A resilient feature extractor in SAXS images

6th Round Table on Deep Learning @ DESY

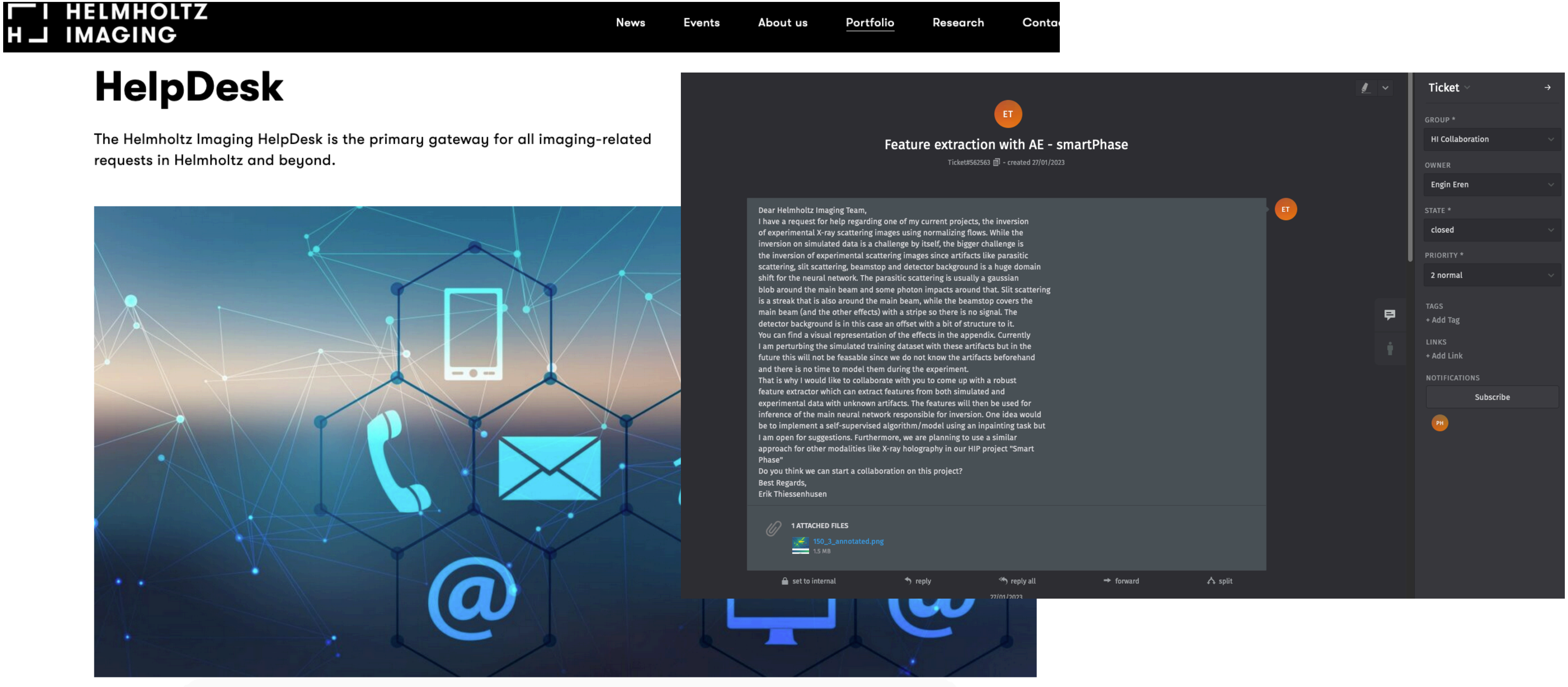
Engin Eren (HI), Philipp Heuser (HI), Erik Thiessenhusen (HZDR), Lingen Huang (HZDR)

HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

HELMHOLTZ IMAGING

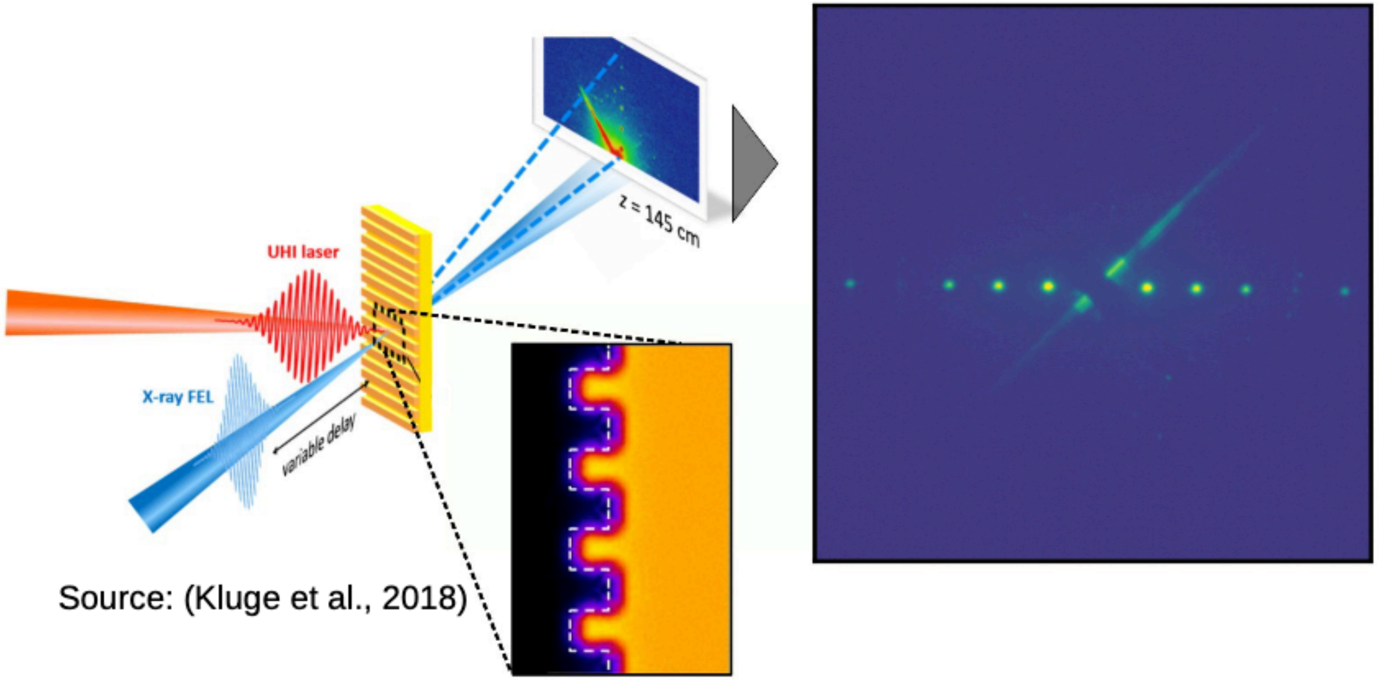
DESY.

Story begins with… Helmholtz Imaging HelpDesk



Experiment

- Goal: understanding laser-solid and laser-plasma interactions + Ion Acceleration
- Simulations for interactions exist → need verification

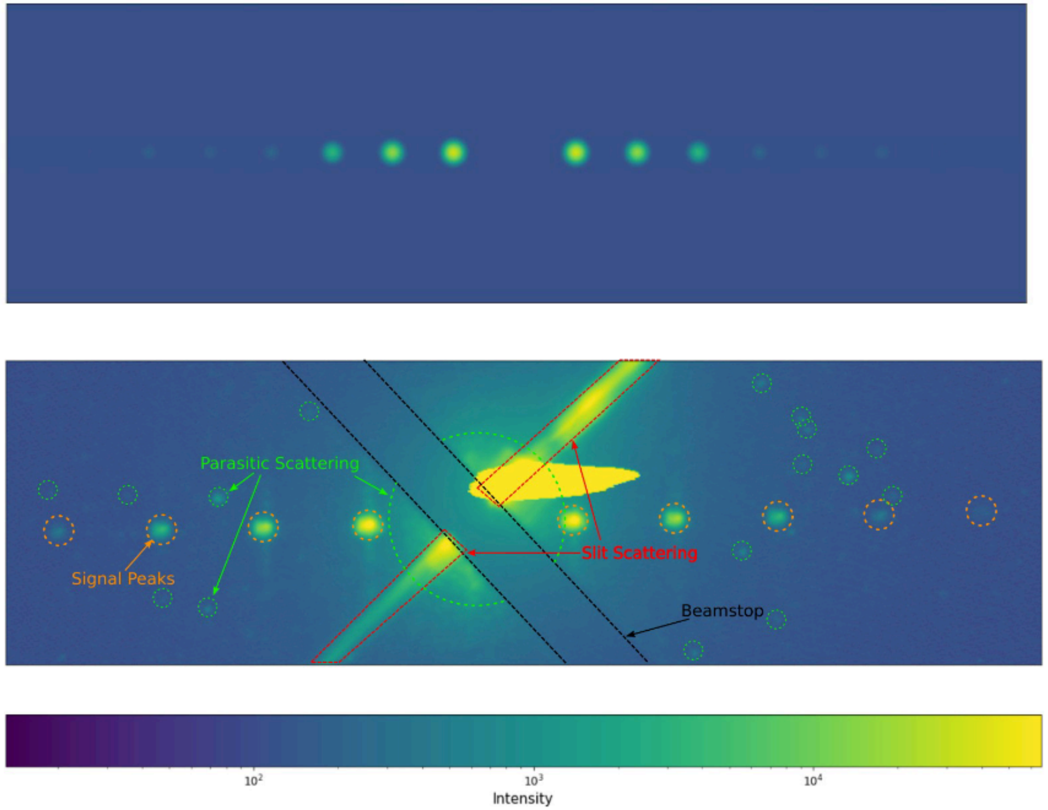


Source: (Kluge et al., 2018)

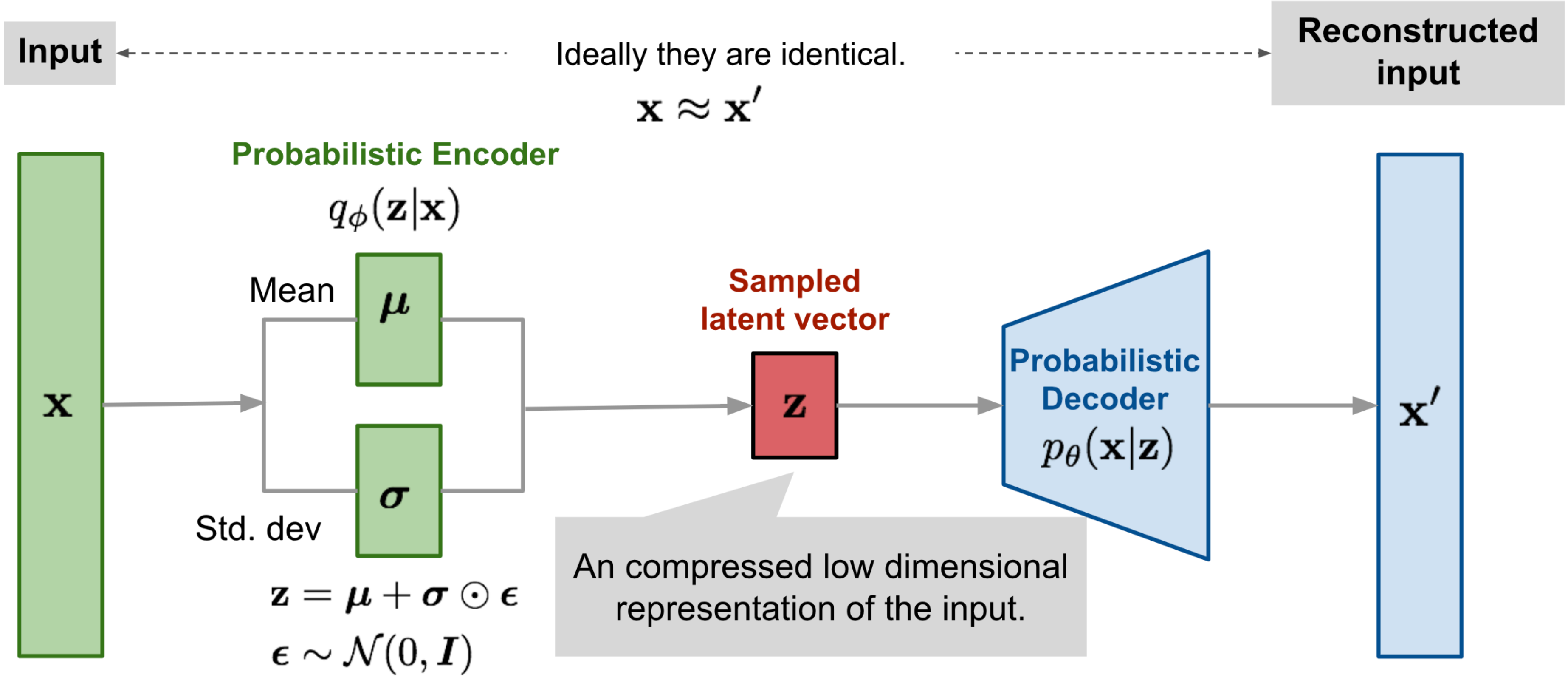
- Sensor only sums up intensity of photons, not phase → phase problem

Solution – A robust Feature Extractor

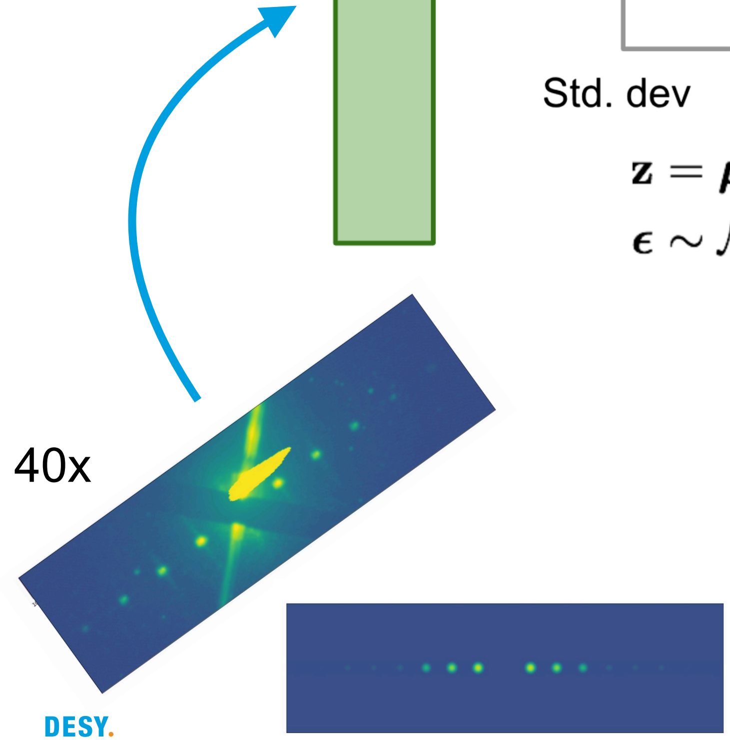
- Need a feature extractor that **works both on simulated and experimental data** (and for different targets)
- Features are used to train cINN
- Additional challenge: **data imbalance** (very few experimental images)
- Available data:
  - **SAXS grating** data both experimental and simulated (LCLS)
  - **SAXS + PCI wire** data; experimental data available, simulated data would need some work (EuXFEL, Hibef)



β-VAE: Learning disentangled representations



Source: https://lilianweng.github.io/posts/2018-08-12-vae/



40x

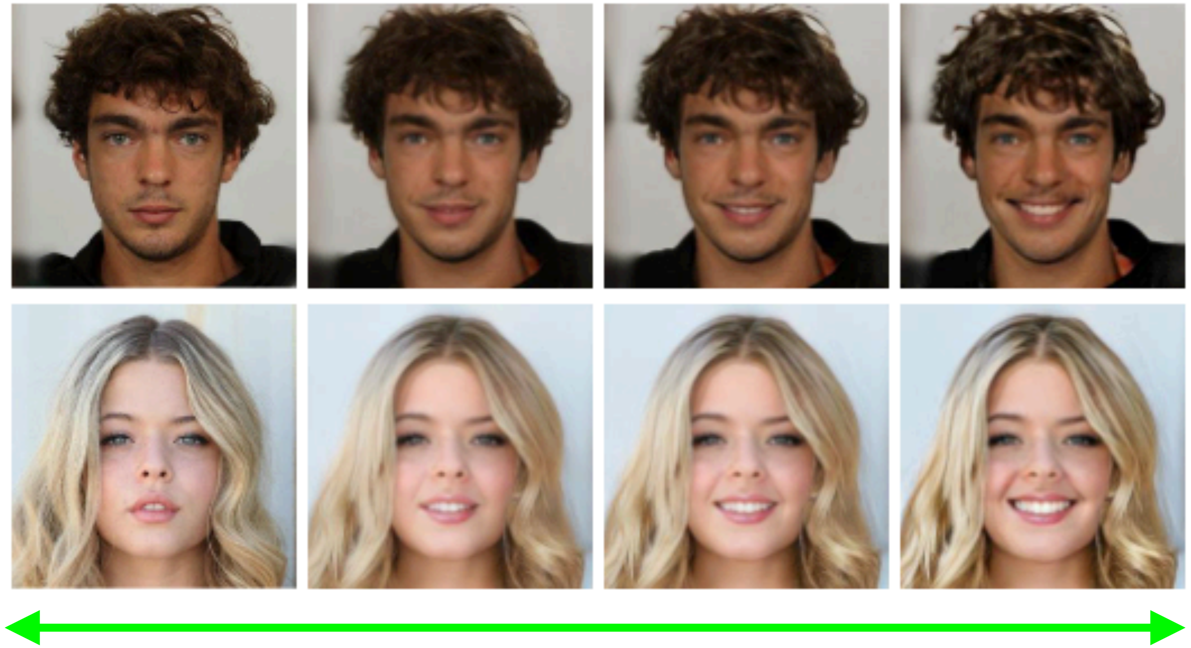
x200

$$\mathcal{L}(\theta, \phi; \mathbf{x}, \mathbf{z}, \beta) = \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\log p_\theta(\mathbf{x}|\mathbf{z})] - \beta\, D_{KL}\big(q_\phi(\mathbf{z}|\mathbf{x}) \,\|\, p(\mathbf{z})\big)$$

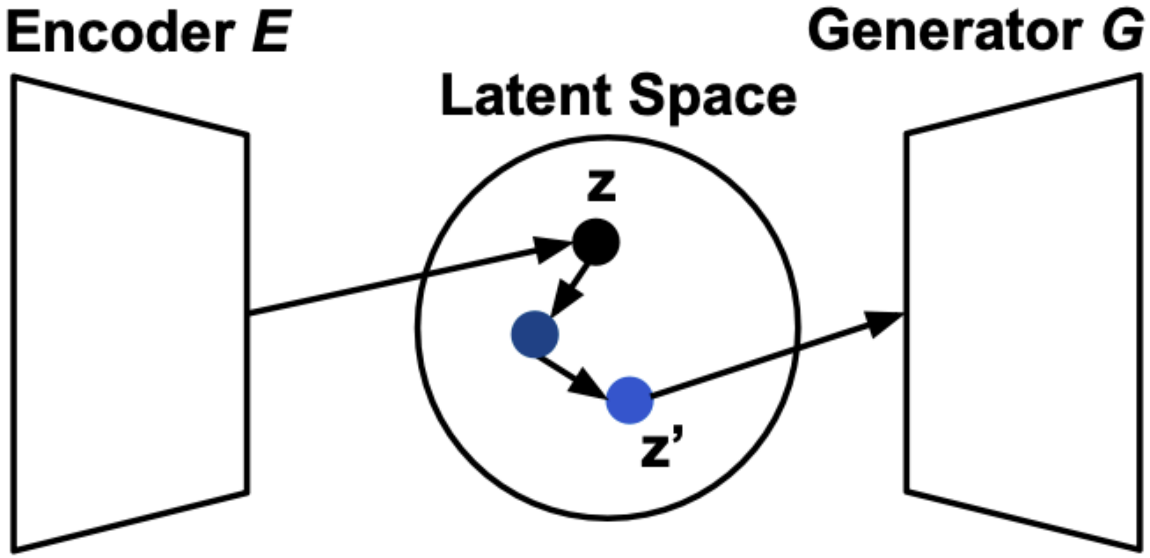
a stronger constraint on the latent bottleneck and results more disentangled latent representations $\mathbf{z}$

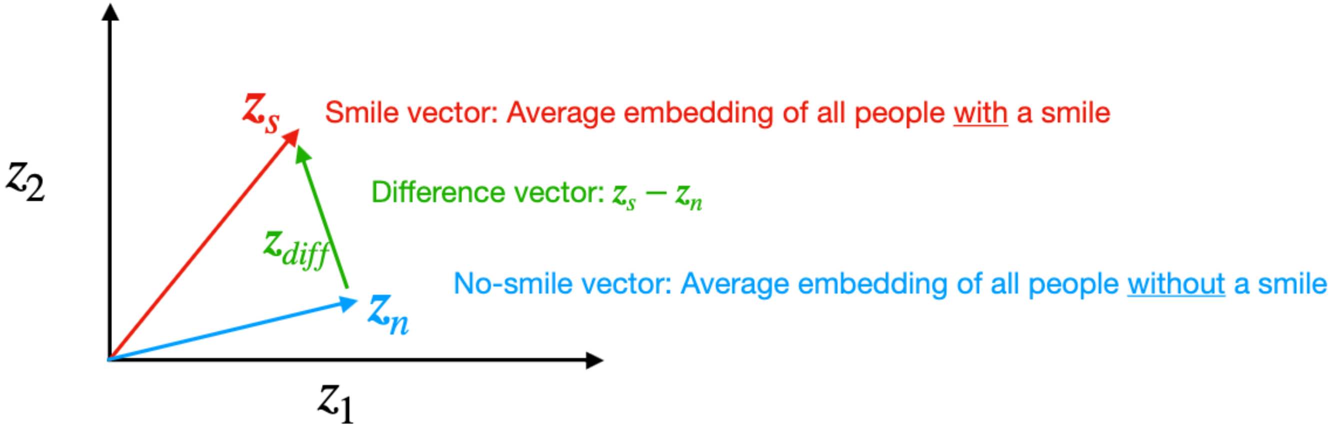
β-VAE: Latent Space Manipulation

Moving in the latent space…



unsmiling smiling

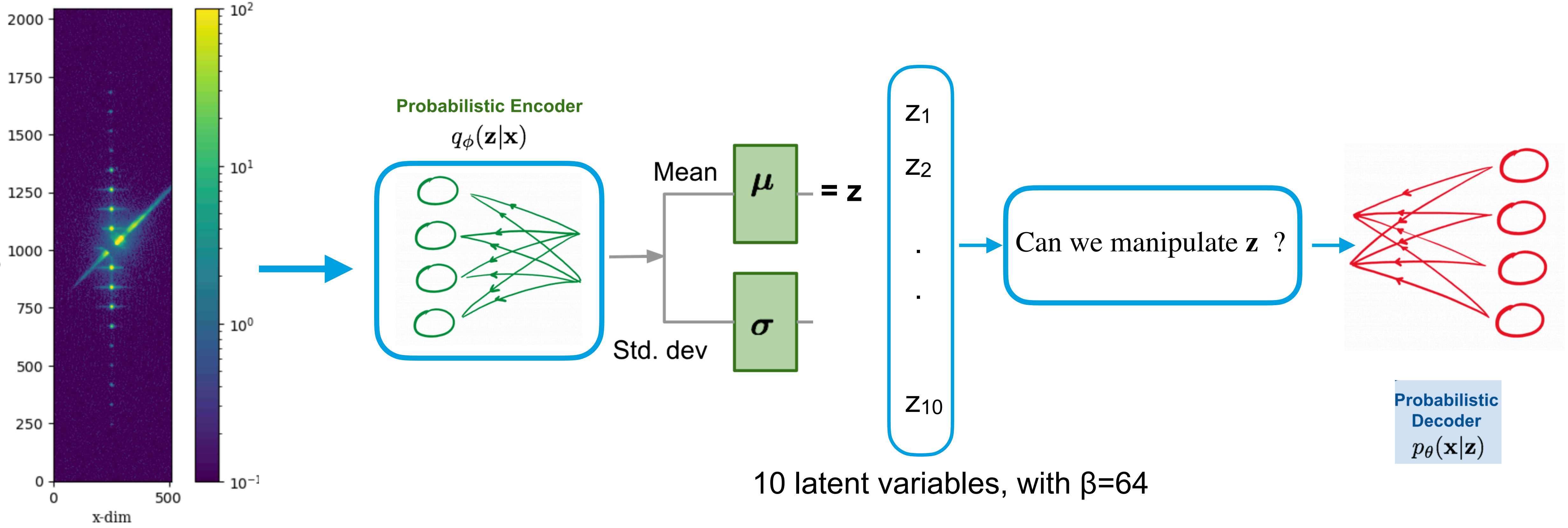




Source: https://sebastianraschka.com/pdf/lecture-notes/stat453ss21/L17_vae__slides.pdf

β-VAE: Results

Inference

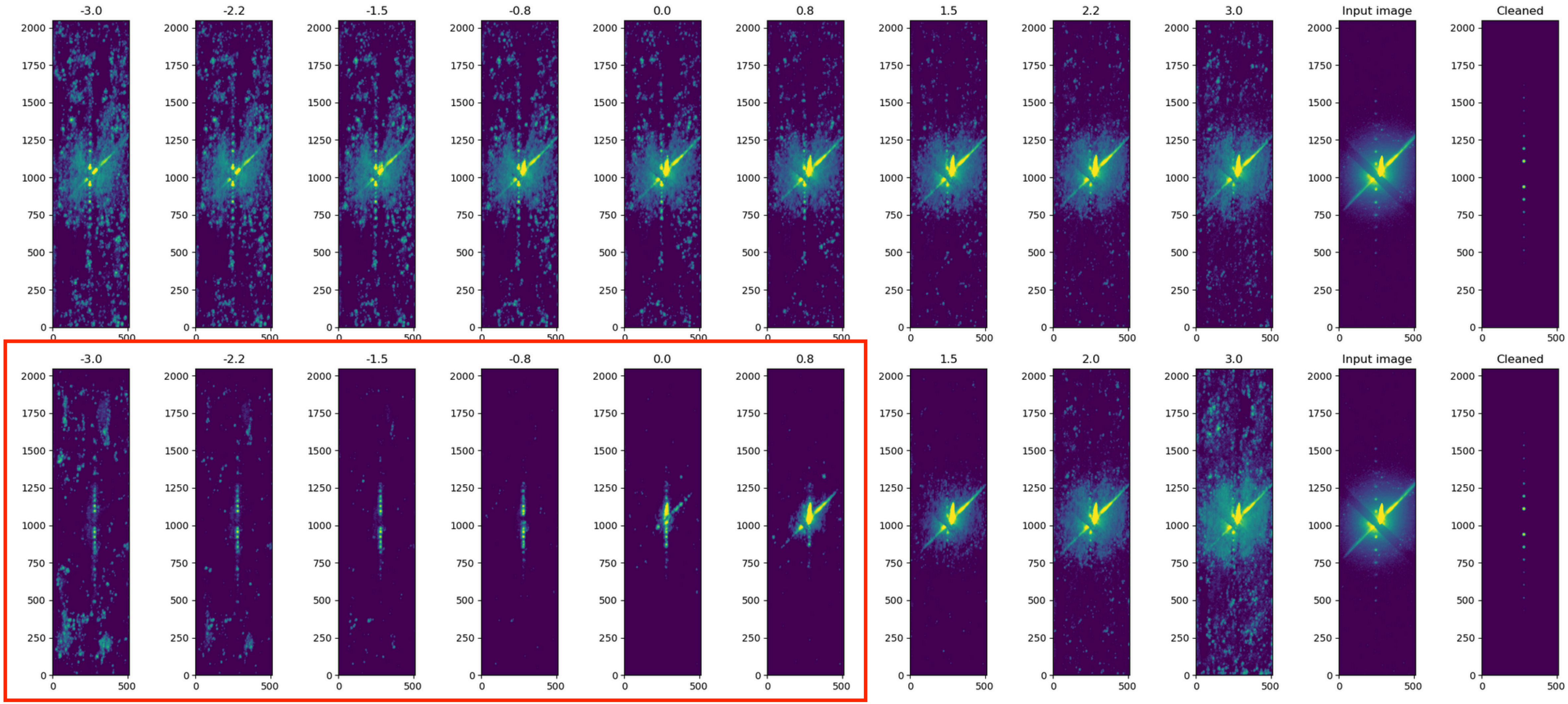


Latent Space Traversal

Changing 1 variable while keeping others fixed !!!

z9

z10



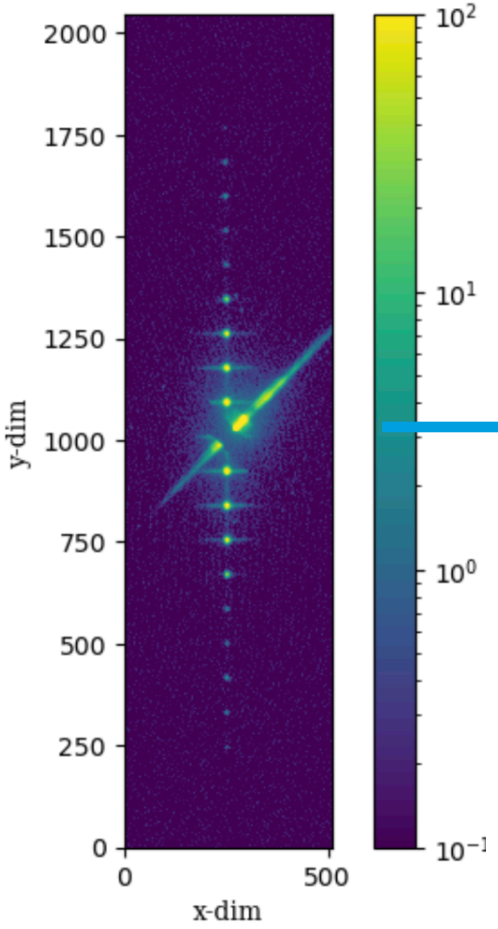
Glimpse of disentanglement ??

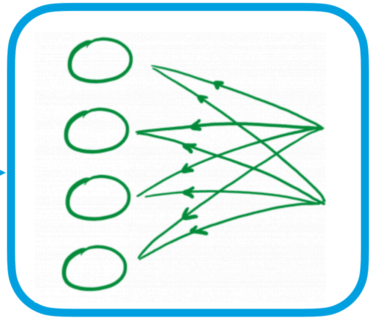
DESY.

Manipulation

Encoding the image and manipulating the z

Original





= z

z_1

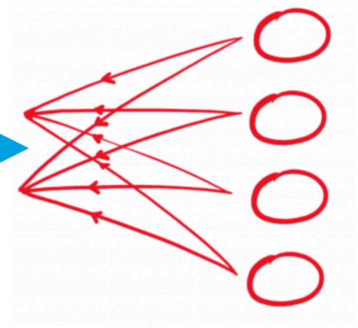
z_2

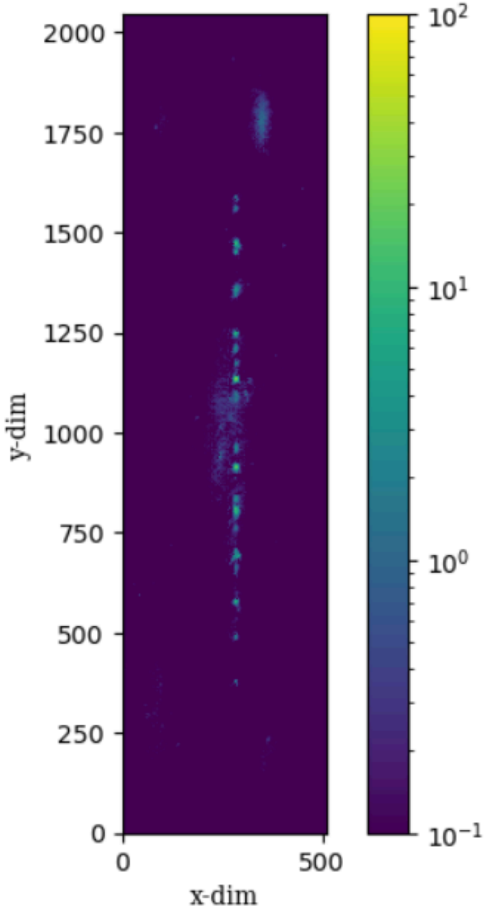
.

.

z_{10}

Set it to -2.5 ?



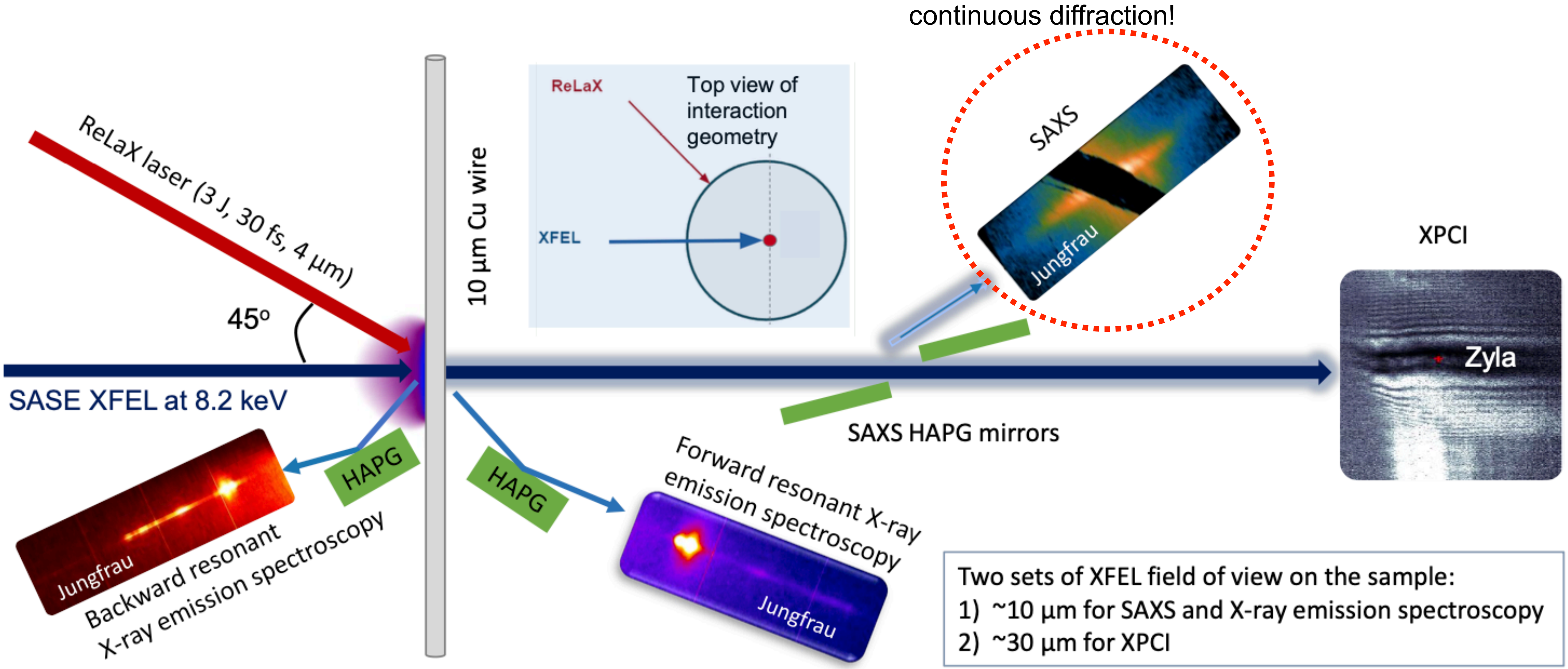


Some artefacts are gone! But.. preservation of the <u>signal quality</u> is not achieved

SAXS + Wire @ European XFEL

10-µm Cu Wire

(© Lingen Huang)

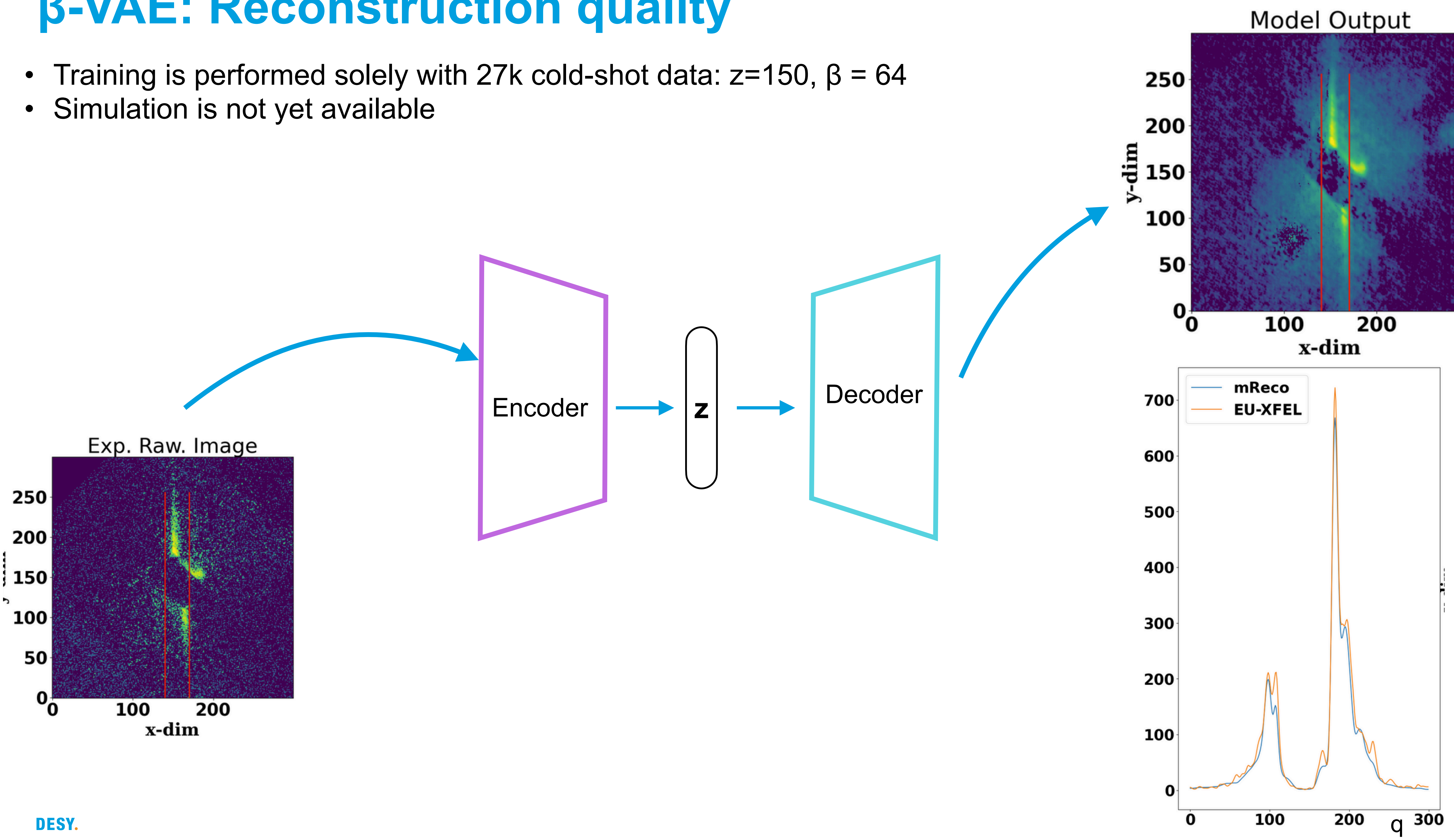


Two sets of XFEL field of view on the sample:

1) ~10 µm for SAXS and X-ray emission spectroscopy
2) ~30 µm for XPCI

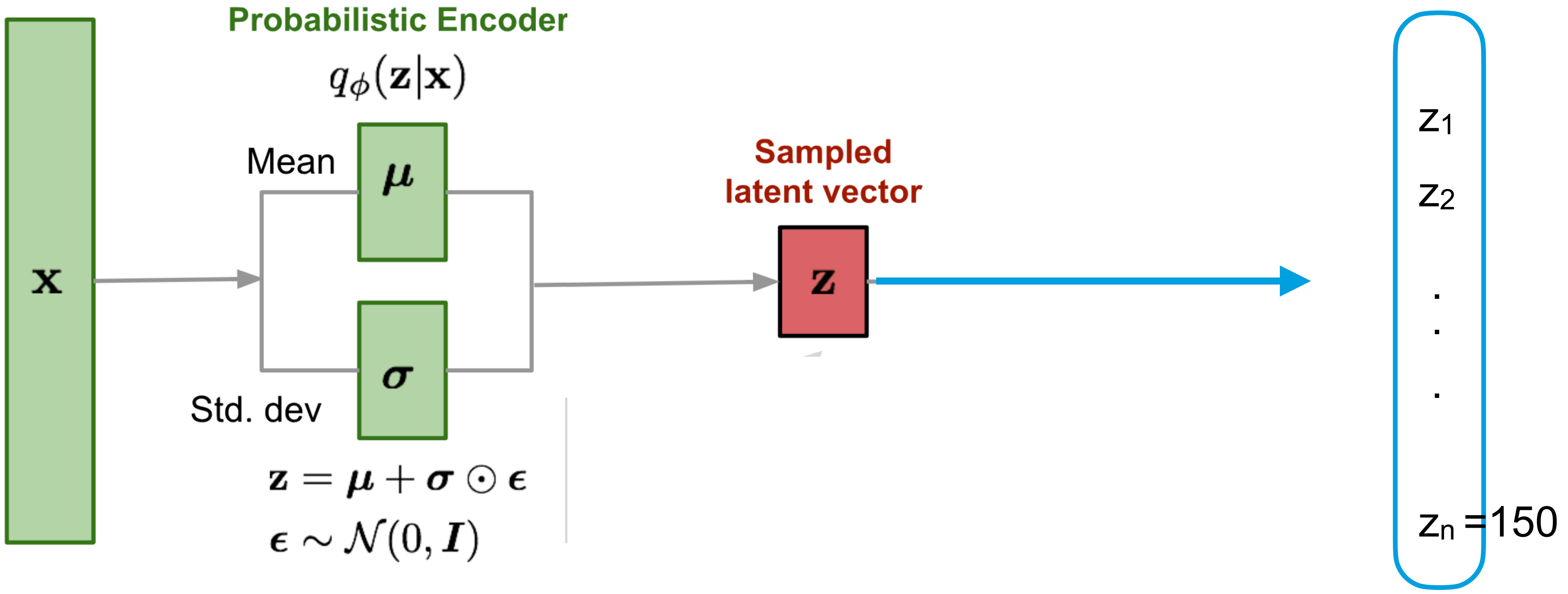
β-VAE: Reconstruction quality

- Training is performed solely with 27k cold-shot data: z=150, β = 64
- Simulation is not yet available

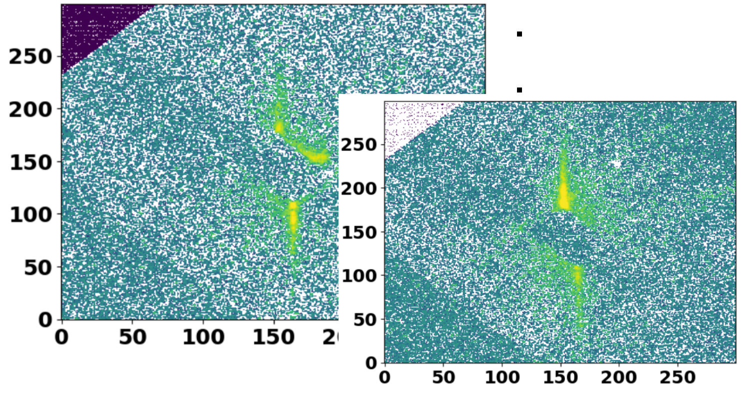


β-VAE: Get the Latent Space

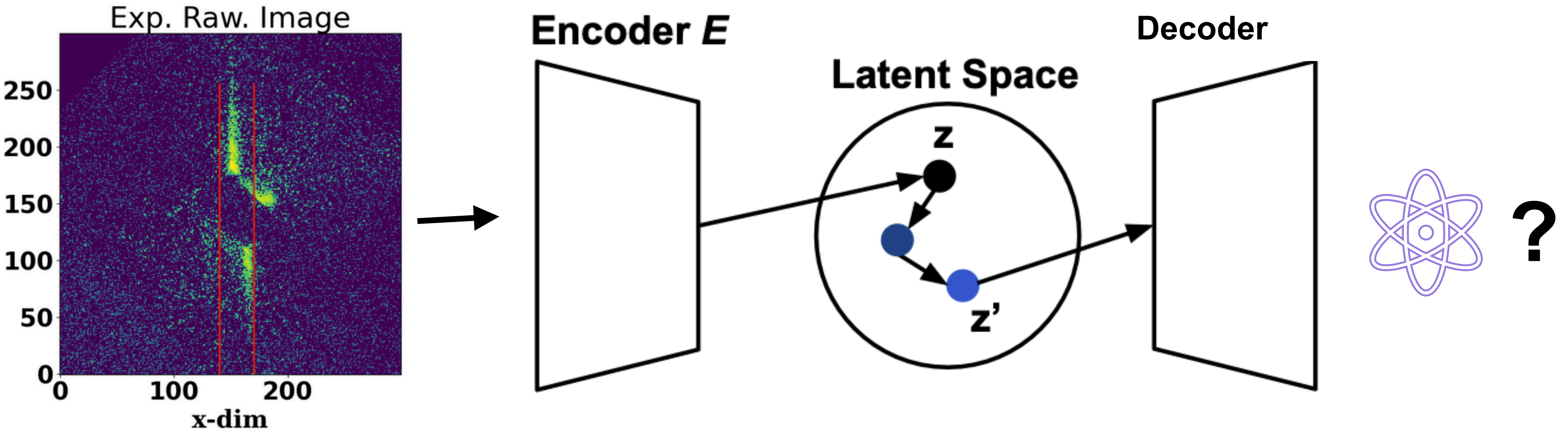
After training the β-VAE, need to construct the latent space



Take a batch of 1k images …



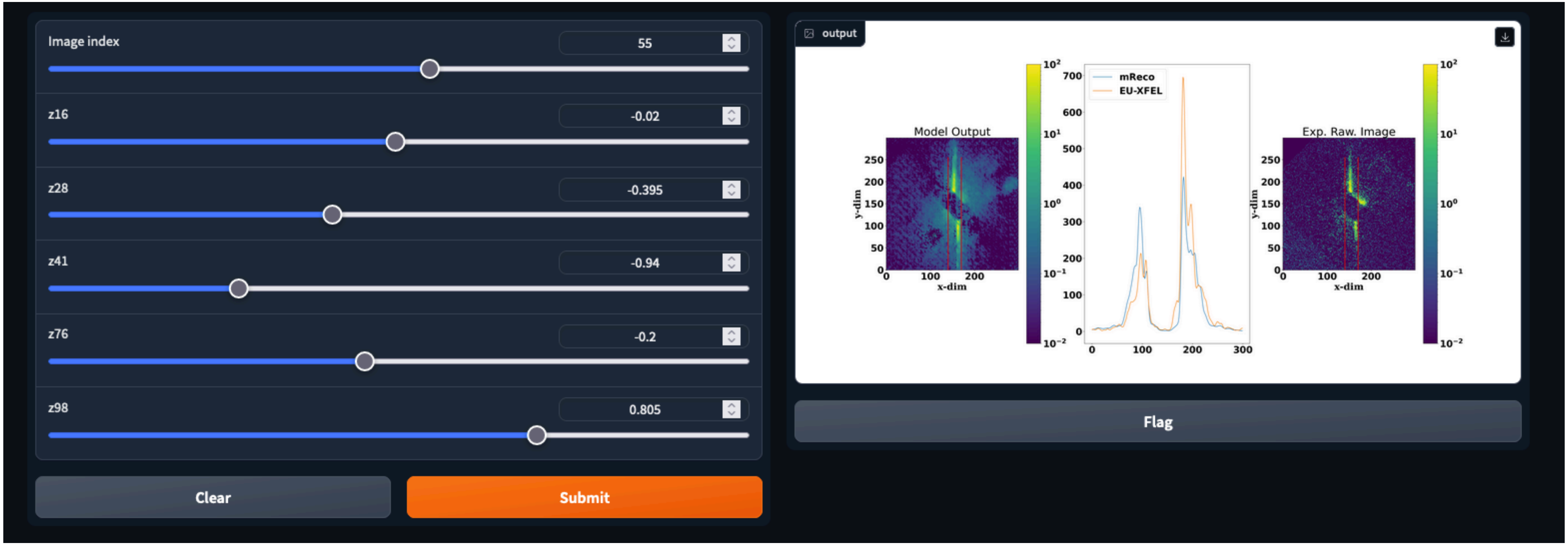
β-VAE: Manipulation



How can we move in our **z** <u>in the direction of **no-artefact** space</u> ?

β-VAE: Latent Space Manipulation

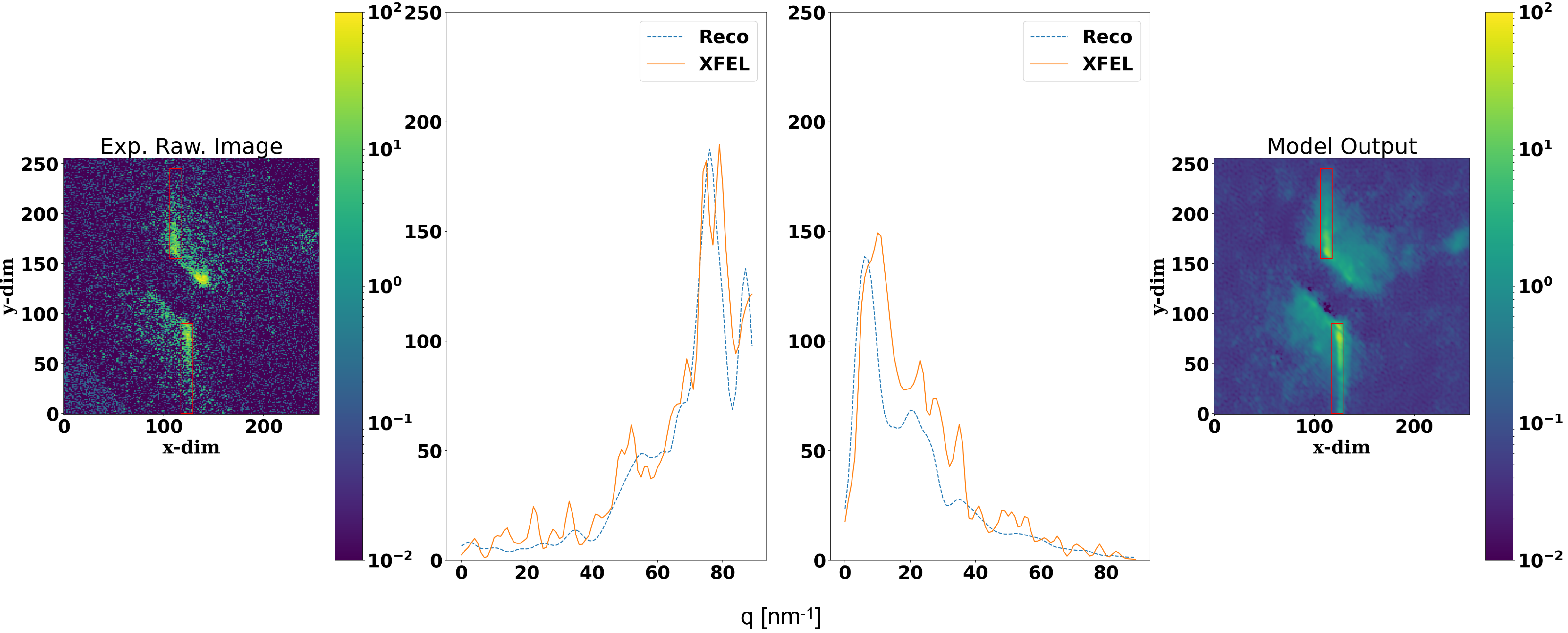
```
Running on local URL:  http://127.0.0.1:7860
Running on public URL: https://47787e1c13e6fa8a69.gradio.live

This share link expires in 72 hours. For free permanent hosting and GPU upgrades,
spaces)
```



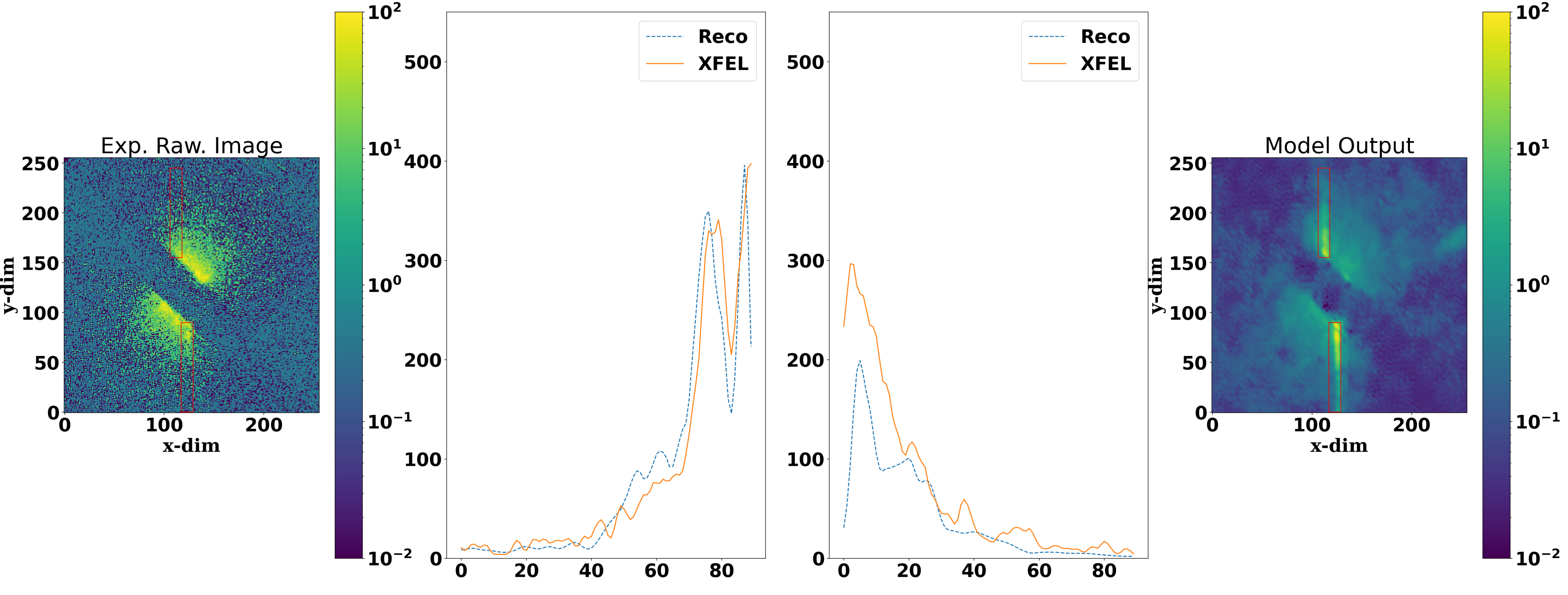

```
Default values these z's are:  -0.02007344365119934 -0.3955821394920349 -0.6009646058082581 -0.5929316282272339 0.8053598403930664
```

```
Default values these z's are:  -0.02007344365119934 -0.3955821394920349 -0.6009646058082581 -0.5929316282272339 0.8053598403930664
```

β-VAE: Latent Space Manipulation

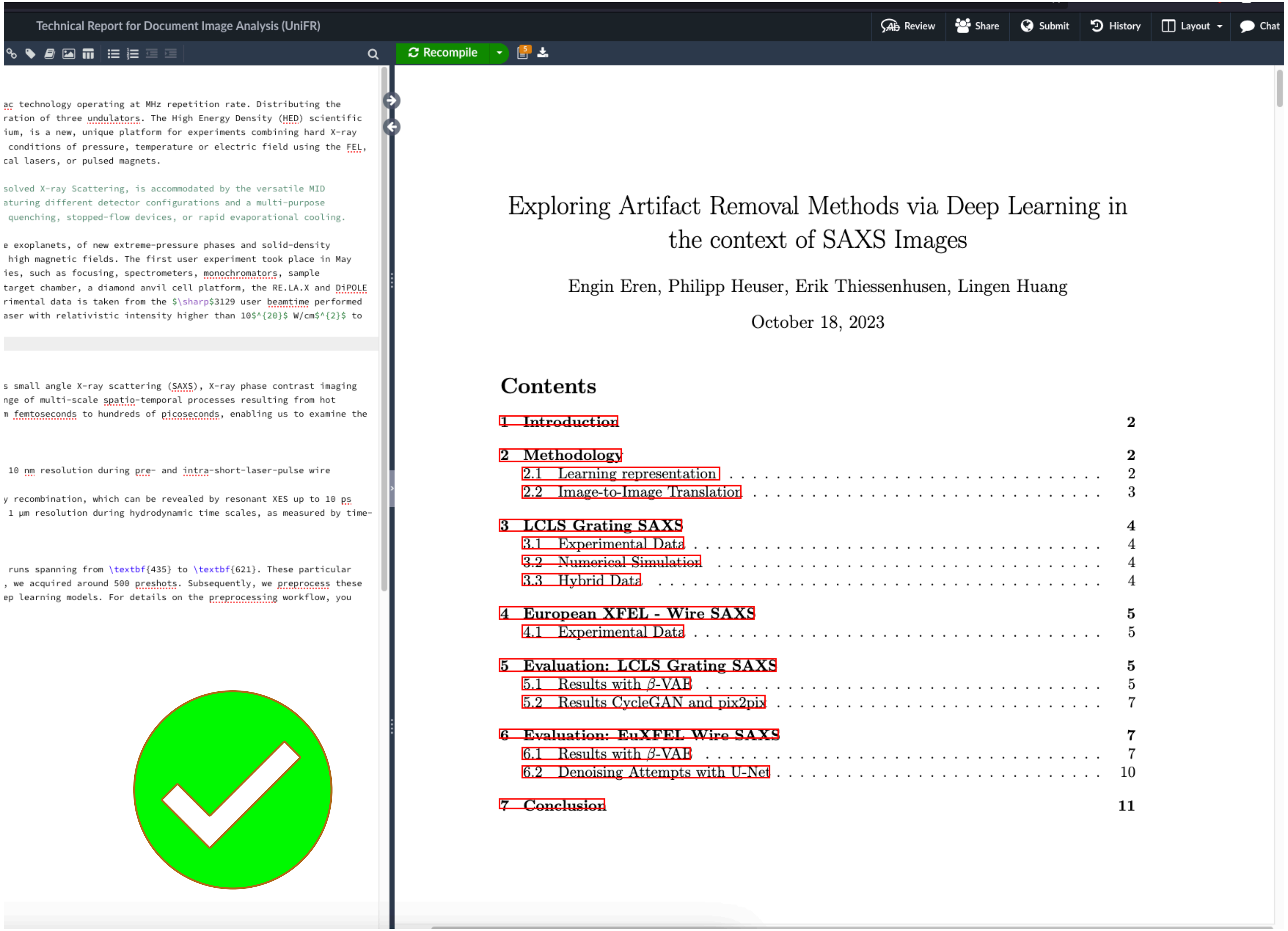


β-VAE: Latent Space Manipulation



q [nm⁻¹]

More information



More information

Beta-VAE with EuXFEL wire data

The project consists of two main parts, each responsible for a specific task.

Part 1: Creating Training Data

To create the training data, follow these steps:

```
python flowXFELwire.py run --outputF 'demo.hdf5'
```

METAFLOW

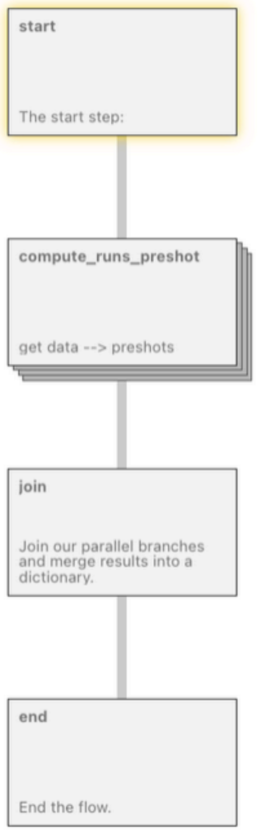
XfelWireFlow/1691064082765476/start/1

Task Metadata

Task Info

- Task Metadata
- Flow Parameters
- Artifacts
- DAG

Task Created On	2023-08-03 02:01:22 PM
Task Finished On	2023-08-03 02:01:30 PM
Task Duration	0:00:07
Tags	python_version:3.10.9, user:eren, runtime:dev, metaflow_
User	eren



Part 2: Starting Training

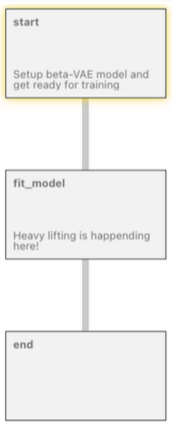
To start the training process, you need to modify the `flowXFELwire.py` file as follows:

```
if __name__ == "__main__":
    #XfelWireFlow()
    bvaeFlow()
```

now you can run

```
python flowXFELwire.py run --tagg TEST --max_iters 100
```

Parameters used here:



RIC > Helmholtz Imaging > xfel-saxs-wire

xfel-saxs-wire

Project ID: 7809

16 Commits | 1 Branch | 0 Tags | 317 KiB Project Storage

main README
Engin Eren authored 4 months ago

main | xfel-saxs-wire / | + | History

README | Add LICENSE | Add CHANGELOG | Add CONTRIBUTING | Enab

Add Kubernetes cluster | Set up CI/CD | Add Wiki | Configure Integrations

Name	Last commit
beta-vae_xfelwire	adding pics and DAG
unet_xfelwire	typo
.gitignore	Test2

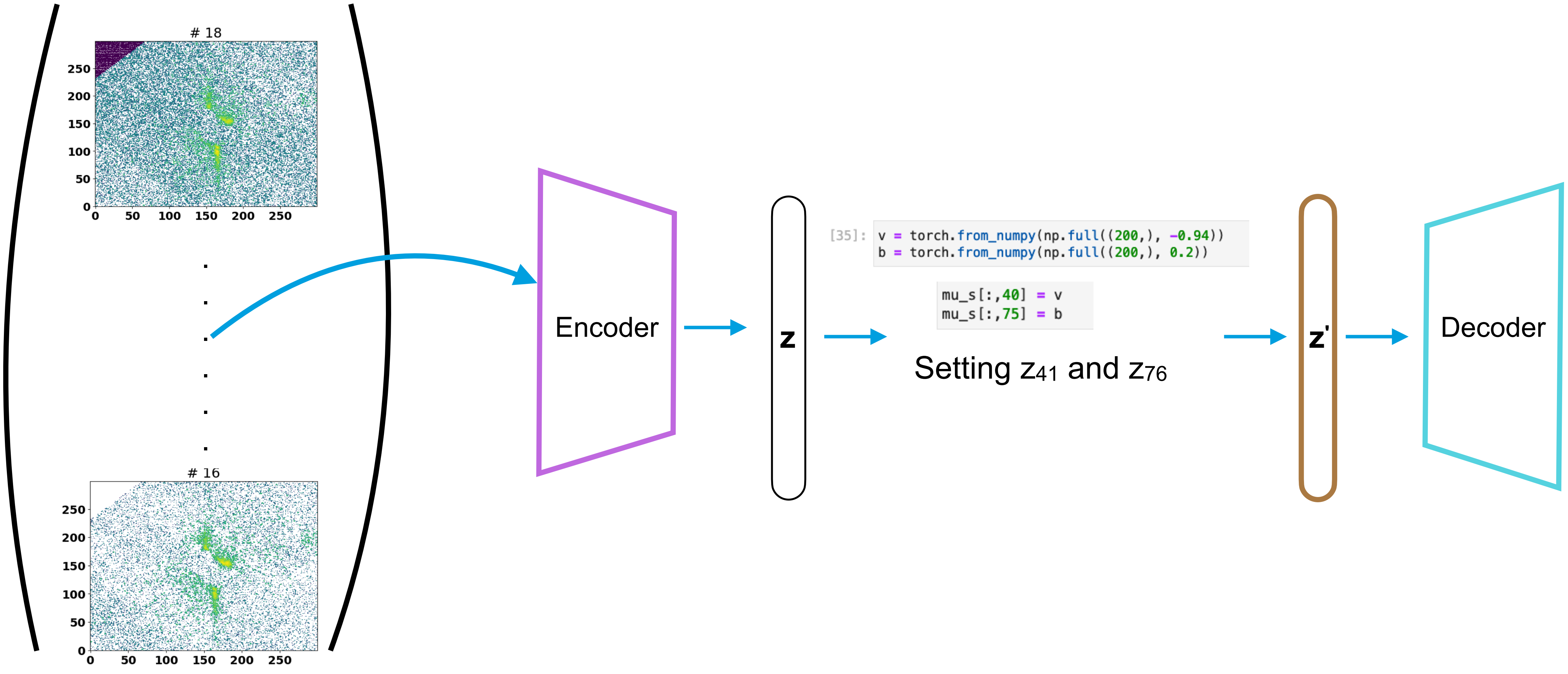
https://gitlab.desy.de/ric/helmholtz_imaging/xfel-saxs-wire

Backup

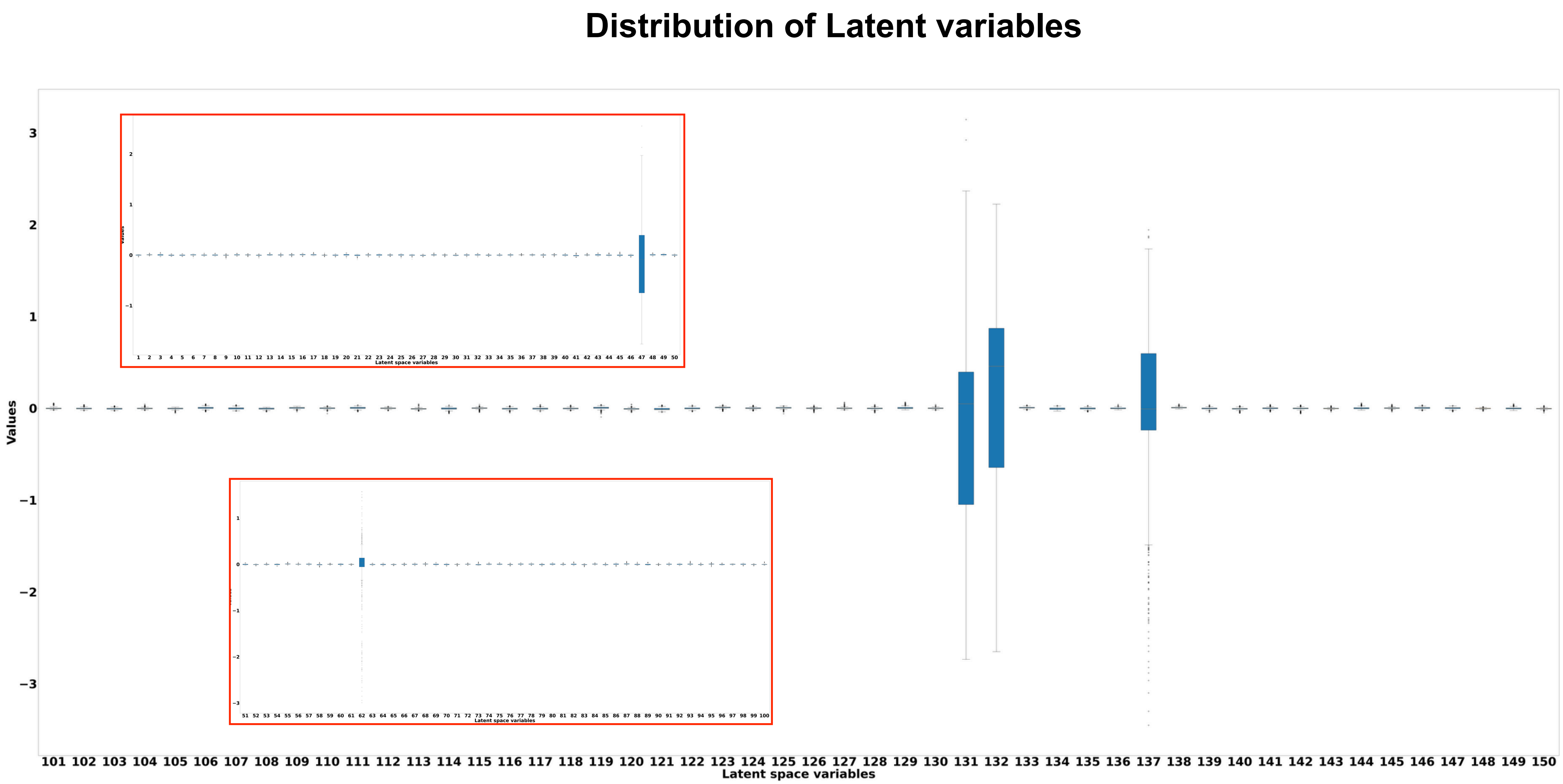
β-VAE: Latent Space Manipulation

Batch-wise

Take a subset of 200 images with obvious artefacts



β-VAE: Latent Space



5 latent variables are responsible for artefacts + signal ??