Versatile Inverse Problem Software Framework

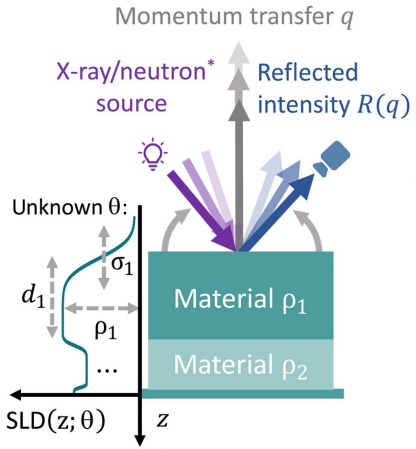


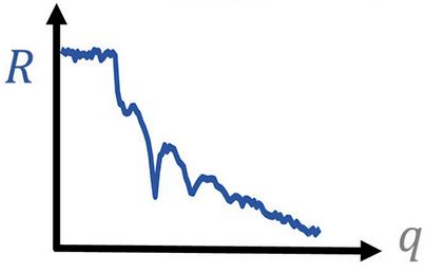
VIPR: A Modular Machine Learning Framework for Inverse Problems with Application to Reflectometry

S. Creutzburg[1,6], J. Rustamov[2], A. Koutsioumpas[4], J. Bornschein[1,6], M. Ganeva[4], S. Häusler[4], B. Helm[1,6], A. Hinderhofer[5], M. Levytskyi[4], V. Munteanu[5], R. Juzak[1,6], V. Pandit[2], F. Schreiber[5], J. Kelling[2,3], and N. Mothes[1,6]

[1]Helm & Walter IT-Solutions GmbH, [2]HZDR , [3]TU Chemnitz, [4]JCNS, Heinz Maier-Leibnitz Zentrum, [5]University of Tübingen, [6]Saxony.AI

Motivation

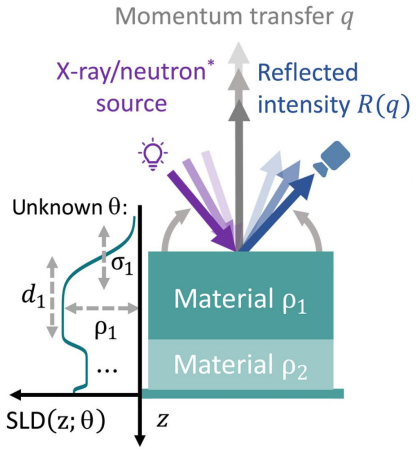


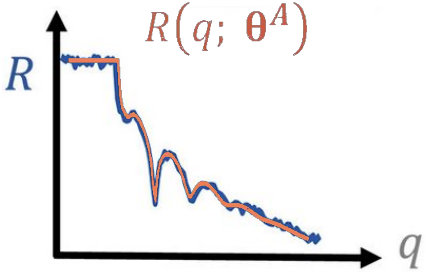


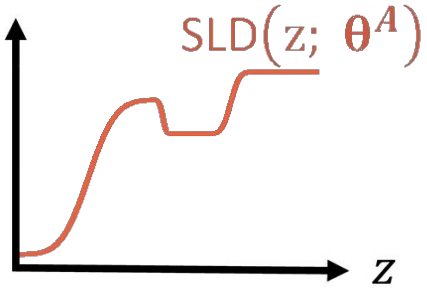
Reflectometry
Goal: determination/reconstruction of layer properties

Adapted from V. Starostin et al., Science Advances, 11(11), eadr9668 (2025)

Motivation



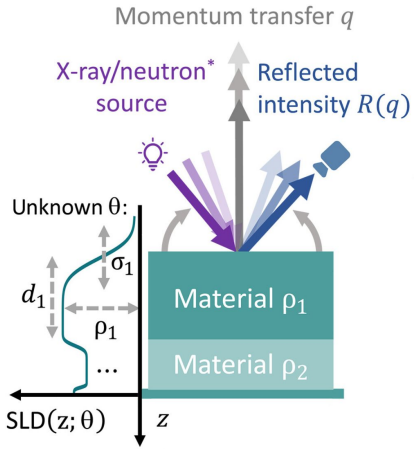


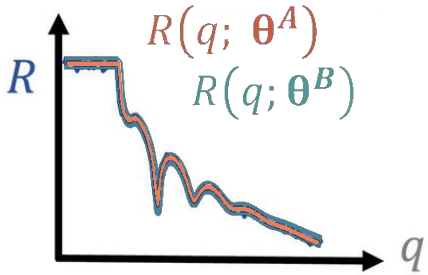


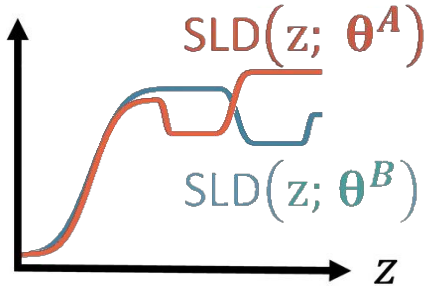
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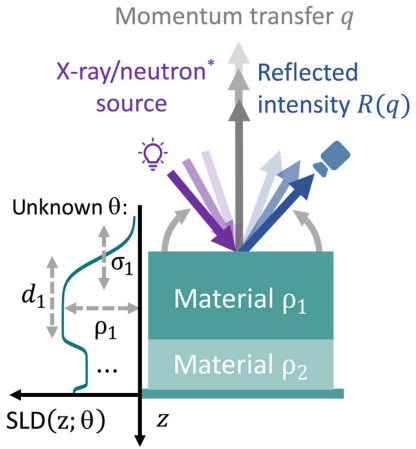


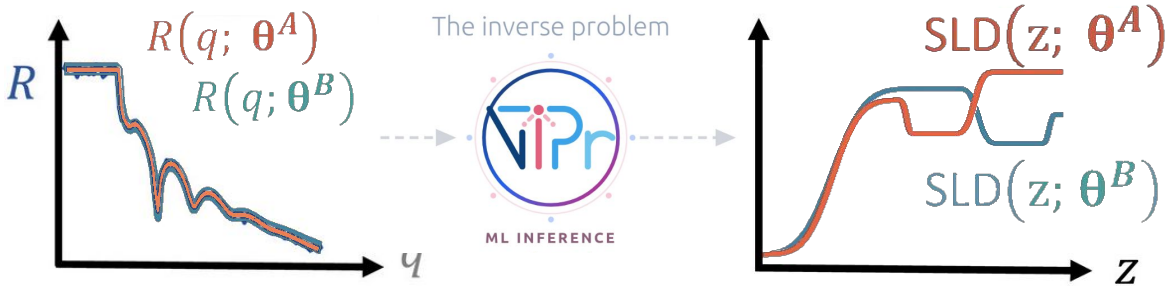


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Motivation





Reflectometry
Goal: determination/reconstruction of layer properties

VIPR is a modular ML framework for solving ambiguous inverse problems.

Adapted from V. Starostin et al., Science Advances, 11(11), eadr9668 (2025)

Inference Engines: From Fast Fit to Full Posterior

Reflectorch

- Yields single solution
- Very fast (~1 s)
- Prior bounds as network input



V. Munteanu et al., J. Appl. Cryst. 57(2):456 (2024) & JOSS, 10(115), 8169 (2025).

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- Built-in statistical refinement



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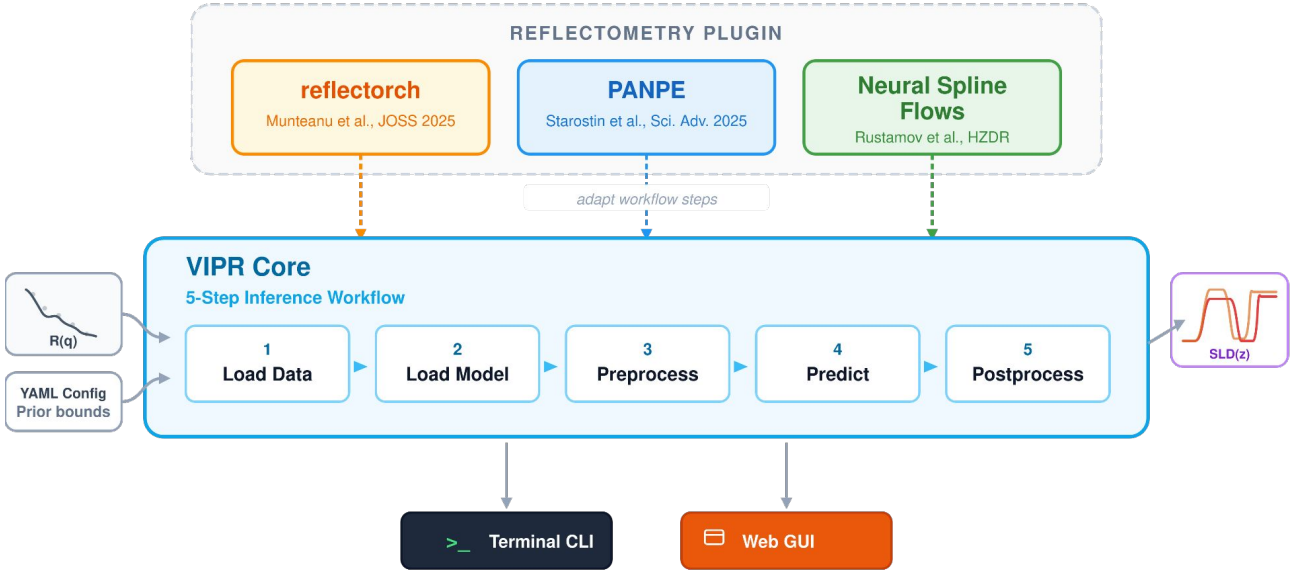
Neural Spline Flows

- Posterior estimation with fixed prior
- No additional refinement

J. Rustamov et al., HZDR



VIPR: One Pipeline, Three Analysis Approaches



VIPR: Workflow framework for ML-based inference — extensible to other inverse problems via plugins

VIPR CLI: Configuration and Execution

```yaml
vipr:
  inference:
    load_data:
      handler: csv_spectrareader
      parameters:
        data_path: '.../Fe_Pt_DN.dat'
    load_model:
      handler: reflectorch
      parameters:
        config_name: NR-2layers-basic-v1
    filters:
      INFERENCE_PREPROCESS_PRE_FILTER:
      - method: preprocess_interpolate
    prediction:
      handler: reflectorch_predictor
      parameters:
        polish_prediction: true
        prior_bounds:
          thicknesses: [[1, 50], [1, 400]]
          slds: [[6, 6.5], [3, 3.2], ...]
          ...
    postprocess: {}
```

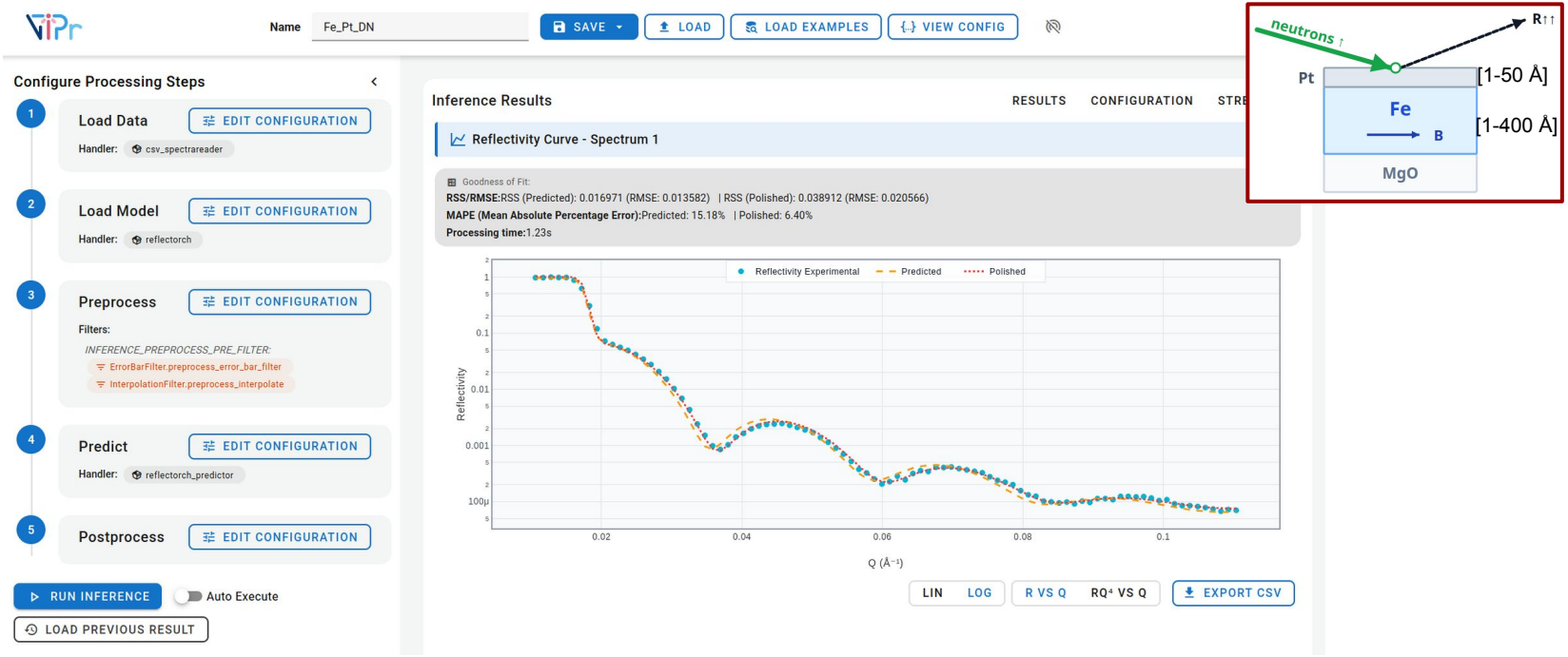
```
$ vipr --config Fe_Pt_DN.yaml inference
run
....

Completed in 1.93 s

Results: storage/results/Fe_Pt_DN_a3b10e34
```

The Web GUI provides a graphical interface for the same workflow steps.

VIPR Reflectorch: Fe/Pt on MgO - Neutron Reflectometry (MARIA)



Reflectorch point estimate in ~1 s (MAPE 6.4% after polishing).

Data: A. Koutsioumpas, J. Appl. Cryst., 54, 1857-1866 (2021)

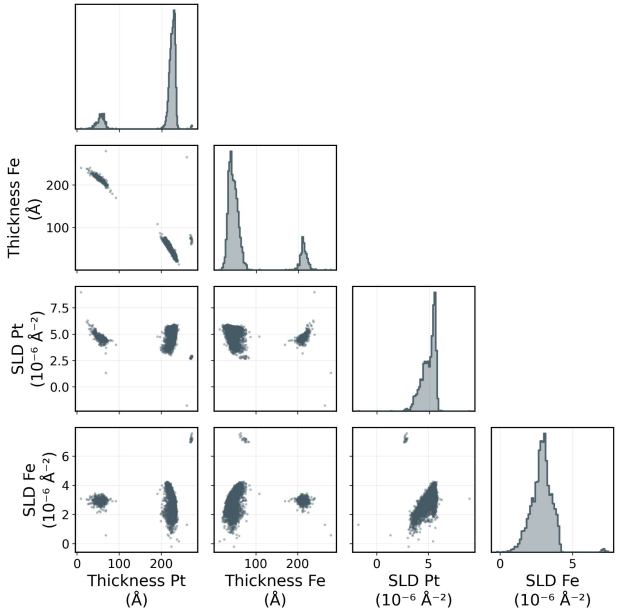
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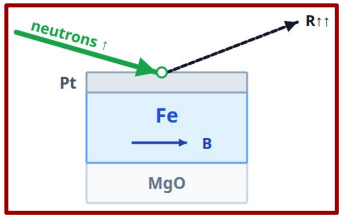


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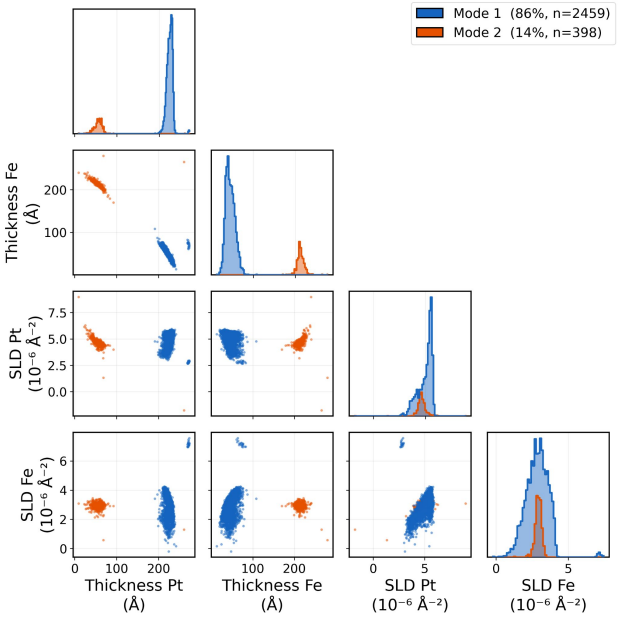
VIPR Neural Spline Flow: Multimodal Posterior (fixed prior)

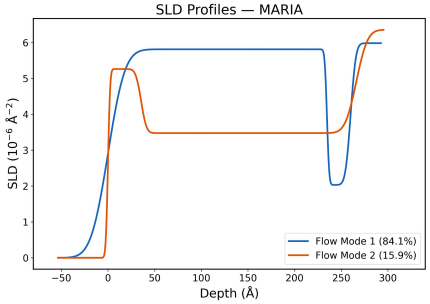


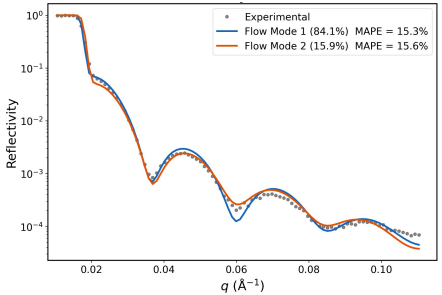


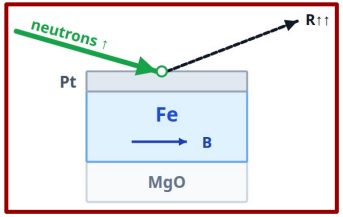
Neural Spline Model: J. Rustamov, HZDR

VIPR Neural Spline Flow: Multimodal Posterior (fixed prior)



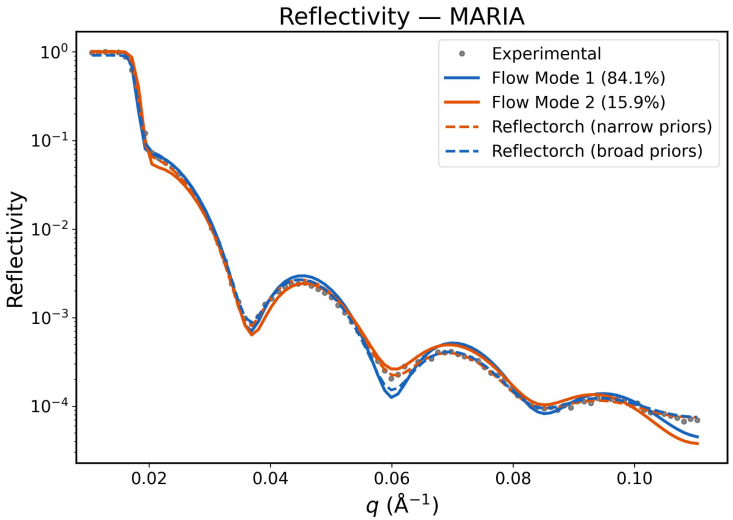


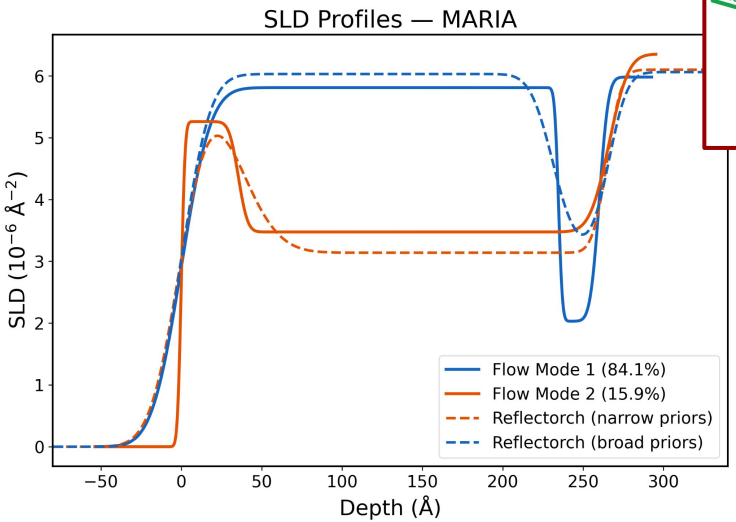


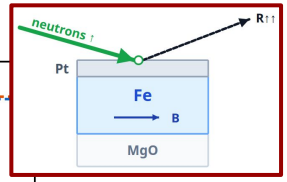


Two posterior modes correspond to different SLD profiles.
Both reproduce the experimental reflectivity.

Reflectorch vs. Neural Spline Flow: Effect of Prior Bounds







With broad priors, Reflectorch defaults to the statistically dominant mode (84%).
The flow model recovers both — including the physically correct Mode 2 (16%).

Narrow priors: Pt [1–50 Å], Fe [1–400 Å] Broad priors: both [1–400 Å]

Data: A. Koutsioumpas, J. Appl. Cryst., 54, 1857-1866 (2021)

Summary & Contact

- VIPR integrates three inference approaches in one workflow — enabling direct comparison of results

- Demonstrated on an Fe/Pt bilayer: broad priors lead Reflectorch to the wrong structure — the flow model recovers both modes, including the physically correct one

- Open source under LGPL via codebase.helmholtz.cloud/vipr/vipr-framework

VIPR Framework Codebase

Direct Contact

Dr. Sascha Creutzburg
sascha.creutzburg@saxony.ai

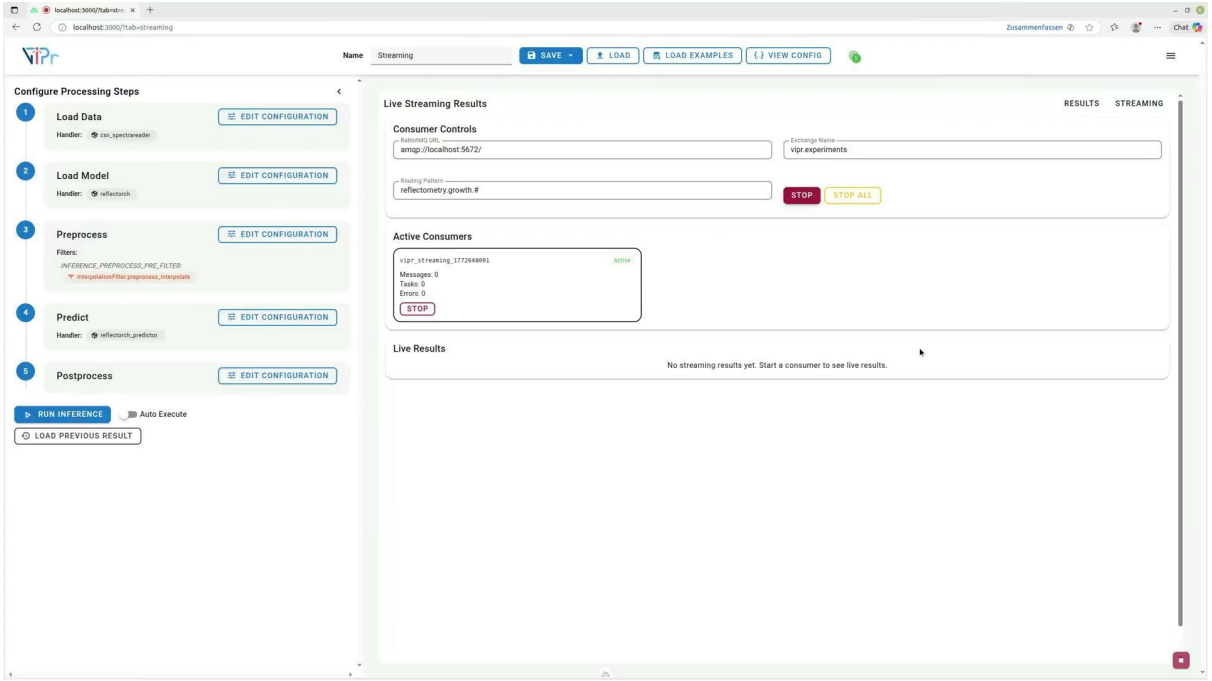
With funding from the:

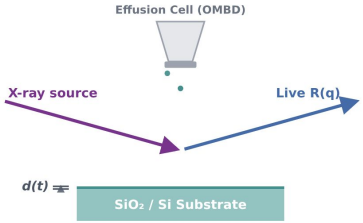
Federal Ministry of Research, Technology and Space

VIPR 05D23VT1 ERUMDATA

Appendix

Outlook: Real-Time XRR Analysis for Growth Monitoring (DIP on SiO_2/Si)

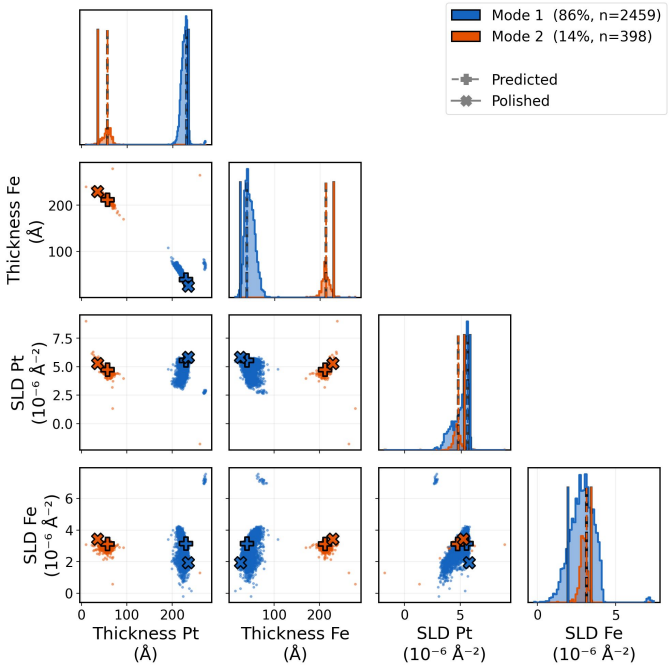


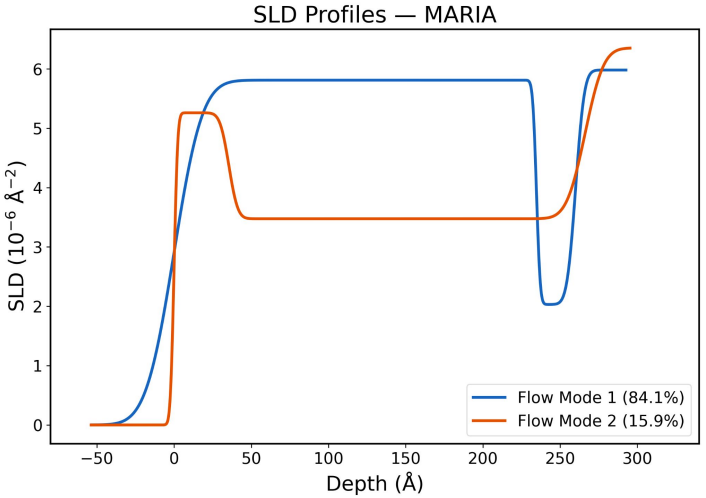


Live tracking of film growth parameters enables on-the-fly decisions during deposition.

Data: https://schreiber-lab.github.io/reflectometry-dataset/

Neural Spline Flow: Multimodal Posterior





Neural Spline Model: J. Rustamov, HZDR

Two posterior modes correspond to different SLD profiles.