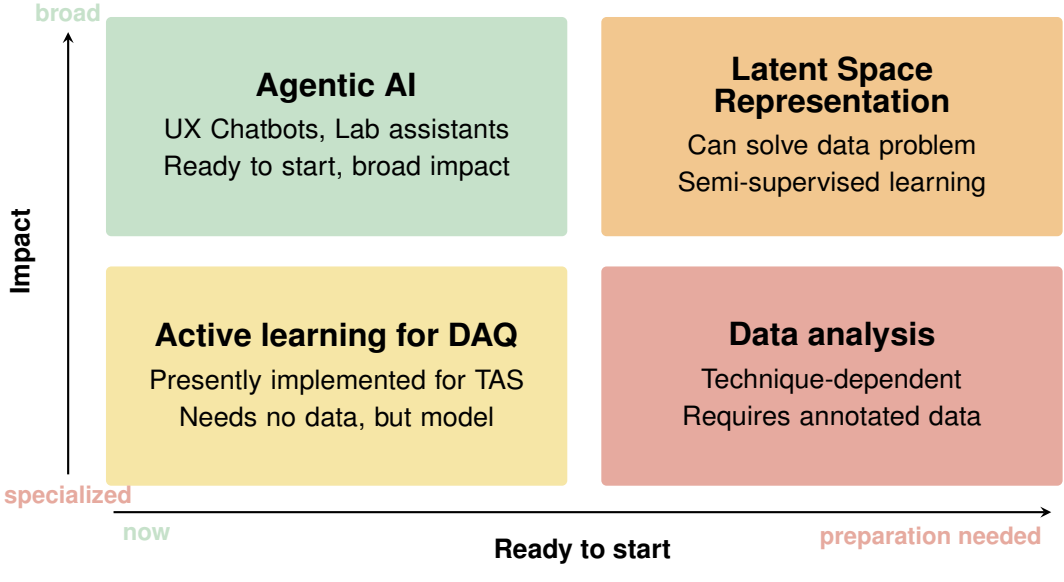
Fourier neural operators (FNOs), Li et al, ICLR (2021)





Use case: Fast, data-efficient predictions
on-the-fly adaptation to experimental settings.

Project candidates for the roadmap



Thank you for your attention!