



VERSATILE INVERSE PROBLEM FRAMEWORK

February 6, 2025 | Marina Ganeva | JCNS

Project partners



HELM & WALTER
IT-SOLUTIONS



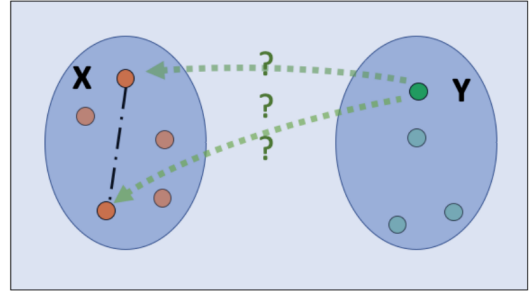
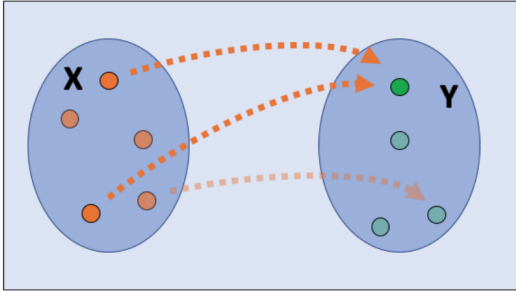
FRM II
Forschungs-Neutronenquelle
Heinz Maier-Leibnitz

EBERHARD KARLS
UNIVERSITÄT
TÜBINGEN



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

Motivation: ill-posed inverse problem

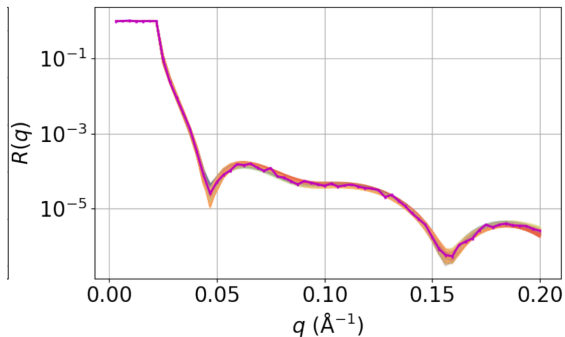


- typical in analysis of x-ray/neutron scattering data
- phase information is lost
- no unique solution

Motivation: use cases

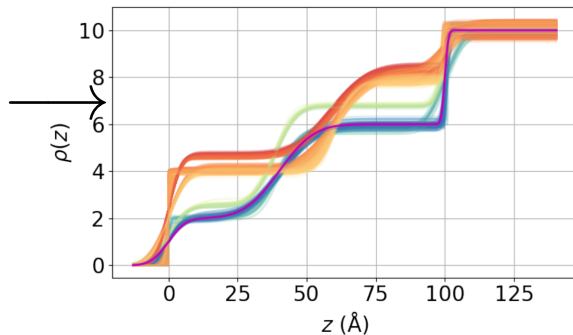
Neutron reflectometry

Experimental curve



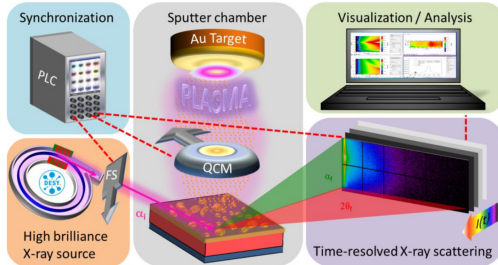
Starostin et. al., in preparation

Sampled SLD profiles



Motivation: use cases

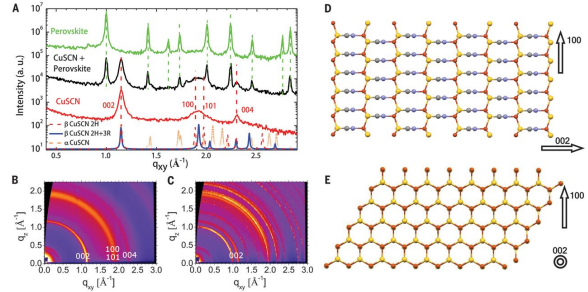
GISAS



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

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

GIWAXS



Arora et al. Science 358 (2017) 768

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

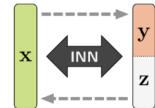
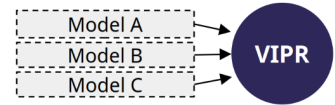
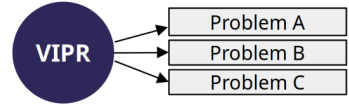
Application areas include, but not limited to:

- 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



Industrial partner

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



HELM & WALTER
IT-SOLUTIONS

- 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

Configuration

1. Fetch experimental data

Experimental Data File:

Click to upload

Model:

mc25

2. Pick pre-trained model from VIPR framework

Prior Bounds

THICKNESSES

Layer 1

0.0 500.0

Layer 2

0.0 500.0

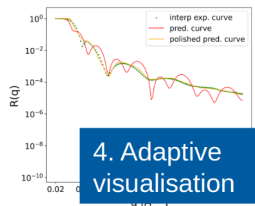
3. Set model parameters & hooks

Layer 3

0.0 20.0

Reflectorch Prediction

4. Adaptive visualisation



Parameters:

Parameter	predicted	polished
Thickness L2	178.8891	186.2426
Thickness L1	206.1531	298.5510
Roughness L2	8.2559	6.1760
Roughness L1	9.8633	20.0000
Roughness sub	12.1632	20.0000
SLD L2	11.6777	10.9404
SLD L1	17.9882	20.2449
SLD sub	9.2583	19.0462

Chatbot as user interface

VIPR Crystal Scatter Chatbot

Change language

DE 

EN 

Hi!



Hello, I'm your Crystal Scatter Chatbot. I'll be guiding you through the creation of the configuration of our simulation code.



Please start by describing the particle type and experiment name.

Crystal Scatter Chatbot



I got spherical particles while the experiment is called "exp"



Hello! It looks like some parameters are missing in your configuration file for the Crystal Scatter neutron beam simulation. Here's a brief explanation of each missing parameter along with a suggested value:

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!