Simulation-based Inference of Beamline Characteristics at BESSY

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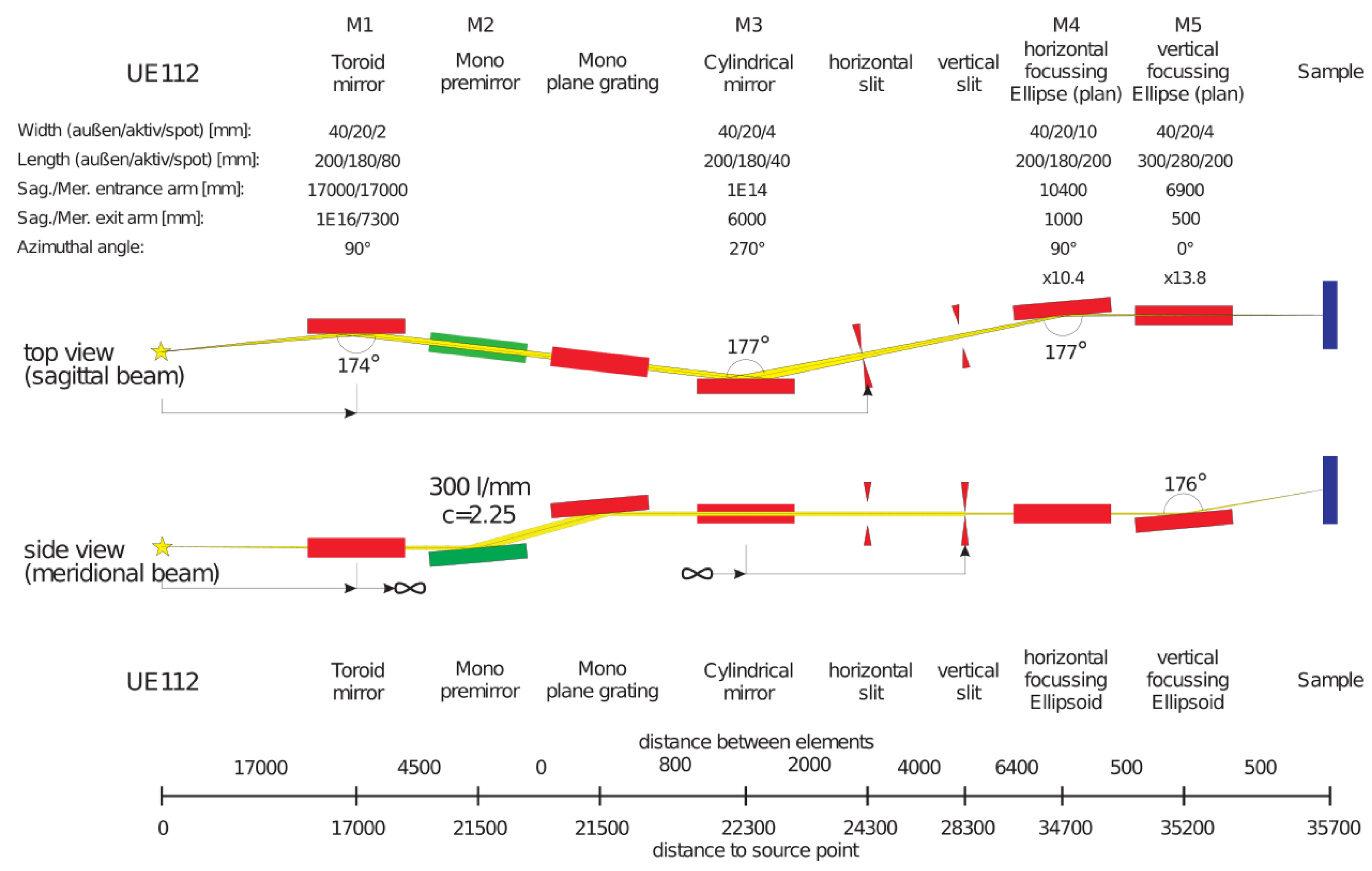
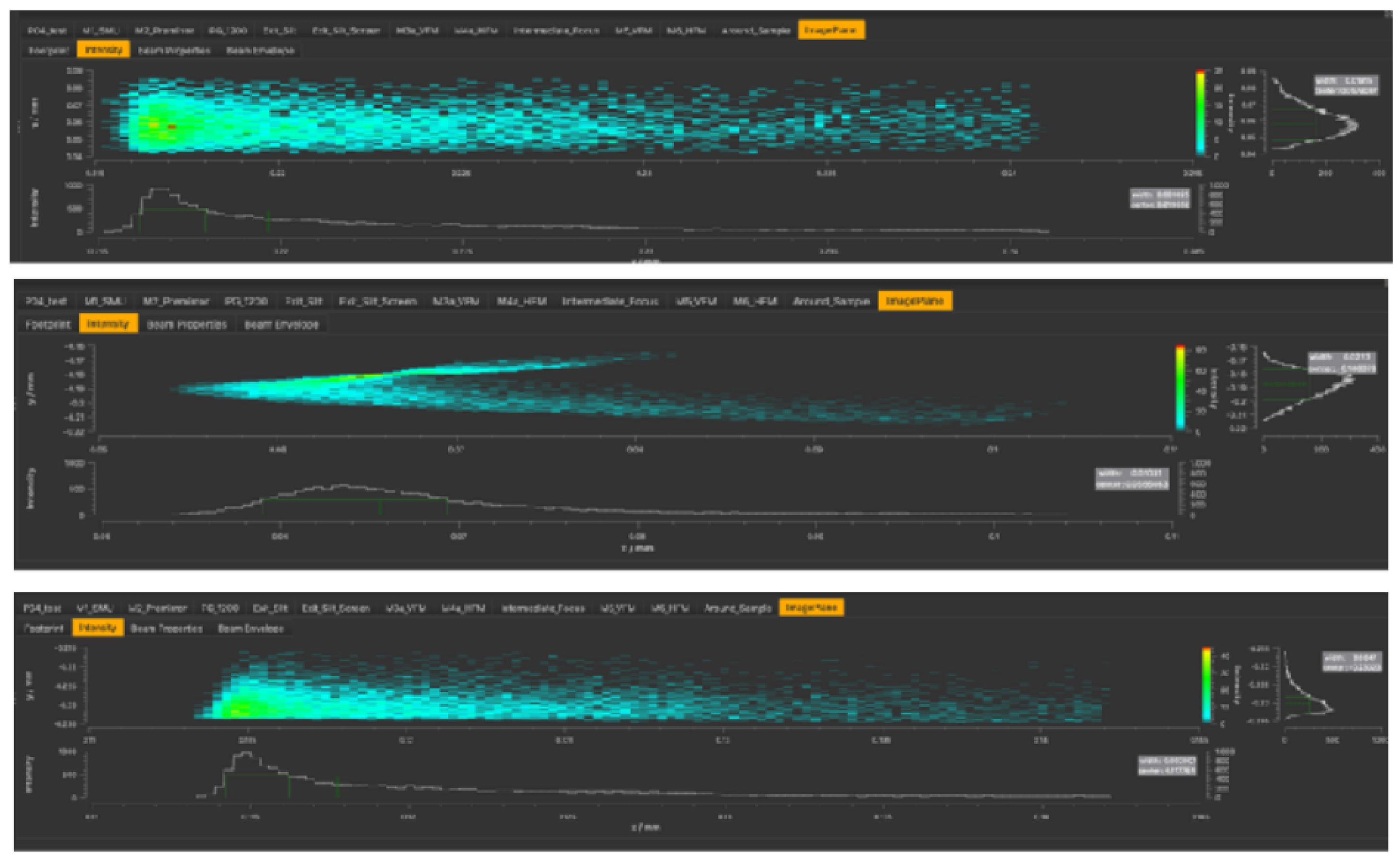
Motivation



Beamline Parameters $\vec{\vartheta}$ towards Sample

Simulation »

« Experiment?



Beam Profile $\vec{x}$ at Sample Position

Bayesian Inference on Inverse Problems

$$p(\vec{\vartheta}|\vec{x}) = \frac{p(\vec{x}|\vec{\vartheta}) \cdot p(\vec{\vartheta})}{\int p(\vec{x}|\vec{\vartheta}) \cdot p(\vec{\vartheta}) d\vartheta}$$

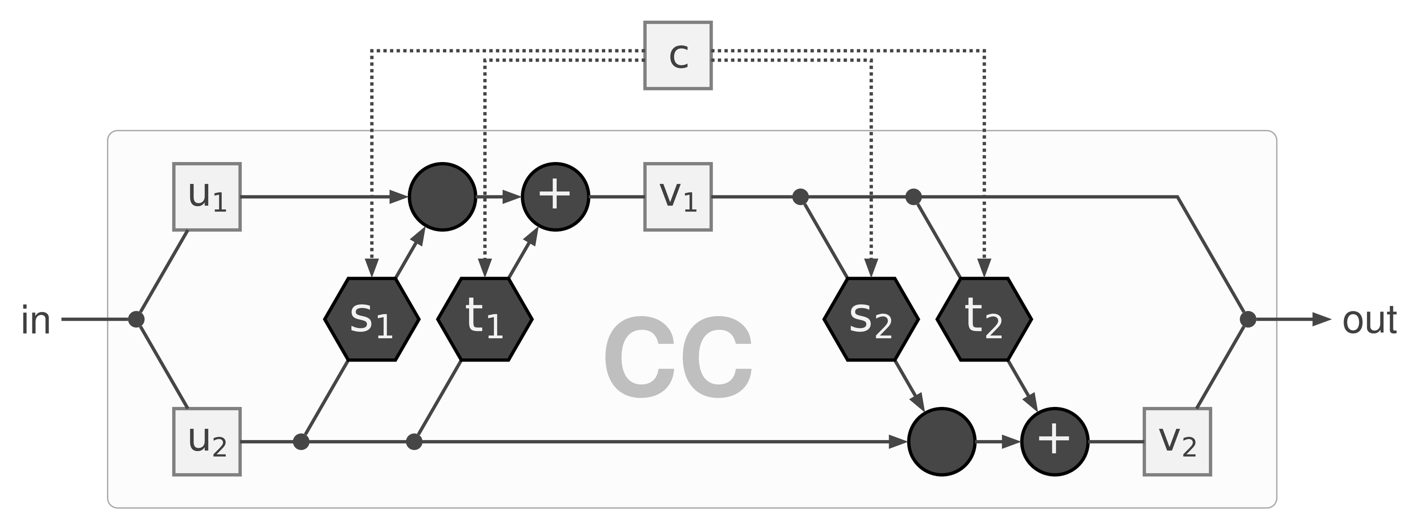
- likelihood $p(\vec{x}|\vec{\vartheta})$ described by simulation (forward process)
- prior $p(\vec{\vartheta})$ known from simulation configuration within meaningful physical limits
- goal:
  obtain posterior $\hat{p}(\vec{\vartheta}|\vec{x})$ from experimental data (backward process)

Normalizing Flows!

- ideal to **map** probability density function $p(\vec{x}_i|\vec{\vartheta}_i)$ **onto** another probability density function $\hat{p}(\vec{\vartheta}_i|\vec{x}_i)$
- using affine coupling blocks inspired invertible neural networks (INN,[1])

$\vec{x}_c$

$\vec{\vartheta}$ «



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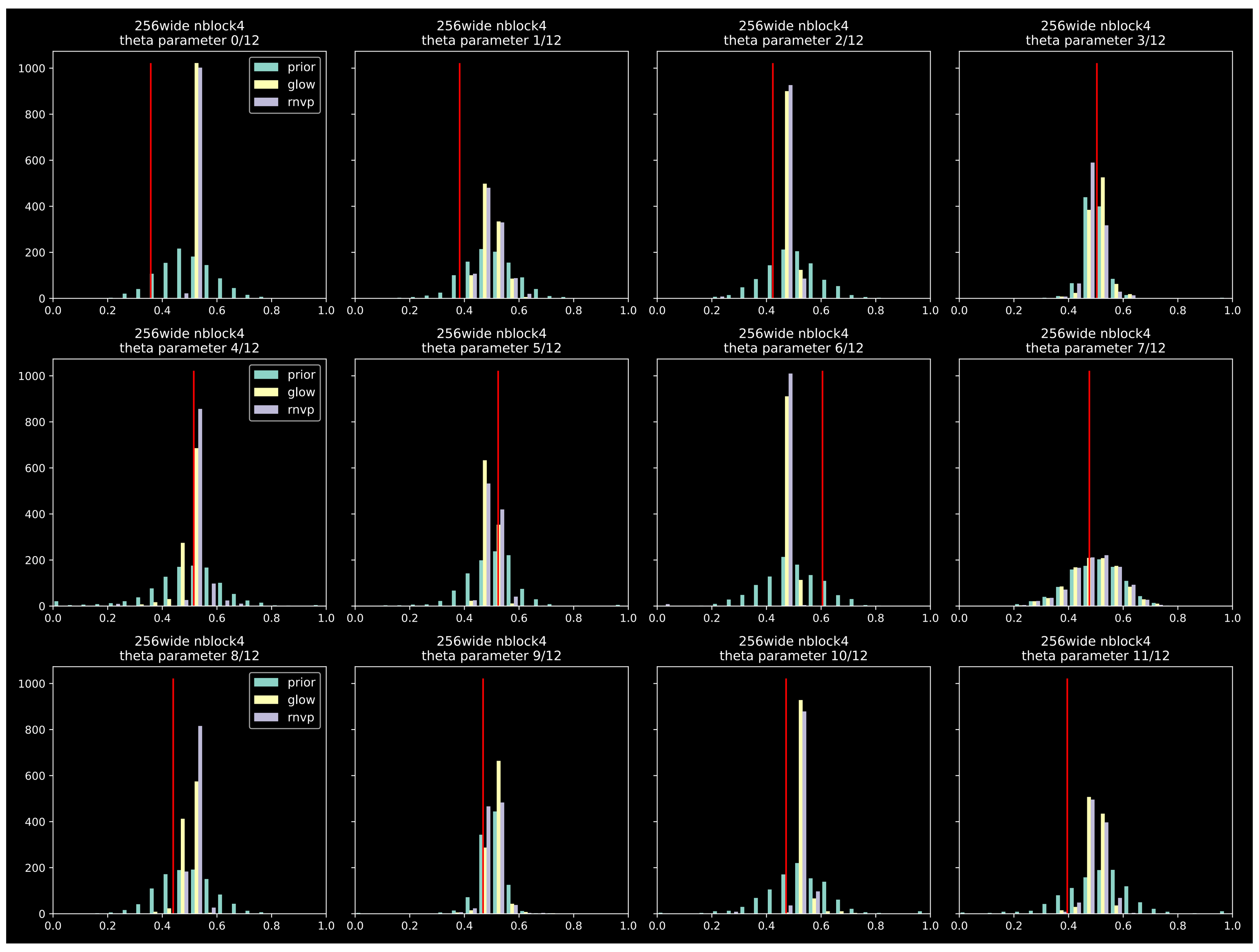
Pre-Alpha-Stage Preliminary Results



Maximum a posteriori (MAP) estimate for single validation sample using conditional INN (based on [3])

- affine coupling blocks based conditional Invertible Neural Network shows promising results
- currently validating architecture, data sets and training
- comparison to SNPE-C [2] (Sequential Neural Posterior Estimator) ongoing

References:

[1] L. Ardizzone, C. Lüth, J. Kruse, C. Rother, and U. Köthe.
Guided image generation with conditional invertible neural networks.

[2] D. S. Greenberg, M. Nonnenmacher, and J. H. Macke.
Automatic posterior transformation for likelihood-free inference.

[3] S. T. Radev, U. K. Mertens, A. Voss, L. Ardizzone, and U. Köthe.
BayesFlow: Learning complex stochastic models with invertible neural networks.