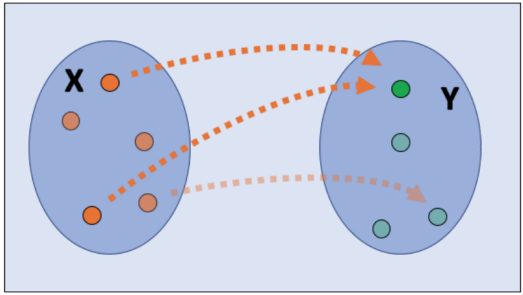
VERSATILE INVERSE PROBLEM FRAMEWORK

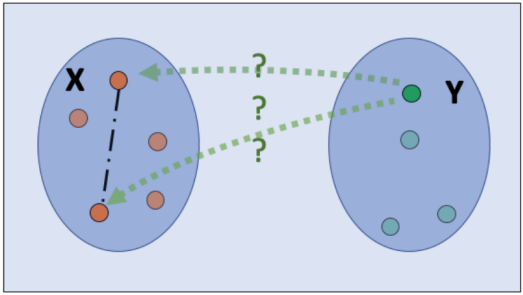
February 6, 2025 | Marina Ganeva | JCNS

Project partners

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

Motivation: ill-posed inverse problem



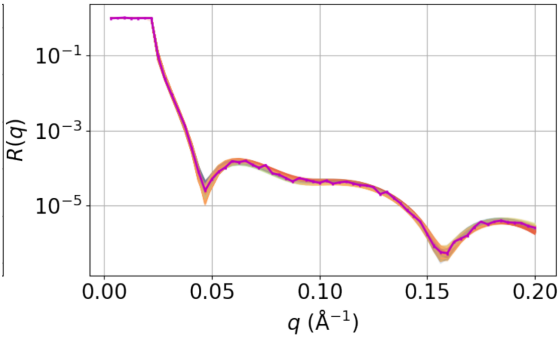


- typical in analysis of x-ray/neutron scattering data
- phase information is lost
- no unique solution

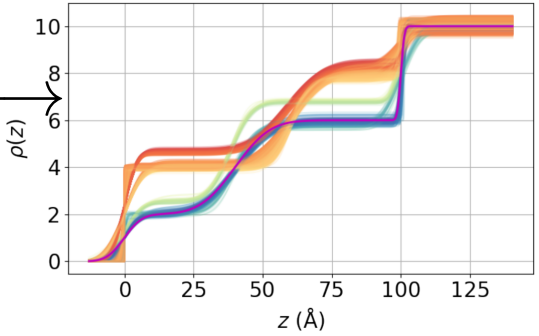
Motivation: use cases

Neutron reflectometry

Experimental curve



Sampled SLD profiles



Starostin et. al., in preparation

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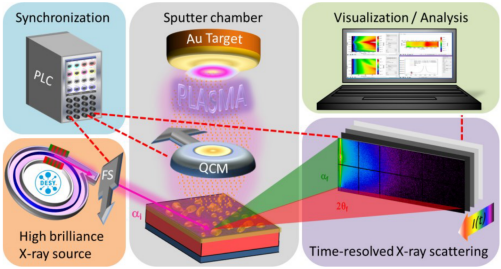
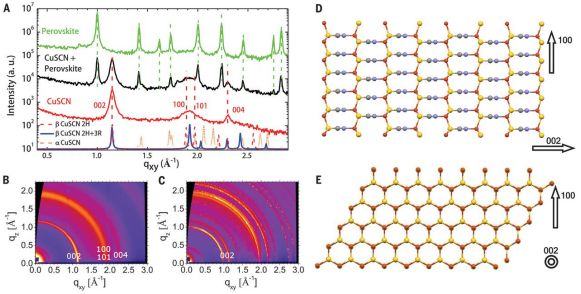
Motivation: use cases

GISAS



M. Schwartzkopf, et. al., Nanoscale Horizons 6, 132 (2021)

GIWAXS



Arora et al. Science 358 (2017) 768

- Investigation of materials properties on nanoscale
- Complex, time-consuming data analysis
- High data rates

Project goal

Develop a software framework for data-driven solution of inverse problems using INNs

Software framework requirements:

- open-source, flexible, easily extendable
- professionally developed, well documented
- maintained on facility level
- deployed as a cloud solution

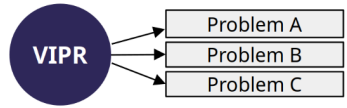
Application areas include, but not limited to:

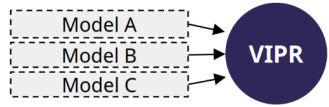
- grazing incidence small- and wide-angle scattering with both neutrons and x-rays
- neutron/x-ray reflectivity
- ptychography

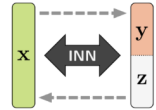
Development will also take into account requirements from spectroscopy and particle physics

VIPR Challenges

- VIPR: versatile inverse problem software framework
- → Development of a flexible software framework for data-driven solutions to inverse problems
- **Interchangeability**
  → Data sources
  → Preprocessing/postprocessing methods
  → Models
- Integration of (conditional) invertible neural networks







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Industrial partner

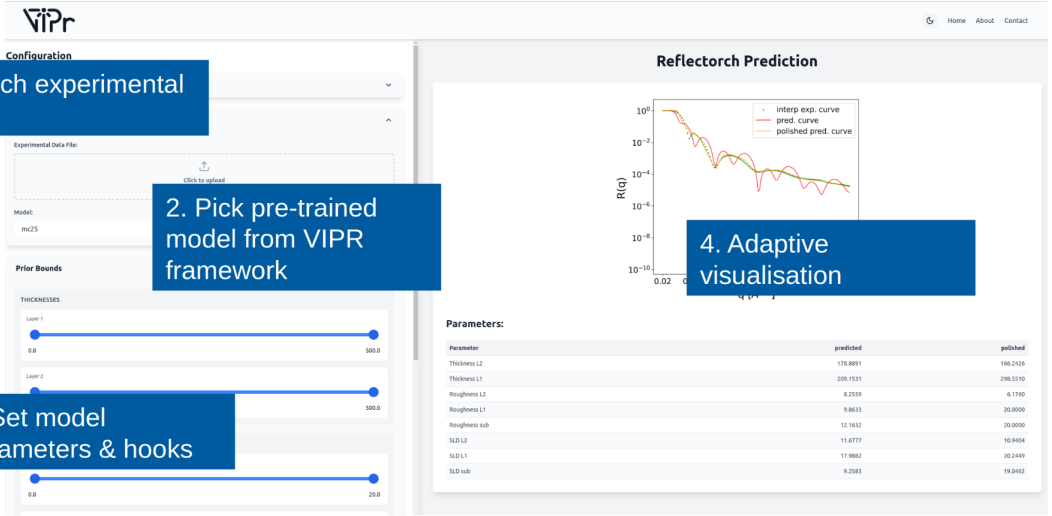
SAXONY.ai – a brand of Helm & Walter IT-Solutions GbR

- Helm & Walter IT-Solutions GbR was founded in Dresden in 2008.
- Agency for customized IT solutions with 19 IT specialists from Saxony

Industrial partner: team involved in VIPR

- Dr. Nico Hoffmann (ML expert)
- Dr. Jens Bornschein (computer scientist, project management)
- Dr. Sascha Creutzburg (physicist, data scientist)
- M.Sc. Anurag Trivedi (mathematician)

VIPR Deployment at partner facilities



1. Fetch experimental data

2. Pick pre-trained model from VIPR framework

3. Set model parameters & hooks

4. Adaptive visualisation

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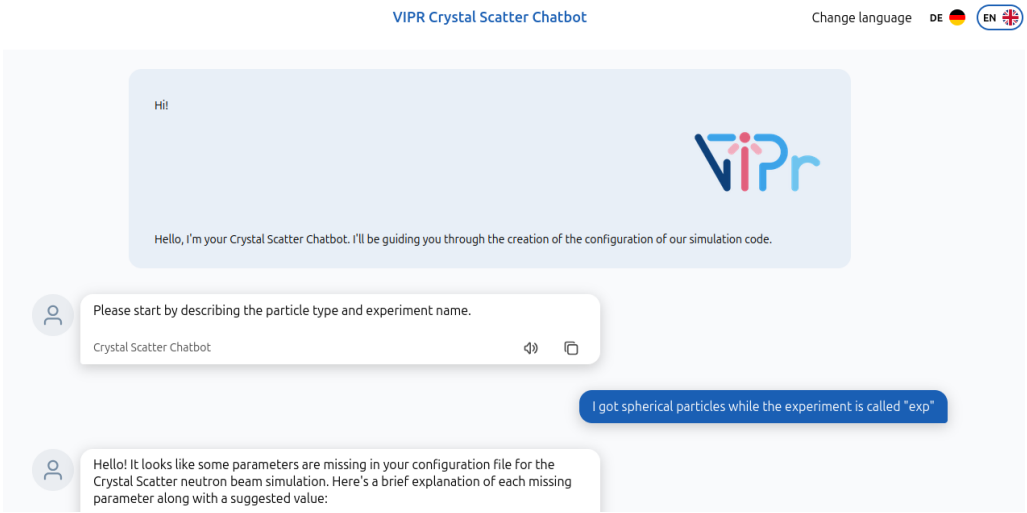
Chatbot as user interface



Technology transfer

Solution: Inference-as-a-Service — pre-trained AI models ready for immediate use

- Powered by VIPR Framework for inverse problem-solving
- Microservices architecture with Kubernetes for maximum scalability
- Standardized API for easy integration

Knowledge gained will be applied to problems in other areas.

Thank you for your attention!