Neural networks for FEL diffraction image separation



Hamburg, 14.11.2025

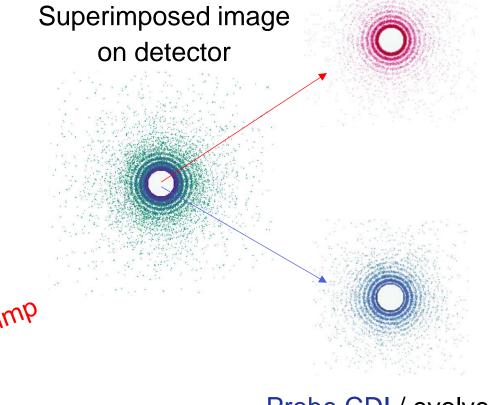
Nikita Morozov

SQS, European XFEL

_At ≤ 1 ps

Pump CDI / initial state

Problem setting



Dataset available:

Pump

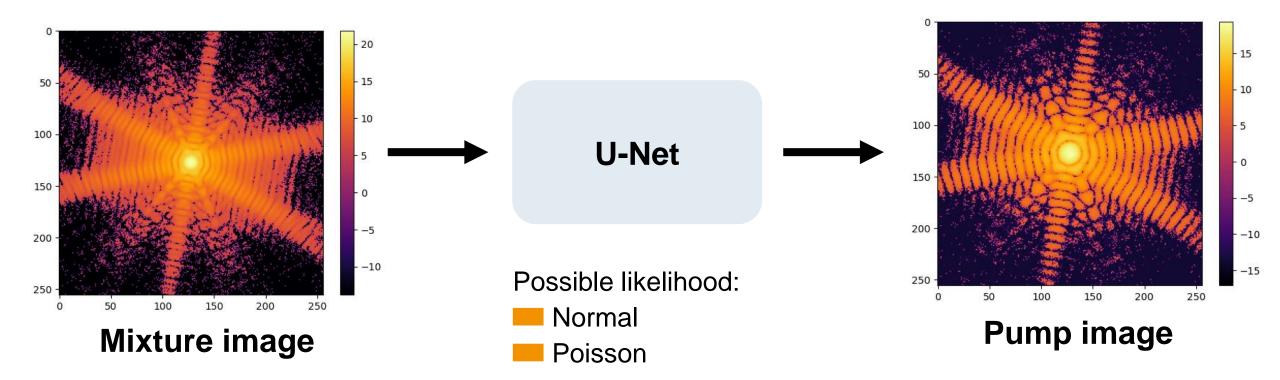
Superimposed images

Datasets are unpaired
No probe dataset

Probe CDI / evolved state

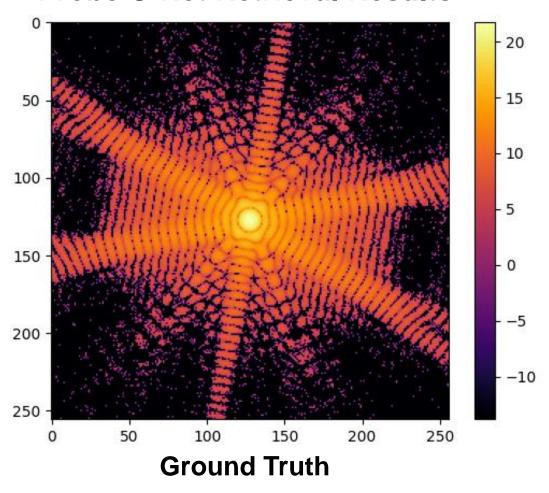
Challenge ⇒ Separate superimposed images

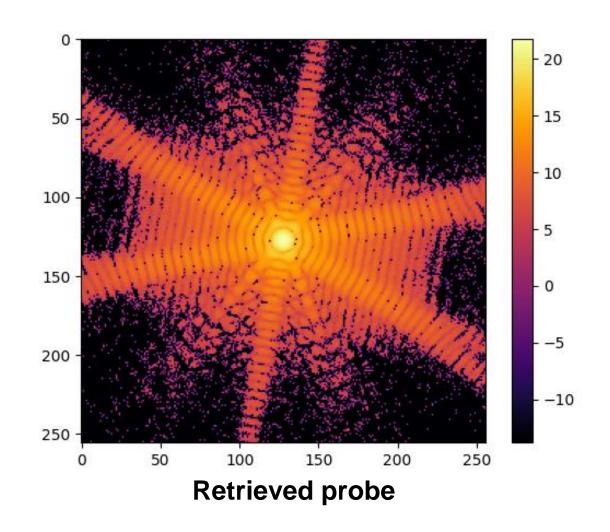
Feed-forward CNN



Trained with realistic pulse simulations

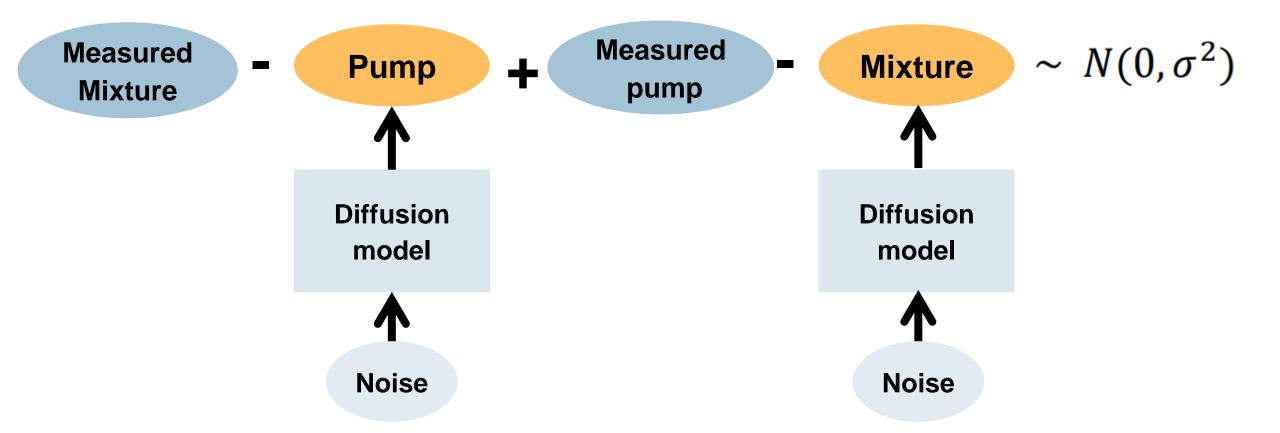
Probe U-Net Retrieval Results



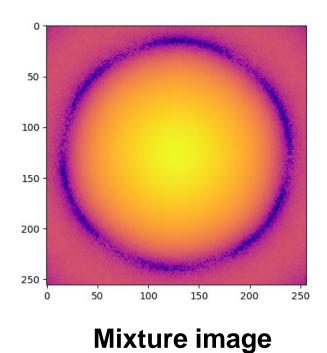


Diffusion model pipeline

How to handle missing pairing and unrealistic simulations?



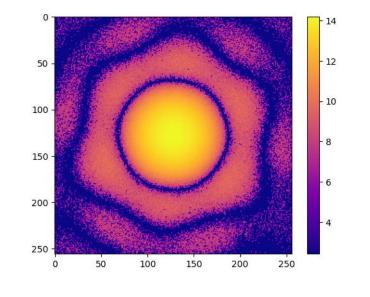
Diffusion Retrieval Results

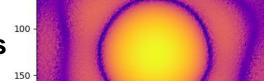


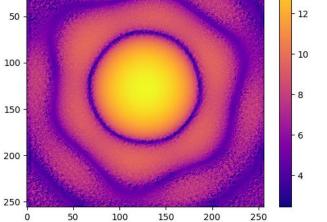
Ground Truth



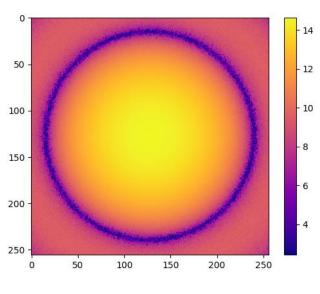


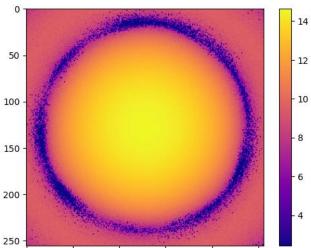






Probe pulse





150

200

250

100

50



Summary and outlook

Developed two strategies: feed-forward NN (validation) and diffusion model approach

Results display high uncertainty around diffraction minima

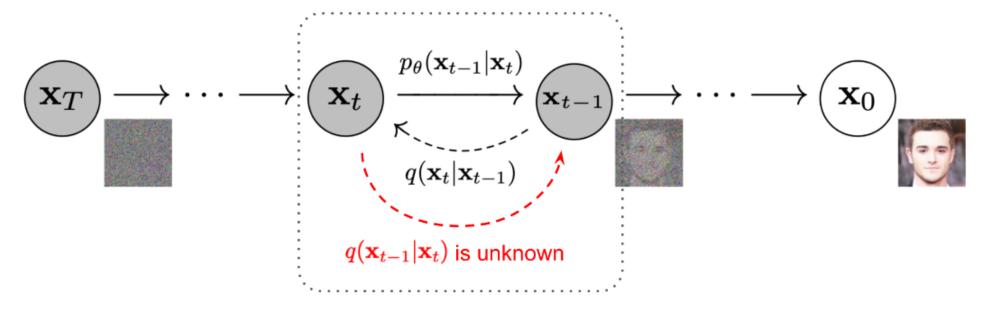
Plans: Improve loss function and preprocessing scheme

Acknowledgements

- Yevheniy Ovcharenko, European XFEL
- Danilo Enoque Ferreira de Lima, European XFEL
- Dmitry Vetrov, Constructor University Bremen

Thank you for your attention!

Diffusion model



- Capable of modeling pump and mixture distributions
- We use U-Net model (5M params) to estimate the parameters of an unknown distribution
- It takes the noisified image and a timestamp to predict parameters

Guidance at timestep t: idea

- Train pump diffusion model and mixture diffusion model
- Compute probe pulse in two different ways
- Difference between these results is a Gaussian with zero mean
- Update conditional distribution parameters for samples at timestep t-1