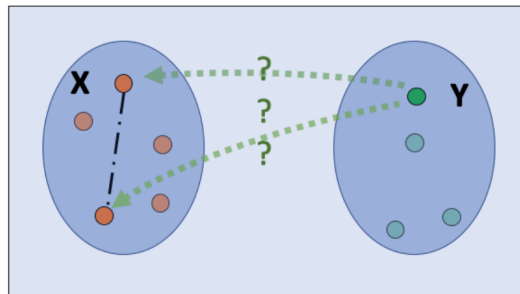
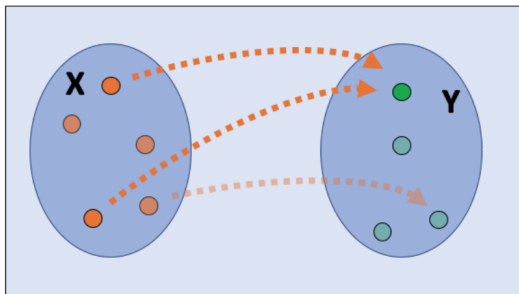




VERSATILE INVERSE PROBLEM FRAMEWORK

February 23, 2023 | Marina Ganeva | JCNS

Motivation: inverse problem

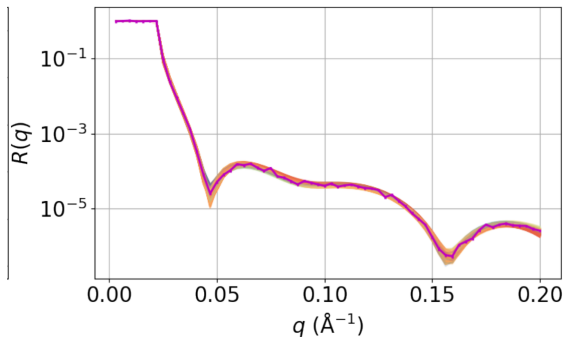


- typical in analysis of x-ray/neutron scattering data
- phase information is lost
- no unique solution

Motivation: use cases

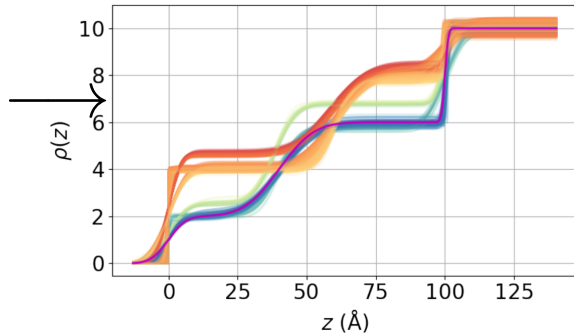
Neutron reflectometry

Experimental curve



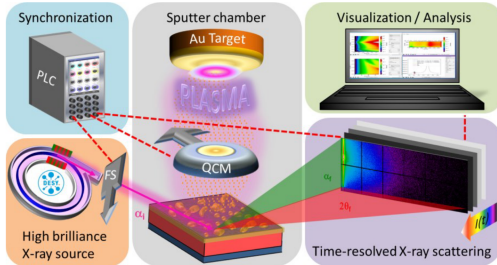
Starostin et. al., in preparation

Sampled SLD profiles



Motivation: use cases

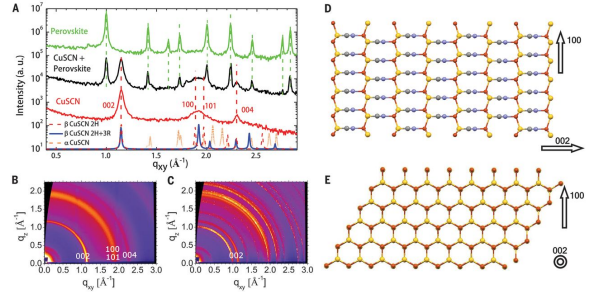
GISAS



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

Project partners

MLZ: large-scale neutron facility

**Forschungszentrum Jülich,
JCNS Neutron SimLab,
VIPR project coordination**

Expertise includes:

- neutron and x-ray scattering: experiment design, DAQ, data reduction and analysis
- HPC, MD simulations, simulation of scattering processes, simulation of neutron experiments
- software development, CI/CD
- cloud infrastructures
- AI-assisted solutions for neutron and x-ray data acquisition, reduction and analysis



**Technical University of Munich,
Group “Functional Materials” led by
Prof. Peter Müller-Buschbaum**

Project partners

Tübingen University. Group of Prof. Dr. h.c. Frank Schreiber

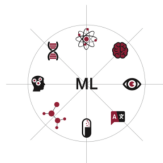
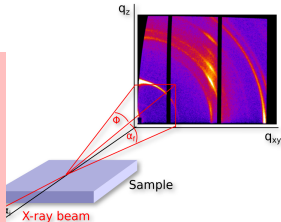
A. Greco, V. Starostin, V. Munteanu, C. Völter, D. Lapkin, L. Pithan.
A. Gerlach, A. Hinderhofer et al.

Years of expertise in:

Neutron and x-ray scattering from soft and hybrid materials

ML for x-ray and neutron scattering data analysis

Different approaches to inverse problem with ML



DFG

Deutsche
Forschungsgemeinschaft



Bundesministerium
für Bildung
und Forschung



Related publications:

- A. Hinderhofer et al., J. Appl. Cryst. (2023), in print
- V. Starostin et al., Synchrotron Radiation News 35 (2022) 21
- V. Starostin et al., npj Comput Mater – Nature 8 (2022) 101
- S. Timmermann et al., J. Appl. Cryst. 55 (2022) 751
- A. Greco et al., J. Appl. Cryst. 55 (2022) 362
- A. Greco et al., Mach. Learn.: Sci. Technol. 2 (2021) 045003
- A. Greco et al., J. Appl. Cryst. 52 (2019) 1342

Project partners



**DESY, Adj. Prof. Dr. rer. nat.
Stephan V. Roth**



**HZDR, Helmholtz AI young
investigator group of Nico
Hoffmann**



**University of Siegen X-ray
science group led by Prof.
Christian Gutt**

- Collaboration to large-scale x-ray facilities (DESY, EuXFEL, . . .)
- Years of expertise in x-ray scattering experiments
- Years of expertise in x-ray scattering data analysis
- Machine learning / AI methods
- Software development, CI/CD, . . .

Project partners

Helm & Walter IT-Solutions



- Currently about 16 employees: software engineers, dev-ops, project managers, designer, UI/UX experts, accessibility experts
- Expertise includes: Web/cloud technologies and applications, e-commerce solutions, mobile apps, hosting, python, C++, Linux, DB solutions, containerized environments, CI/CD ...



Associated partners

5 associated partners:

- Lawrence Berkeley National Laboratory, Advanced Light Source Division, Alexander Hexemer
- DESY/CMS, Dirk Kruecker
- Forschungszentrum Jülich / ER-C, Dieter Weber
- Helmholtz Zentrum Berlin, BESSY II, David Meier
- Rostock University, Prof. Dr. Dominik Kraus

Project partners expertise

Kompetenzen	Partner
Umgang mit experimentellen Daten	FZJ, DESY, TUM, Uni Tübingen, Uni Siegen, Uni Rostock, DESY/CMS, HZB, LBL, HZDR
Verständnis der experimentellen Daten	FZJ, DESY, TUM, Uni Tübingen, Uni Siegen, Uni Rostock, DESY/CMS, HZB, LBL, HZDR
Simulation	FZJ, DESY, LBL, DESY/CMS, HZB, TUM, HZDR
Softwareentwicklung	H&W, FZJ, HZDR, DESY, LBL, TUM, DESY/CMS
Maschinelles Lernen (INN, CNN)	HZDR, FZJ, LBL, DESY, Uni Tübingen, H&W, HZB, DESY/CMS, TUM
Unsicherheit Quantifizierung	HZDR, FZJ, DESY, Uni Tübingen
HPC, Horovod	HZDR, FZJ, LBL, H&W, DESY/CMS
Kooperation zu Großforschungseinrichtung	FZJ, DESY, LBL, HZDR, Uni Tübingen, Uni Siegen, TUM, DESY/CMS
Cloud Infrastrukturen	FZJ, HZDR, LBL, H&W, DESY, DESY/CMS

Workpackages

WP1: Project coordination. Lead: M. Ganeva / FZJ

WP2: Definition of inverse problems, preparation of training data. Lead: C. Gutt / University of Siegen

WP3: Invertible neural networks. Lead: N. Hoffmann / HZDR

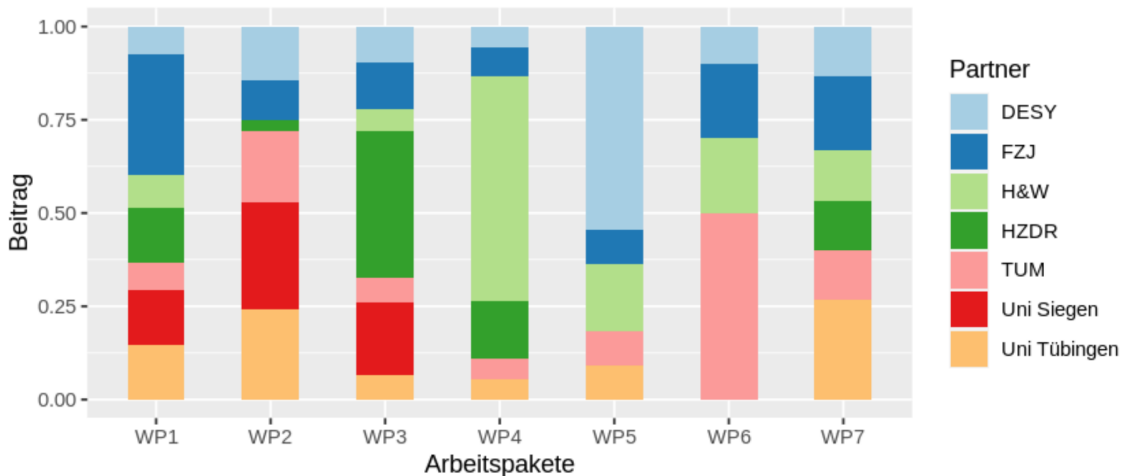
WP4: Design and development of the software framework. Lead: Helm & Walter IT-Solutions

WP5: Quality assurance. Lead: S. Roth / DESY

WP6: Integration in the data pipelines at participating research facilities. Lead: P. Müller-Buschbaum / TUM

WP7: Knowledge transfer. Lead: A. Gerlach / Tübingen University

Partner contribution to workpackages



VIPR project summary

- 7 partners: FZJ, HZDR, DESY, TUM, University of Siegen, Tübingen University, Helm & Walter IT-Solutions
- 5 associated partners: LBL, HZB/BESSY II, DESY/CMS, FZJ/ER-C, Rostock University
- 7 workpackages
- Total budget (as applied) about 2.2×10^6 Euro
- Duration: 3 years

And a lot of work to be done . . .

Thank you for your attention!