PhotonMEADOW 2023

HZB BESSY II Light Source

Efficient simulation and AI surrogate models for real-time optimisation

Peter Feuer-Forson, HZB

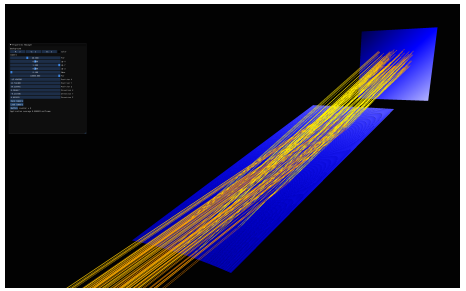
Spectrometer development: Peter Feuer-Forson, Gregor Hartmann, Philippe Wernet, Rolf Mitzner

RAY-X: Peter Feuer-Forson, Peter Baumgärtel, Rudi Schneider, Oussama Sayari, Jannis Maier, Enrico Ahlers, Fanny Zotter

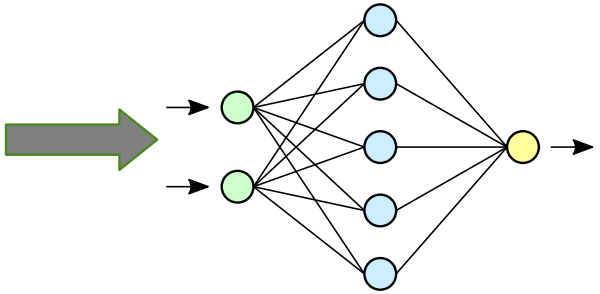
Goals

- Develop ray tracing software with GPU support for the generation of large datasets
- Train neural networks as surrogate models for spectrometers and beamlines
- Optimise alignment and design parameters of optical elements

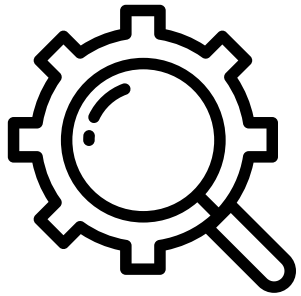
SIMULATION



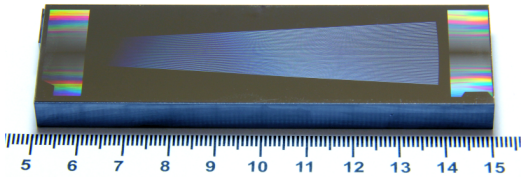
SURROGATE



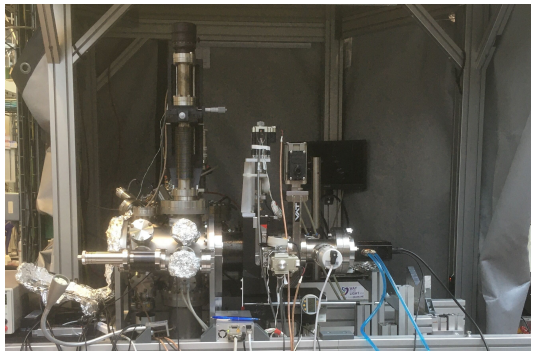
OPTIMISATION



DESIGN



EXPERIMENT



Simulation - Ray-UI

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- Fortran => Migration of code to C++
- Limited CLI => Modern design pattern for modular and maintainable code (adapted MVC)
- Spaghetti code => Robust test suite and documentation
- CPU bound => Tracer which utilises parallel computing / GPU compute

RAY-X

Git Repository:
https://hz-b.de/ray-x

Simulation - RAY-X

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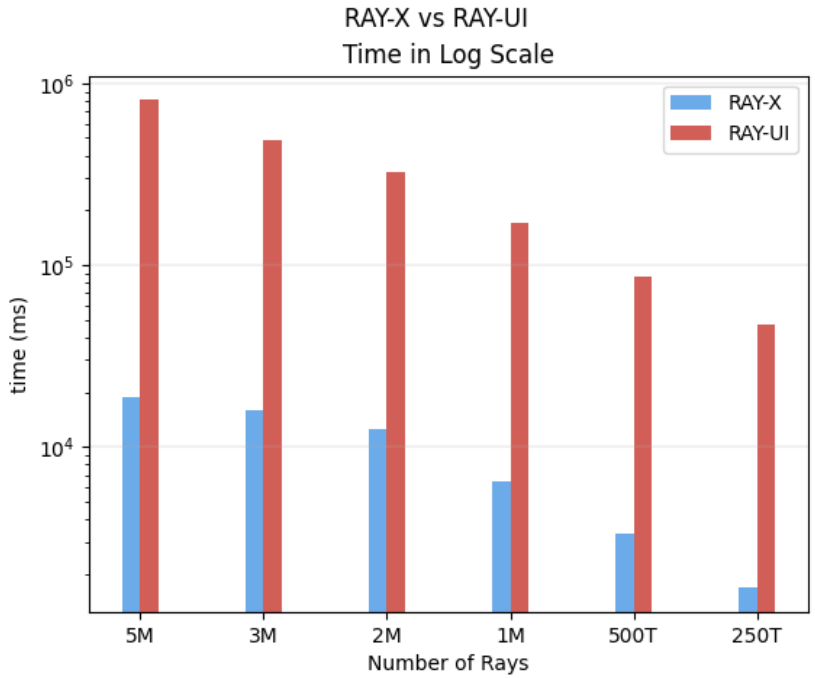
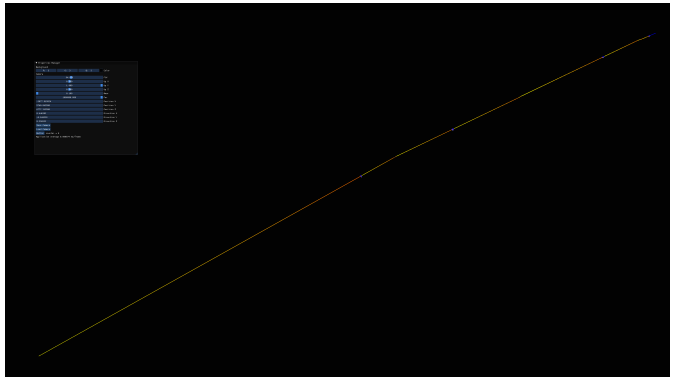
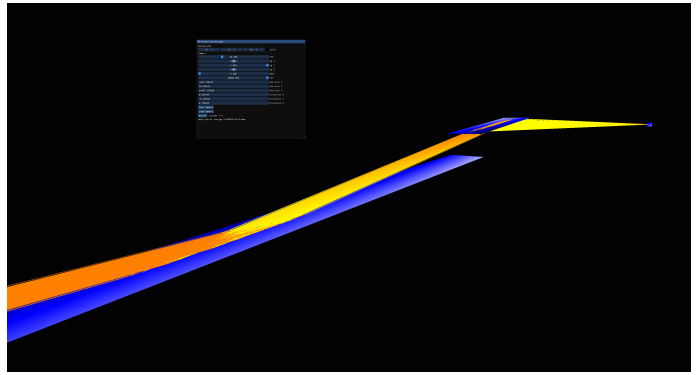
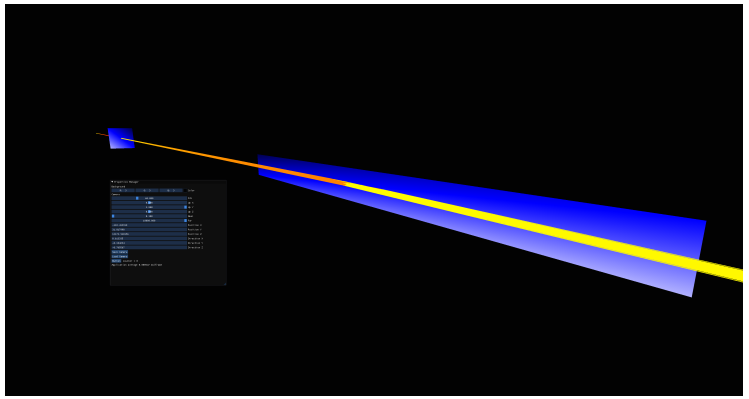
- Improve trace-time via GPU hardware and software (Vulkan)
- Implement support for new optical elements via grouped objects (multi-RZP)
- Dynamic and sequential tracing
- Fully functional CLI
- 3D visualisation (wip)
- (almost) all functionality of Ray-UI



METRIX BEAMLINE







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https://hz-b.de/ray-x

RAY-X

Simulation - RAY-X

- Why Vulkan?
  - AMD and Nvidia support
  - Fine-grained control over GPU pipeline
  - Open source
  - Continued development and support from large companies (google)

Vulkan

Application responsible for memory allocation and thread management to generate command buffers

Direct GPU Control

GPU

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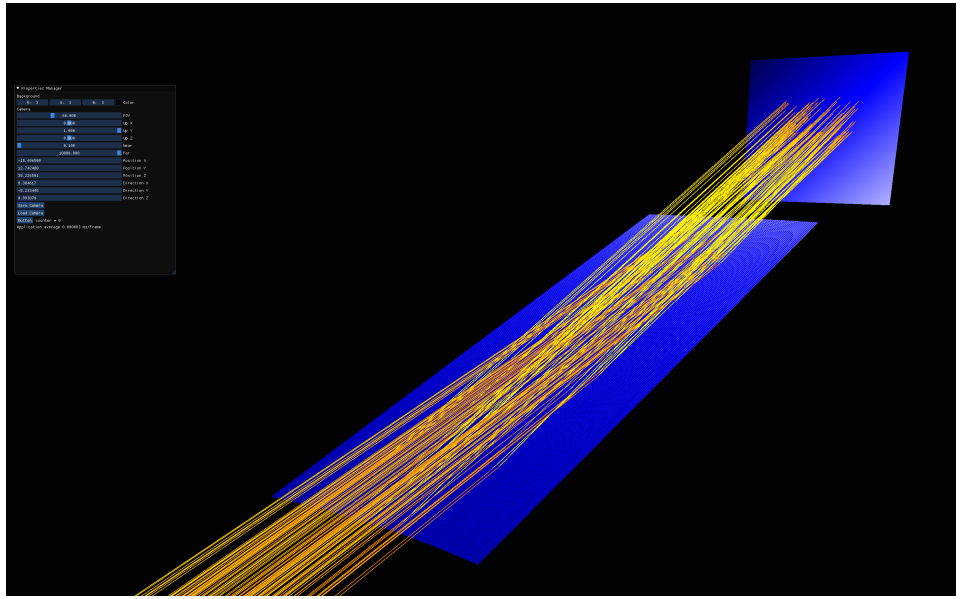
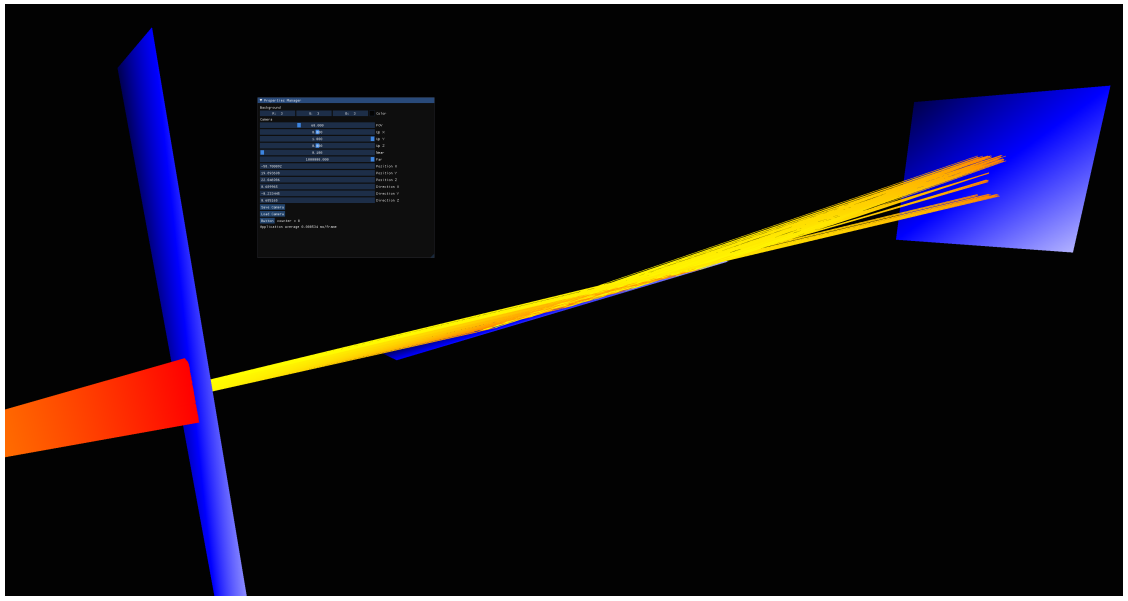
REFLECTION ZONE PLATES





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RAY-X

Spectrometer Alignment

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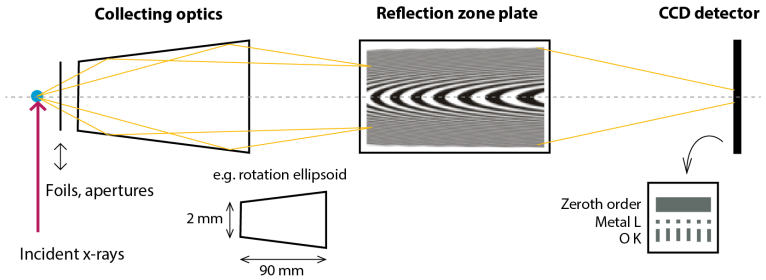
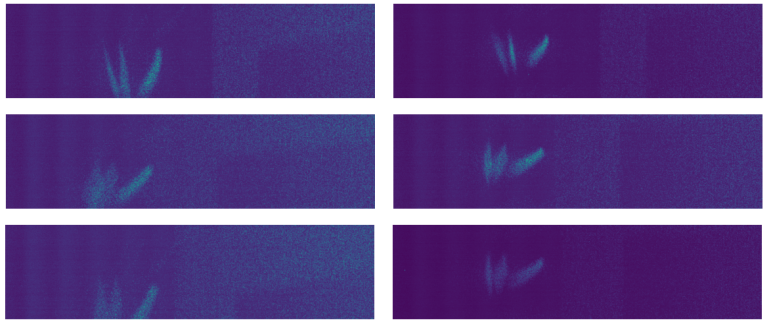
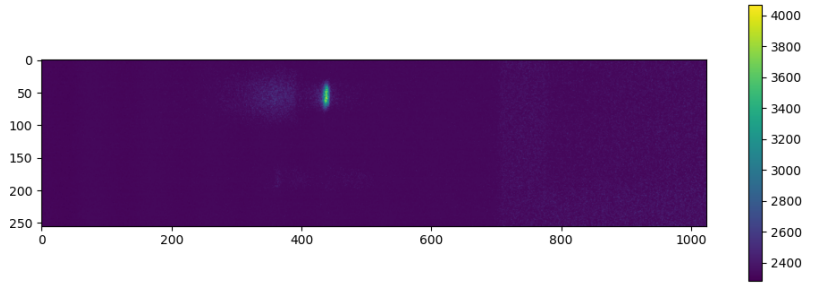
- Record PFY-XAS Spectra on wire Cu86, Mn12, Ni2 – goal: clear separation of Mn from O2
- Manual alignment process ~ 1 hour
- Position of RZP relative to the sample and the camera hard to determine
- If RZP or sample switched, alignment position can be lost
- Optimal alignment requires careful fine-tuning







→ Task: Automate alignment → Find optimal XYZ position of RZP

Spectrometer Alignment

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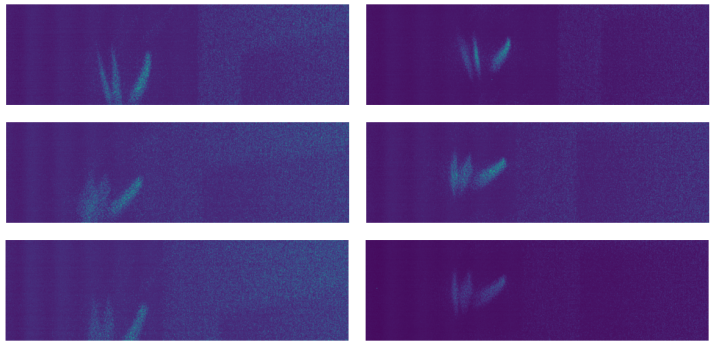
CHALLENGE

High dimensional experiment data



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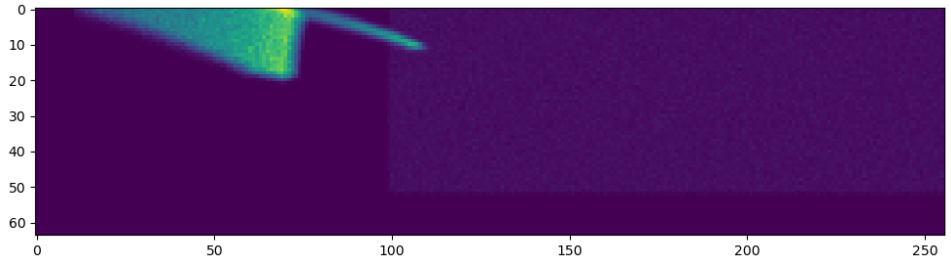
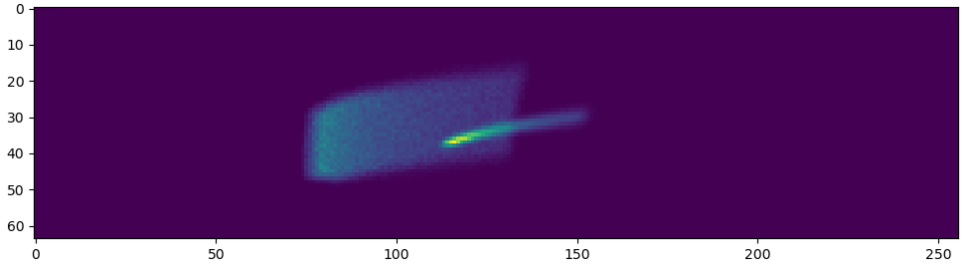
Desired transformation

Low dimensional desired information (X, Y, Z)

- Insufficient experiment data to train a Neural Network (1 week = ~3000 images)
- But… experiment can be simulated with RAYX => 2 millions simulations





Spectrometer Alignment

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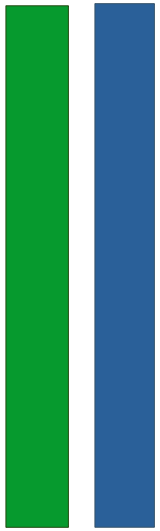
CHALLENGE

High dimensional experiment data

Simulation data



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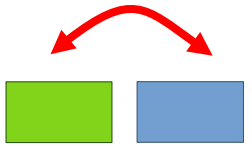
Desired transformation

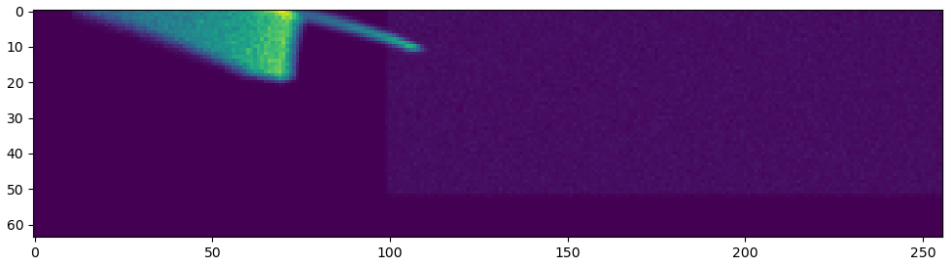


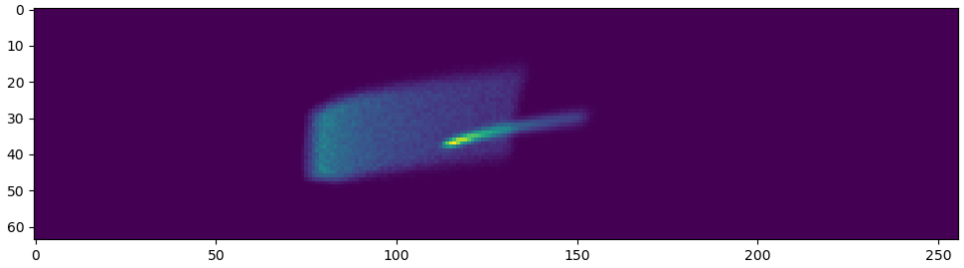
Mismatch

Low dimensional desired information (X, Y, Z)

Simulation parameters (X, Y, Z)

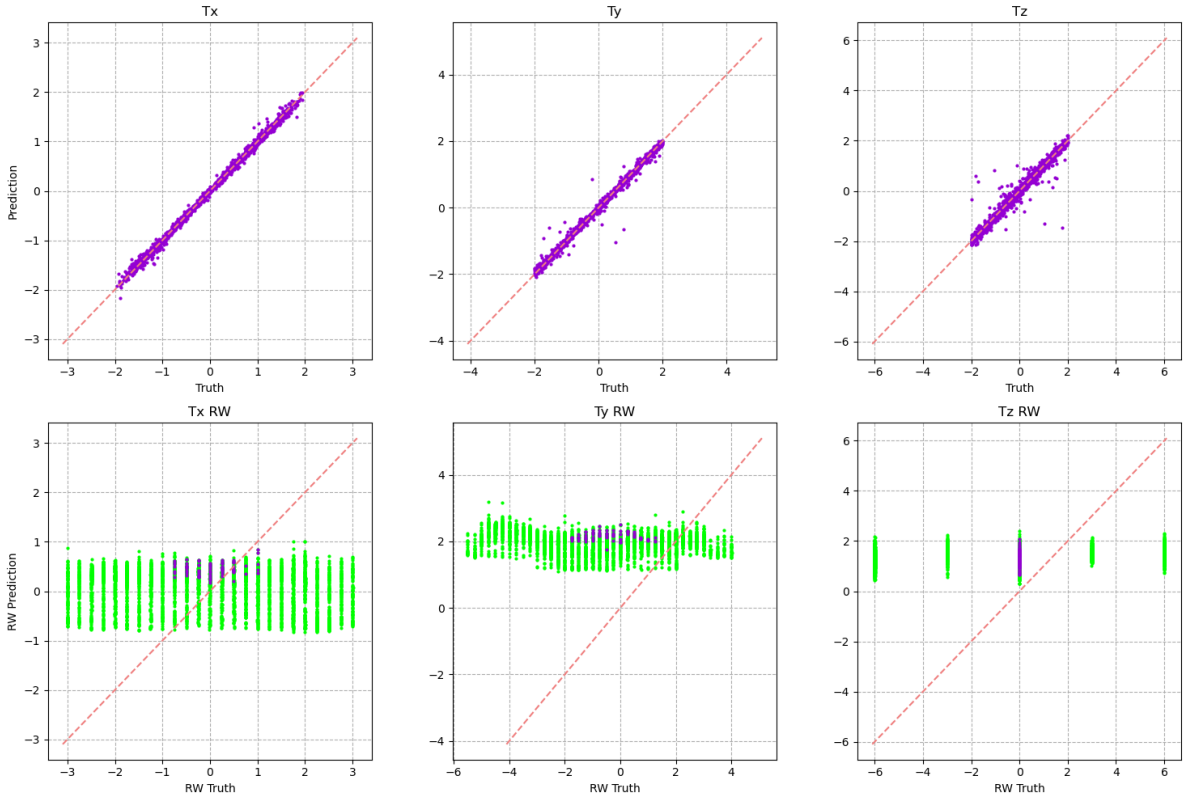
- Insufficient experiment data to train a Neural Network (1 week = ~3000 images)
- But… experiment can be simulated with RAYX => 2 millions simulations





Spectrometer Alignment

FORWARD DIRECTION



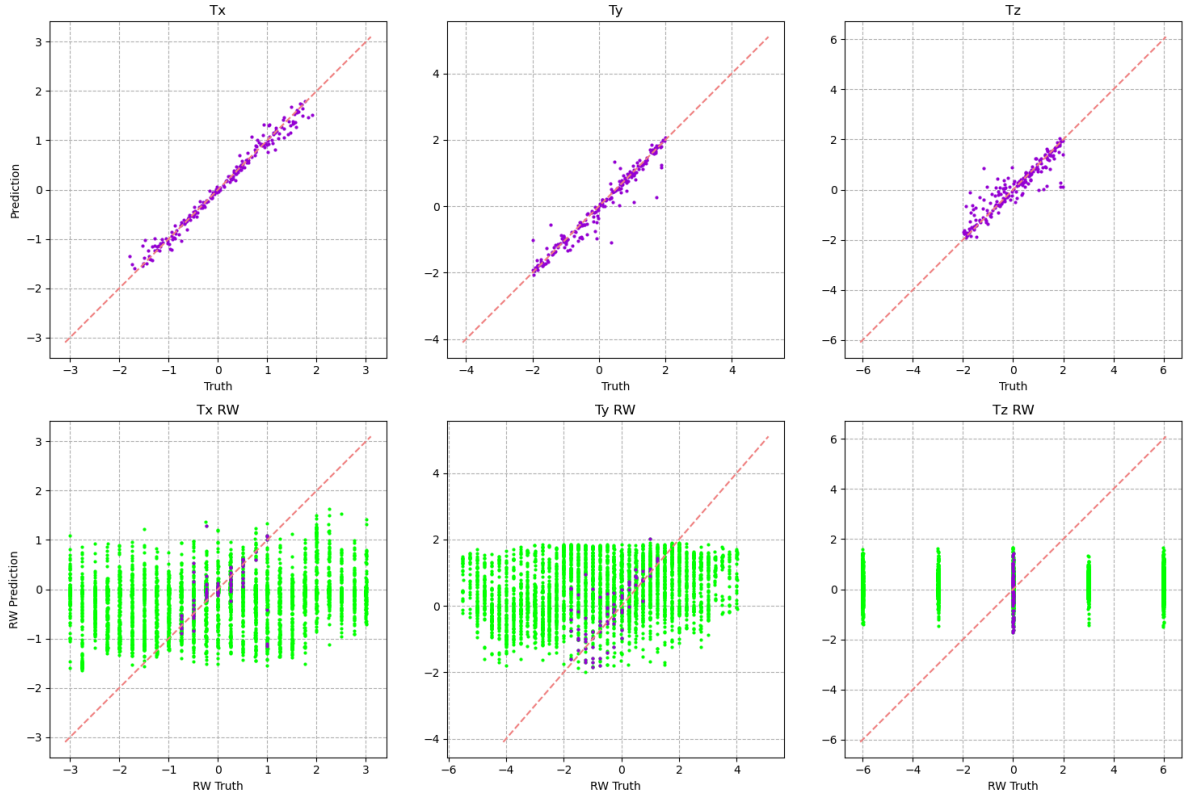
Simulation

Experiment

- Network trained with 500k sims
- Inference 1000 datapoints
- CNN / FCN
- Experiment data filtered to focus on detector images with significant information
- Augmentation required...

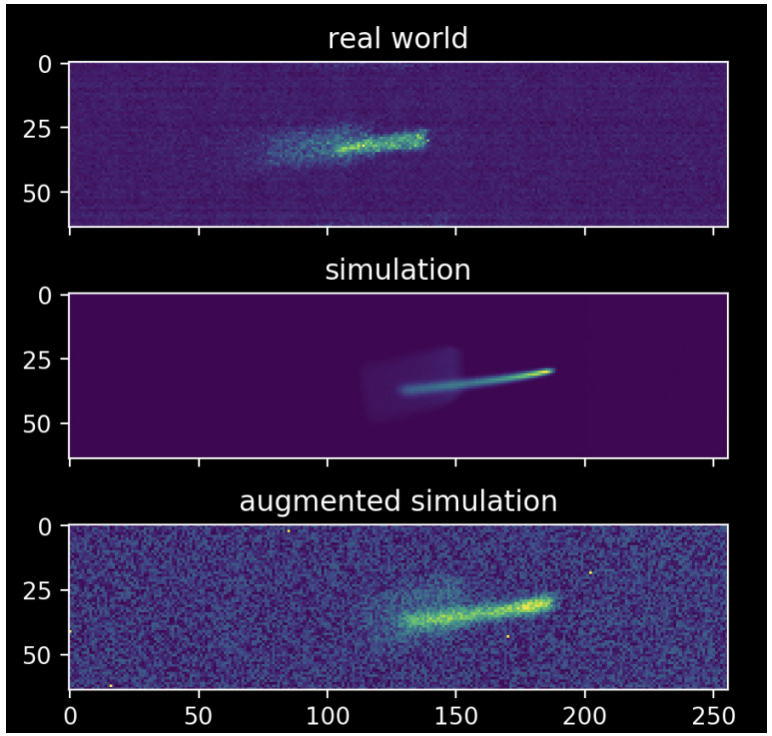
Spectrometer Alignment

BASIC AUGMENTATION



Simulation

Experiment



- Added noise, random hits, variance intensity
- Work continuing on training networks for adaptive simulation

Spectrometer Alignment

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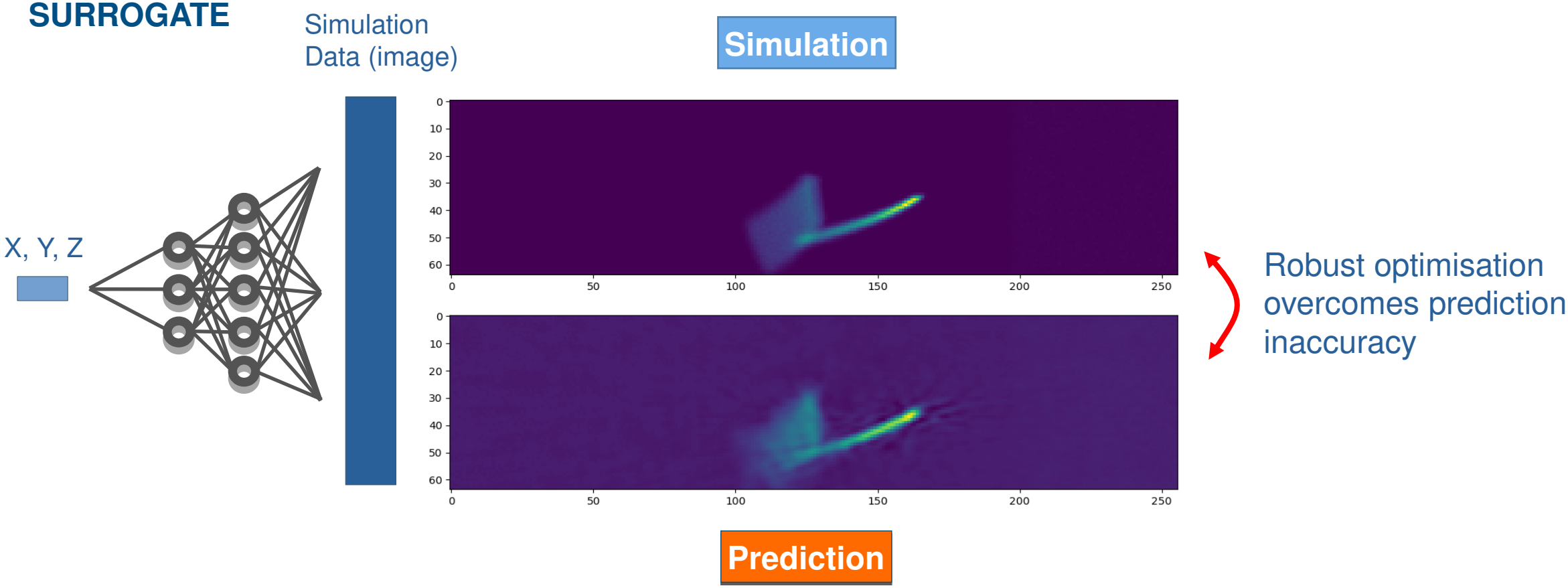
SURROGATE



- Simulation duration ~ 2 seconds per trace. Neural network inference ~ ms
- Use as model for optimisation. But… how to overcome mismatch?

Spectrometer Alignment

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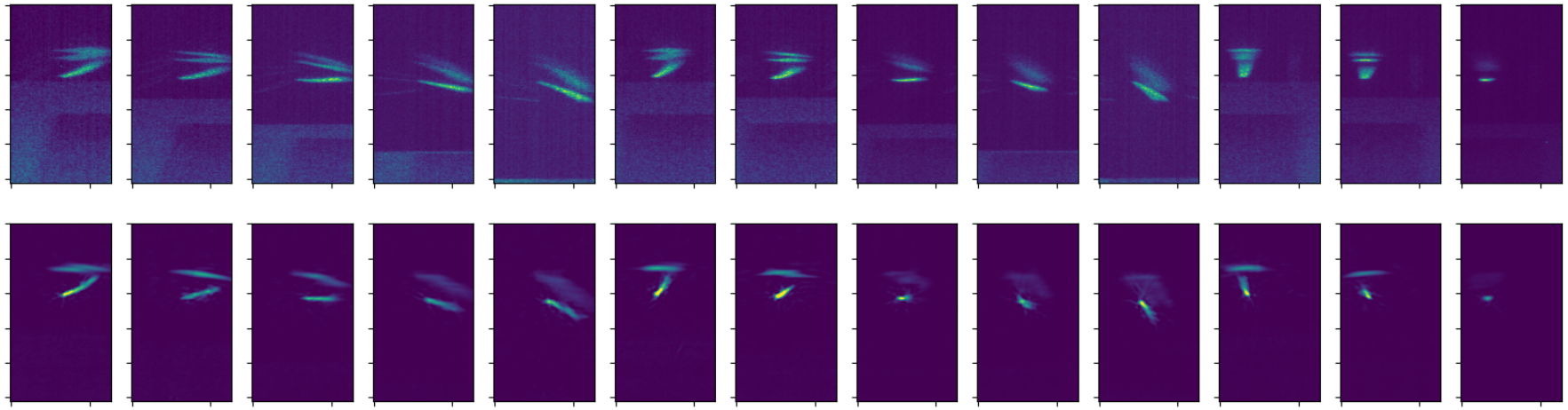
FUNCTION TO MINIMISE

$$\text{diff} = \sum_{i=1}^{N} (Image_i^{exp} - NN(T_i^{exp} + T^{off}, C^{off}, RZP^{off}, Ratio))^2$$

- Record N images and their corresponding T_exp
- Use Optimiser to minimise diff by searching for T_off
- Result of T_off => Absolute position of perfect alignment



Precision: ~0.01mm
Runtime: ~5 min

Reflection Zone Plate Design

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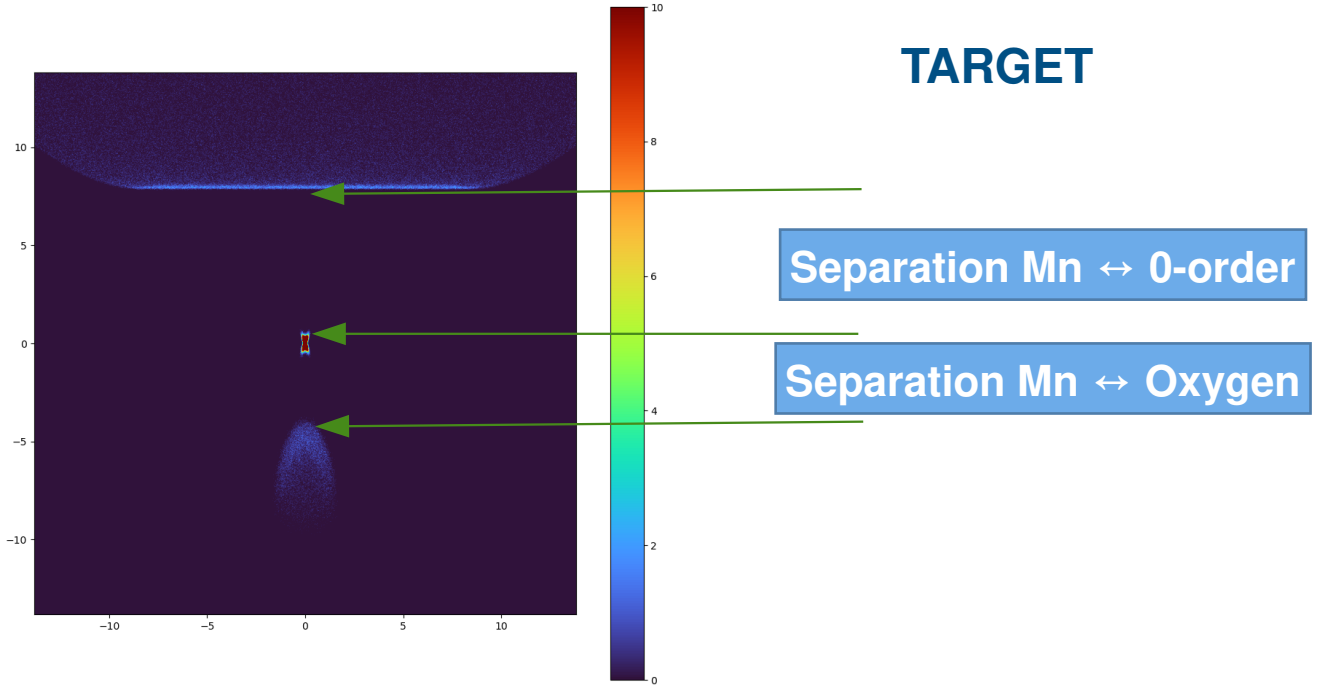
- Optimise 7 design parameters of a spherical RZP (with constraints)
- Target: maximise separation between manganese, oxygen and zero-order
- Utilize same method – simulate, train neural network as surrogate model, optimise

SIMULATION → **SURROGATE** → **OPTIMISATION** → **DESIGN**

PARAMETERS

- Design angle alpha: [1.5 - 3.0]
- Design Angle beta: [0.5 - 7.0] (beta < alpha)
- Sagittal entrance arm length: [70mm - 150mm]
- Sagittal exit arm length: [300mm - 800mm]
- Long Radius R: [3000mm, 5000mm, 10000mm]
- Slope Error Sagittal: [0.0 - 100.0]
- Slope Error Meridional: [0.0 – 100.0]

TARGET



Reflection Zone Plate Design

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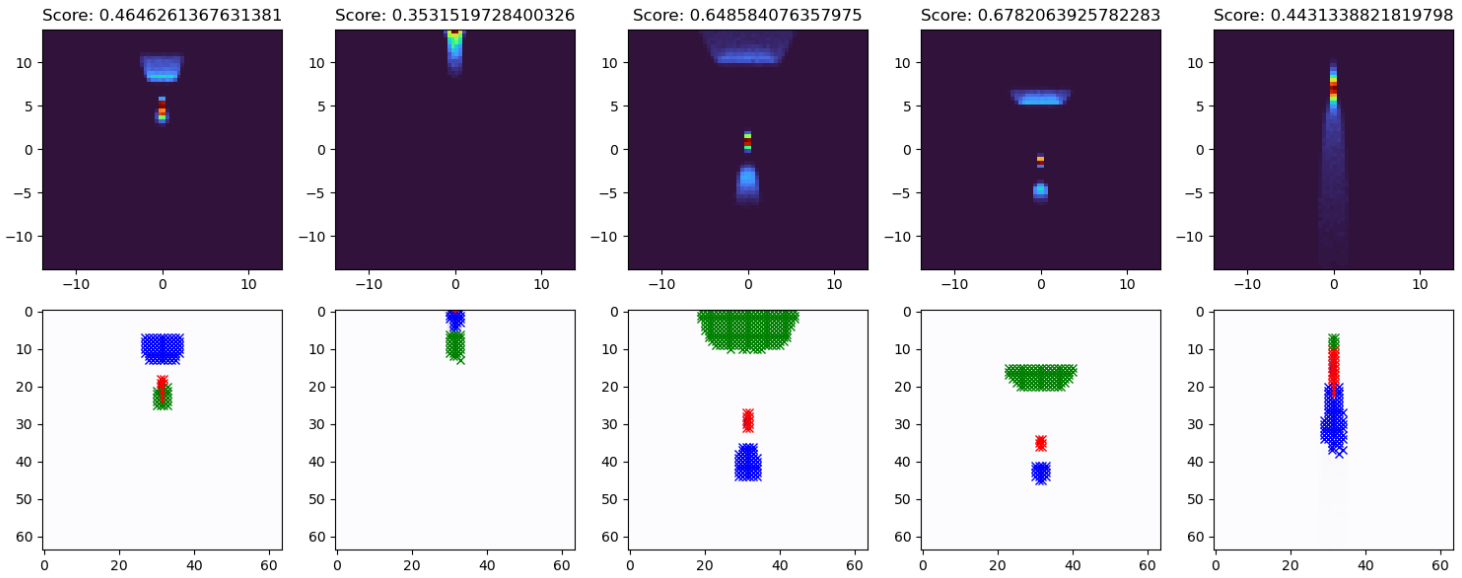
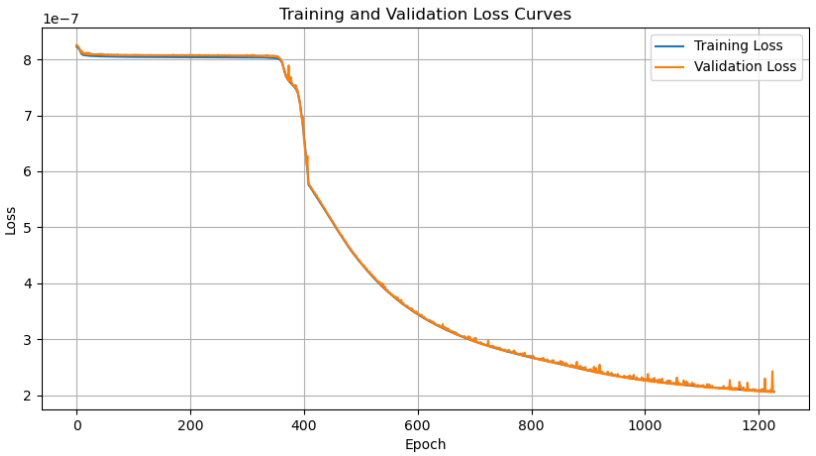
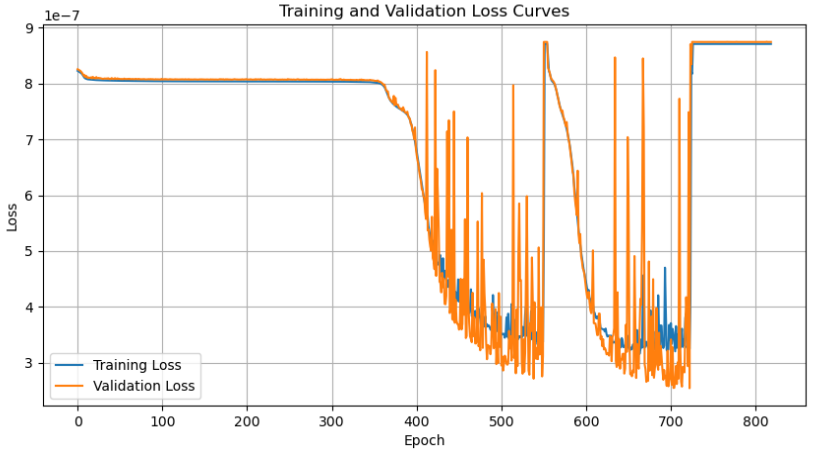
- Simulate 2 million traces, bin to 64x64 and normalise (0, 1)
- FCN followed by deconvolutional layers → params to histogram
- Clustering algorithm and silhouette score to measure separation







- score = (b - a) / max(a, b)
- a: cohesion, average distance between datapoint and all other in cluster
- b: separation, average distance from datapoint to datapoints in nearest other cluster

Reflection Zone Plate Design

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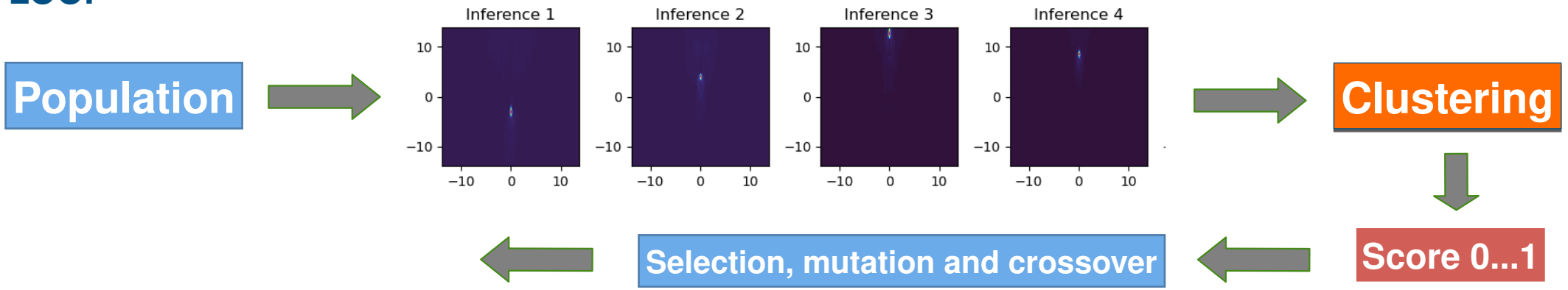
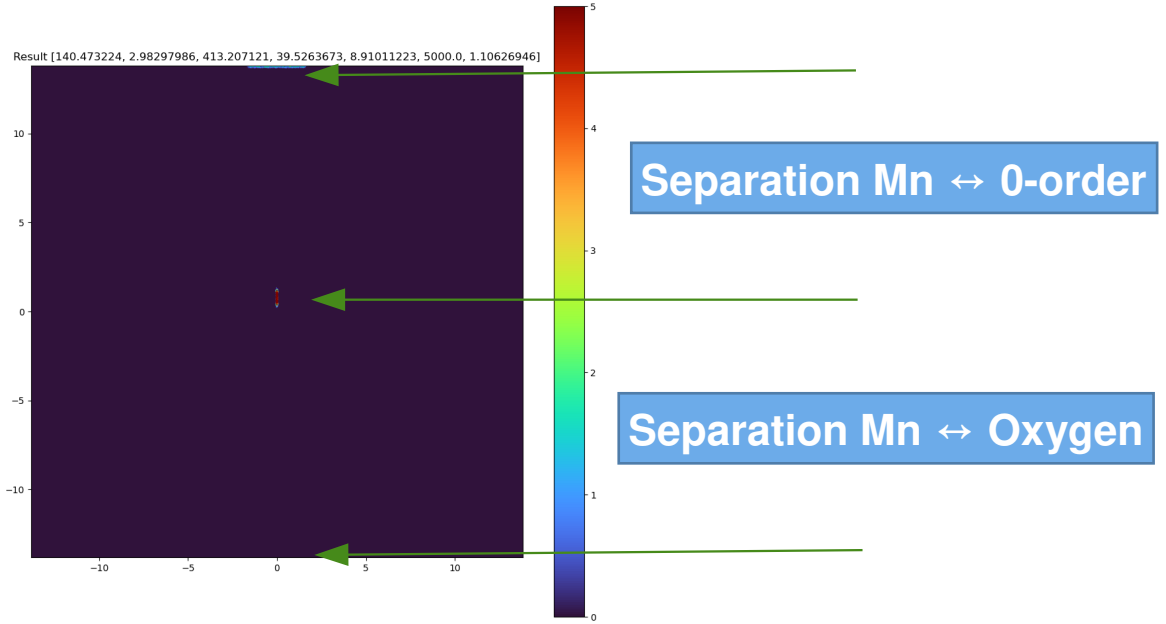
OPTIMISATION LOOP



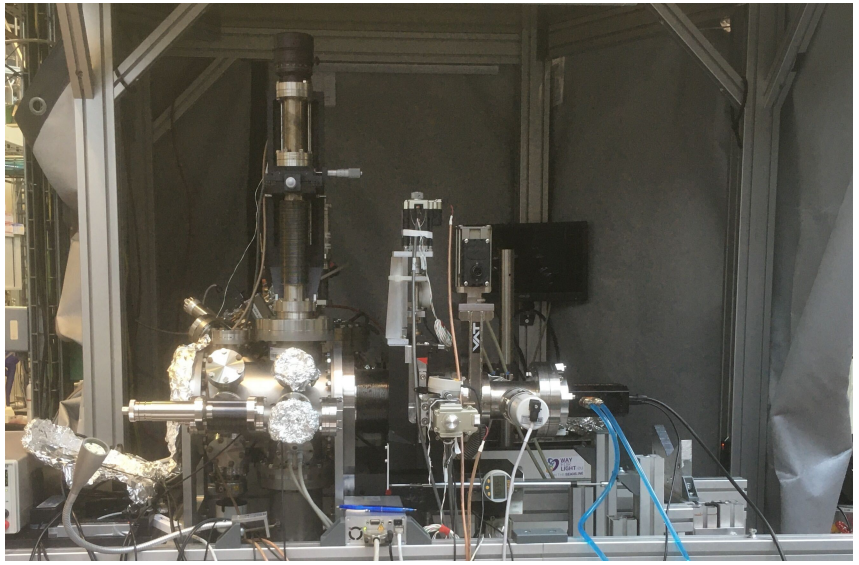
RESULT

- Design angle alpha: 2.98297986
- Design Angle beta: 1.10626946
- Sagittal entrance arm length:140.473224
- Sagittal exit arm length: 413.207121
- Long Radius R: 5000.00000
- Slope Error Sagittal: 39.5263673
- Slope Error Meridional: 8.91011223



Outlook

- Utilise domain adaption and augmentation to realise the training of surrogate models (Histogram->params)
- Expand scope to the alignment of entire beamlines (Rock-IT project) – Metrix beamline 62 parameters
- Further optimise RZP design in order to improve signal intensity
- Design new RAC Spectrometer based on AI feedback – in progress
- RAY-X deliverable (docker…)
- Integration of RAY-X into Bluesky (Simone Vadilonga, HZB)



Git Repository:
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Acknowledgements

- Jens Viefhaus and Lars Grunske
- HZB Machine Learning Group
  - Gregor Hartmann, David Meier, Gesa Goetzke, Felix Moeller
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  - Peter Baumgärtel, Rudi Schneider, Oussama Sayari, Jannis Maier, Enrico Ahlers, Fanny Zotter
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Swedish
Research
Council

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