

# Deciphering FEL pulse profiles with autoencoder networks

Gesa Goetzke – FLASH Photon Diagnostics

Longitudinal photon diagnostics Workshop

Gesa Goetzke<sup>1</sup>, Rajan Plumley<sup>2</sup>, Felix Möller<sup>3</sup>, Thorsten Otto<sup>1</sup>, Daniel Ratner<sup>2</sup>,  
Joshua Turner<sup>2</sup>, Stefan Düsterer<sup>1</sup>, Gregor Hartmann<sup>3</sup>

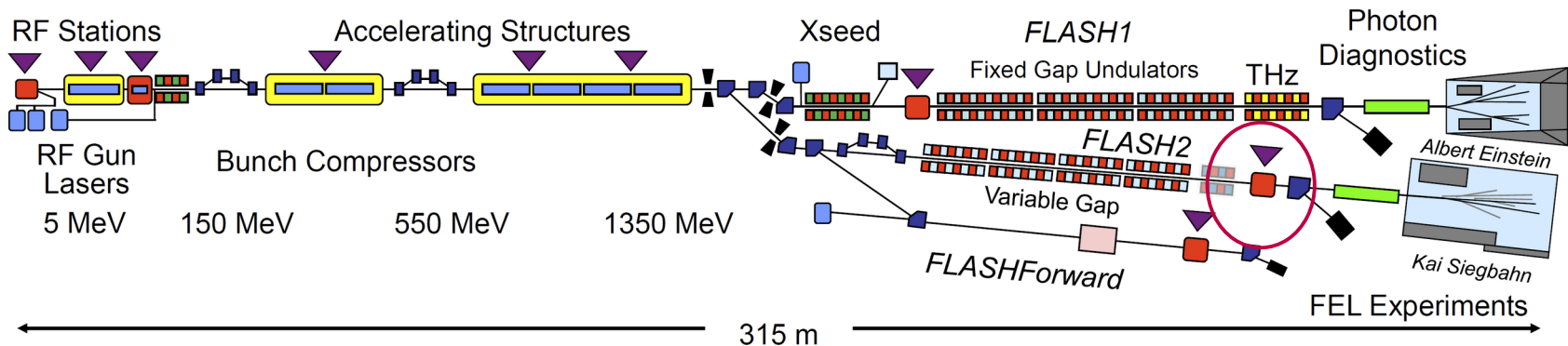
<sup>1</sup> Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

<sup>2</sup> SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA

<sup>3</sup> Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, German



# Pulse length diagnostics



[https://flash.desy.de/sites2009/site\\_vuvfel/content/e66400/infoboxContent259146/FLASH\\_layout-2022.png](https://flash.desy.de/sites2009/site_vuvfel/content/e66400/infoboxContent259146/FLASH_layout-2022.png)

- We want photon pulse length information.
- We analyze the energy of the electrons that created this photon pulse.

# Obtaining power profiles

## Few-femtosecond time-resolved measurements of X-ray free-electron lasers

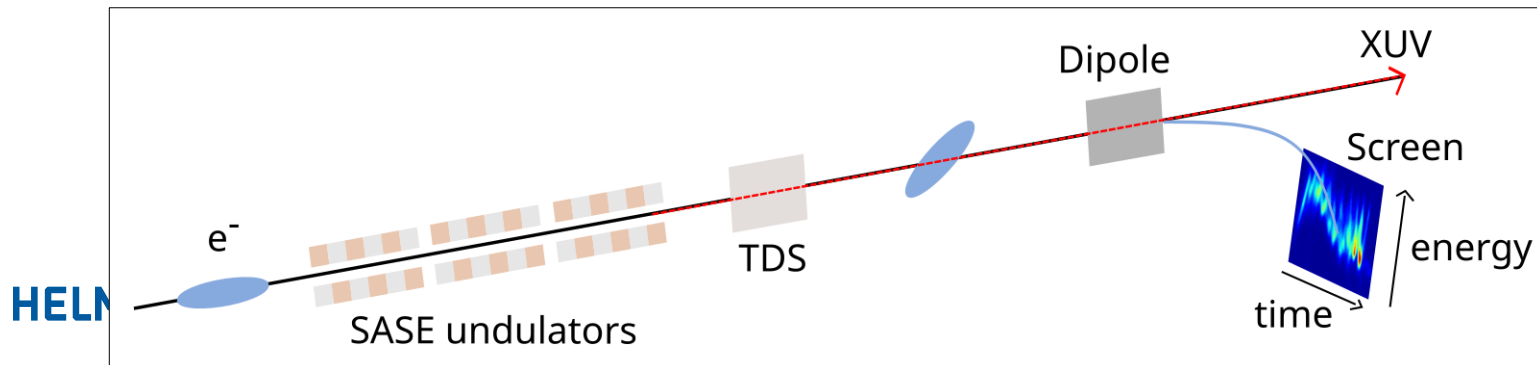
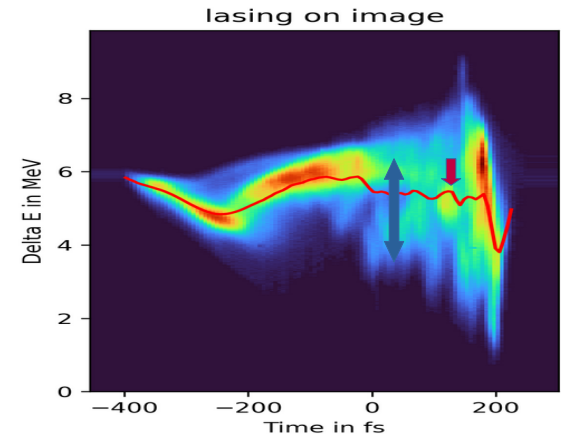
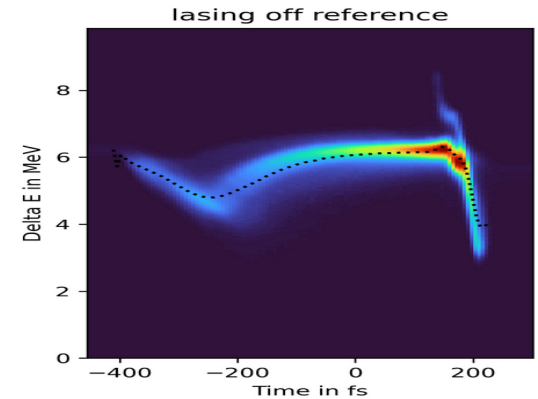
C. Behrens, F.-J. Decker, Y. Ding , V. A. Dolgashev, J. Frisch, Z. Huang, P. Krejčík , H. Loos, A. Lutman, T. J. Maxwell, J. Turner, J. Wang, M.-H. Wang, J. Welch & J. Wu

*Nature Communications* 5, Article number: 3762 (2014) | [Cite this article](#)

- to get a power profile you have to compare lasing on images with the matching lasing off images.
- you can compare the **center of mass** or the **energy spread**.

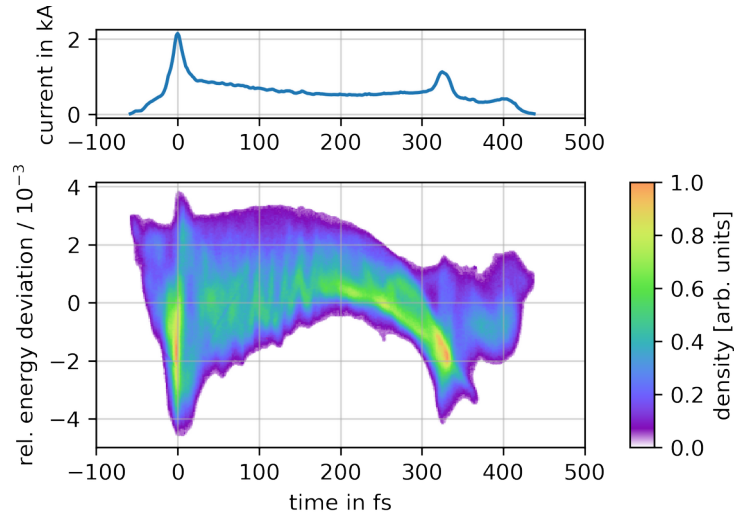
**Com:**  $P = \Delta E \cdot I / e$

**Spread:**  $P \propto I^{2/3} (\sigma_{E,on}^2 - \sigma_{E,off}^2)$

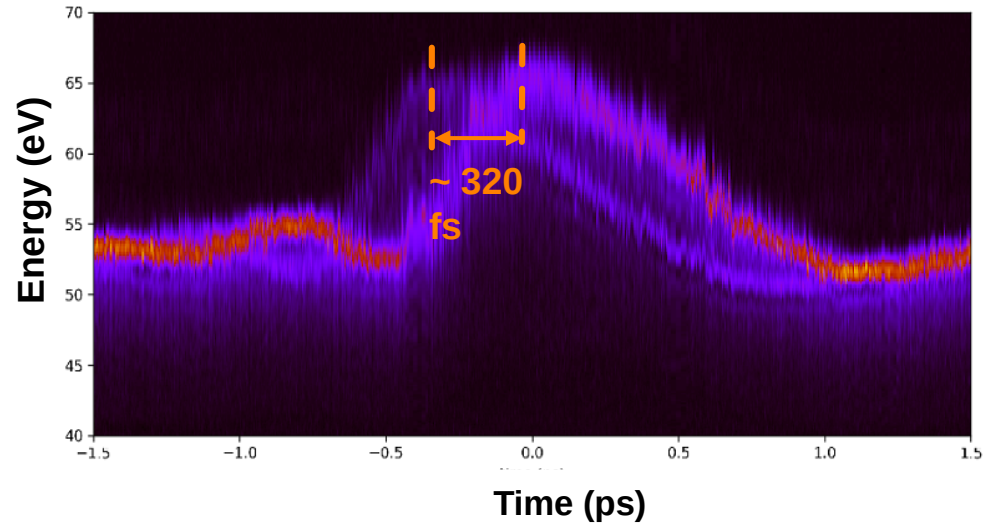
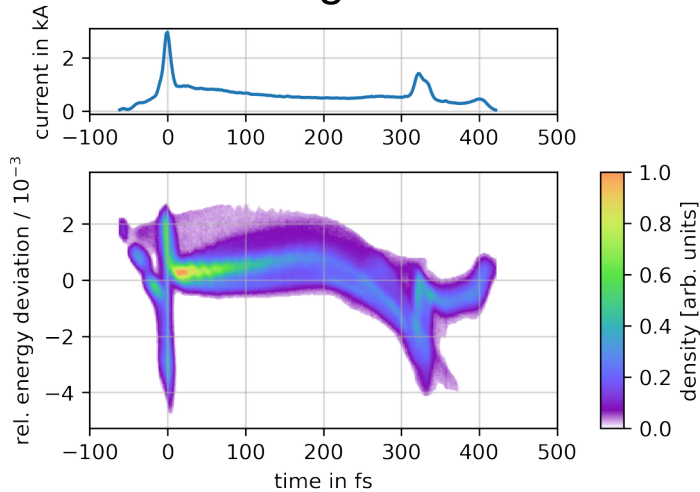


# Polarix and THz streaking

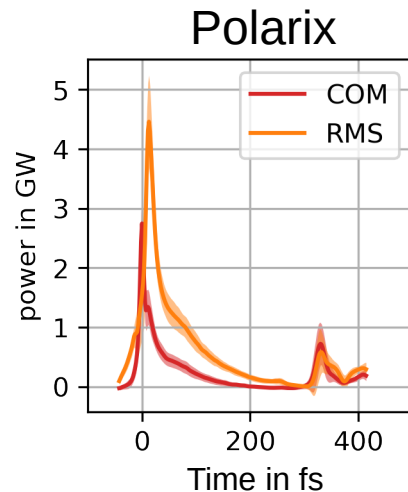
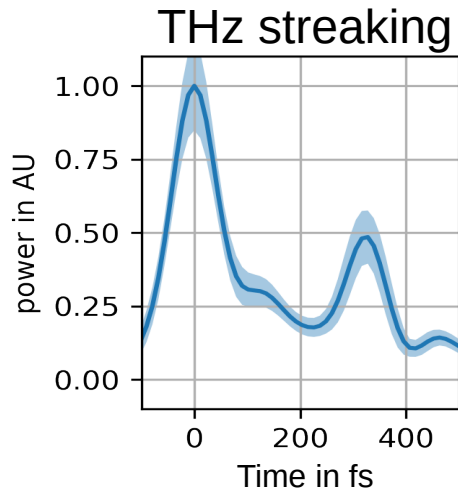
## Lasing on



## Lasing off



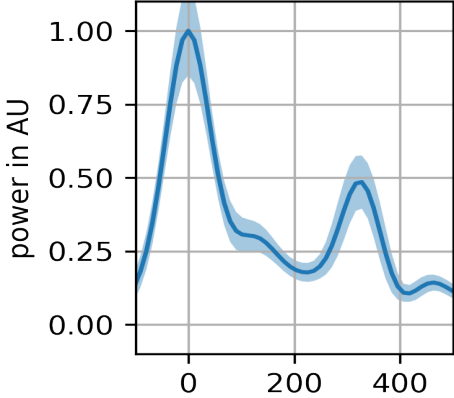
# Polarix and THz streaking



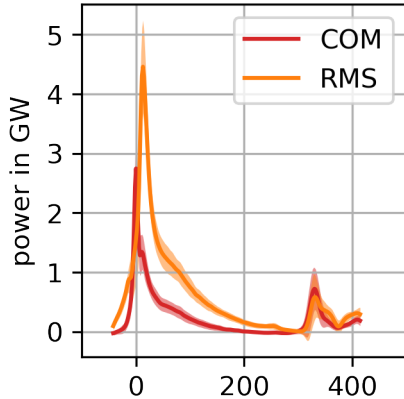
- THz pulses are much broader
- This has to do with the long THz streaking ramp
- For better comparison of the pulse shapes:
  - convolve the Polarix profiles with the THz streaking instrument function

# Polarix and THz streaking

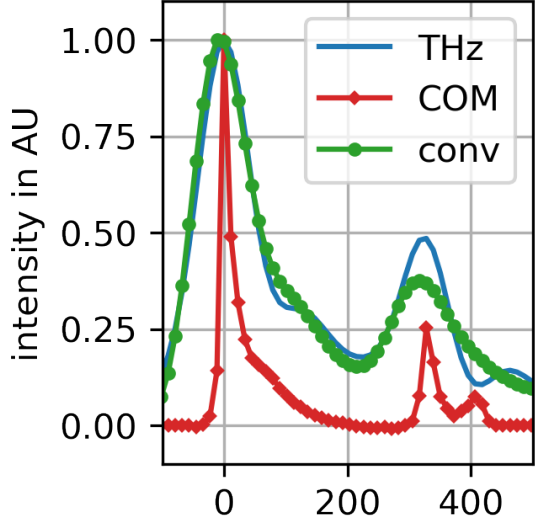
THz streaking



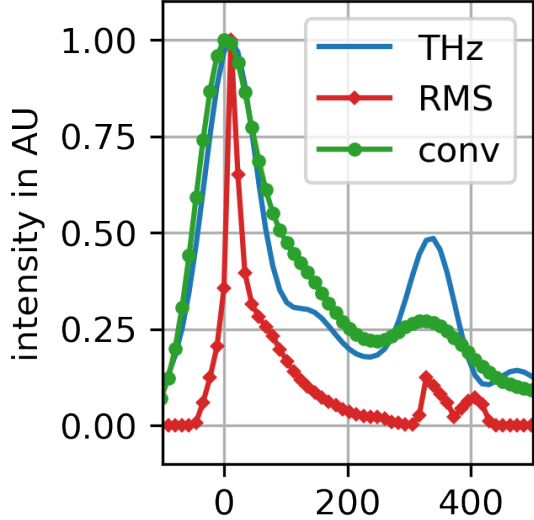
Polarix



COM (energy loss)



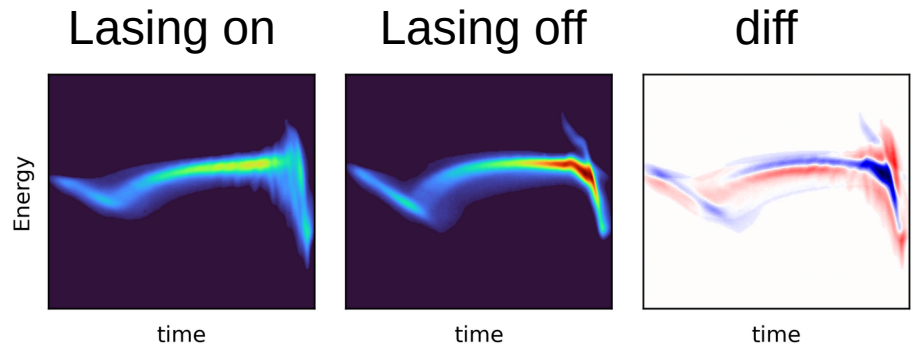
RMS (energy spread)



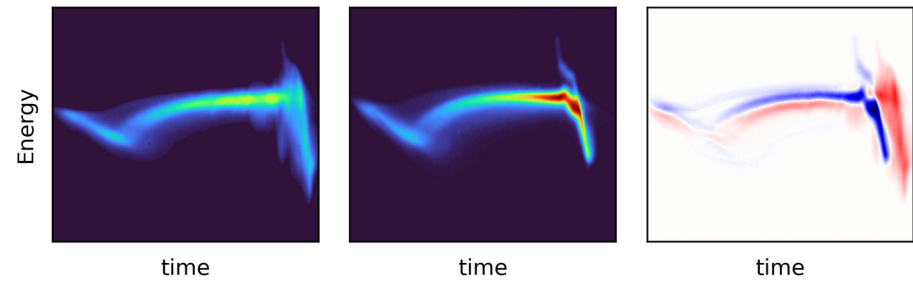
# Challenges in TDS analysis

## Finding matching lasing off references

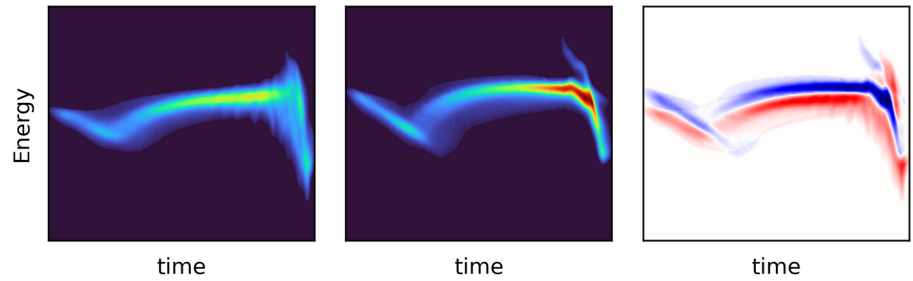
Finding the 'perfect' reference:



Isolating the signal / matching in x:



Matching in y:



# How to adress those challenges

“for foundational discoveries and inventions that enable machine learning with artificial neural networks”

“for protein structure prediction”



Machine learning is really good in pattern recognition, and with handling of large datasets.



# How to address those challenges

“for foundational discoveries and inventions that enable machine learning with artificial neural networks”

“for protein structure prediction”



**Ich** Write a sentence that contains the letter G exactly three times.

**KI** Sure! Here is a sentence that contains the letter G exactly three times: "The gentle breeze was gliding through the garden."

GPT4 omni

But sometimes fail in most basic tasks

You should never blindly trust them.

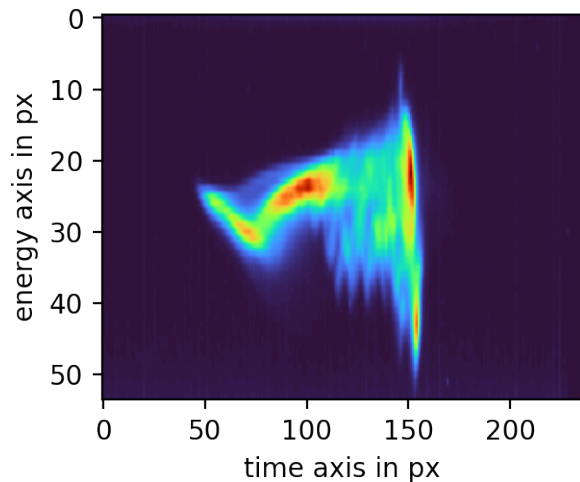


# Two projects with XTCAV and machine learning



## @FLASH (DESY)

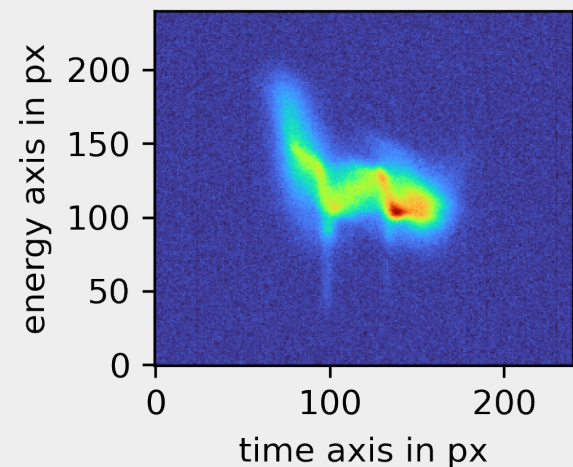
- SASE
- strong lasing signal



## @LCLS (SLAC)

With Rajan Plumley, Daniel Ratner, Joshua Turner

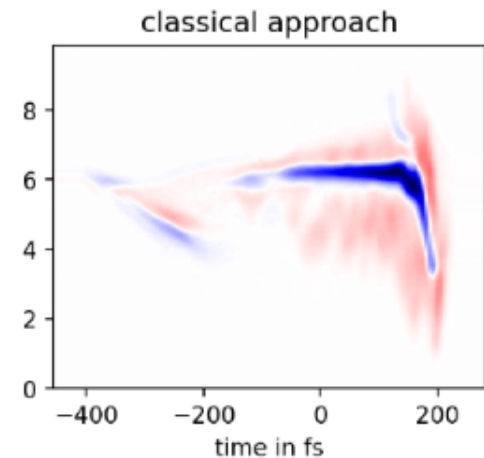
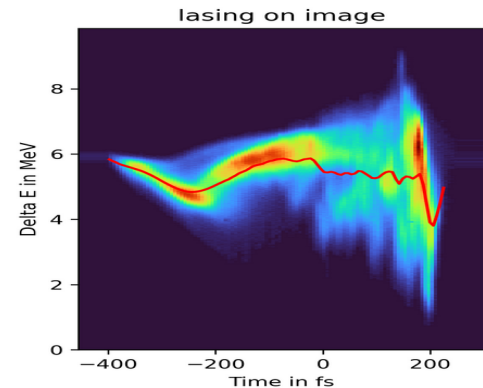
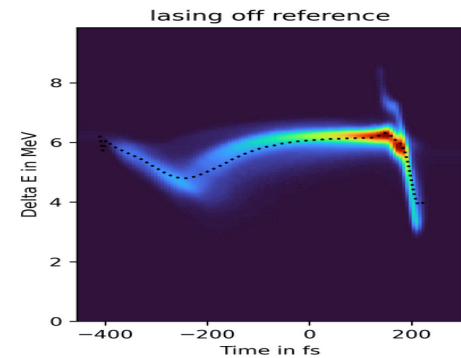
- self seeded
- emittance spoiling foil
- very weak lasing signal



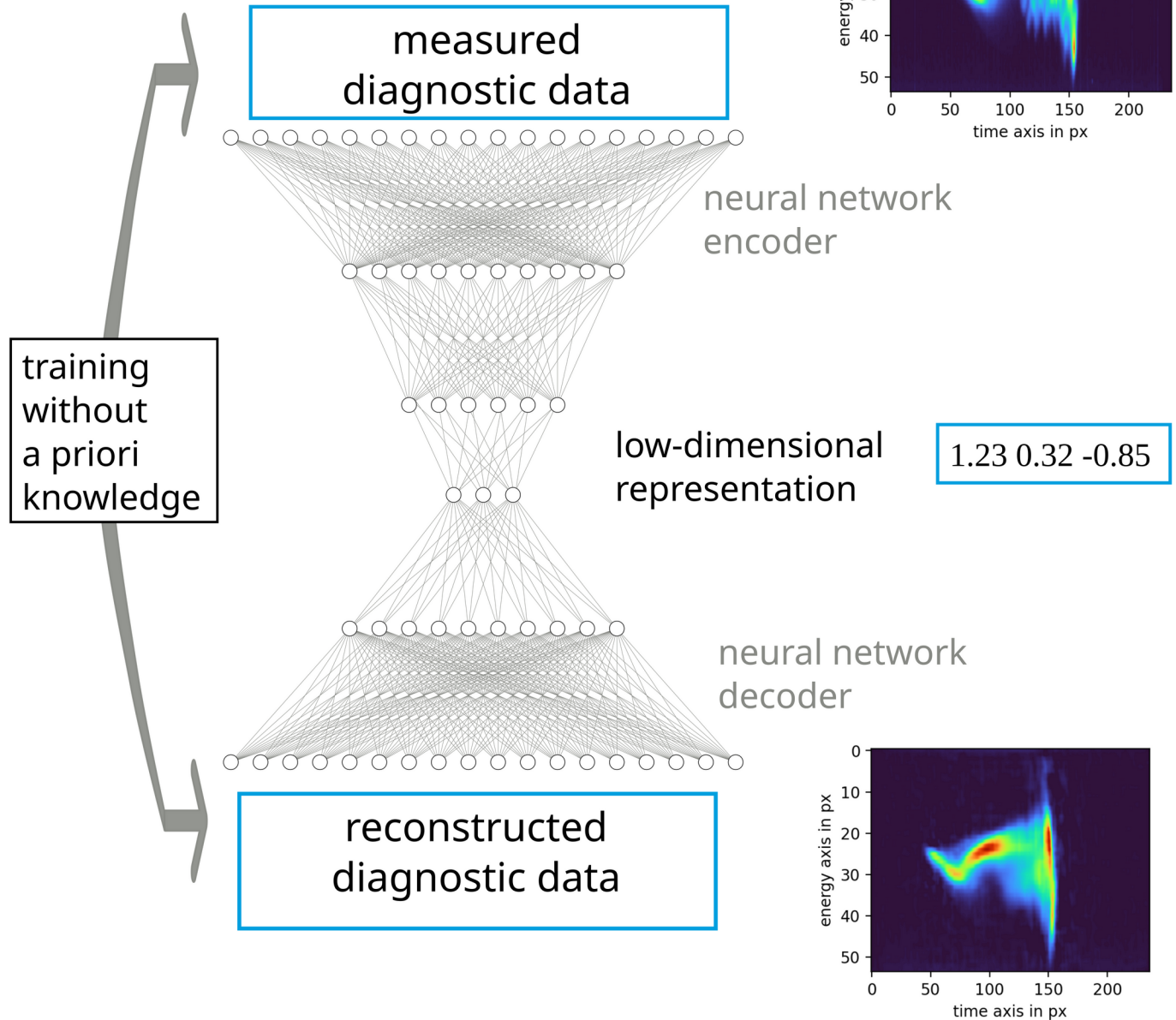
# SASE Data from FLASH

- Electron energy distribution changes from shot to shot.
- We want a method that can learn lasing off representations and can interpolate between them.
- We want a method that can solve the x,y matching problem for us.

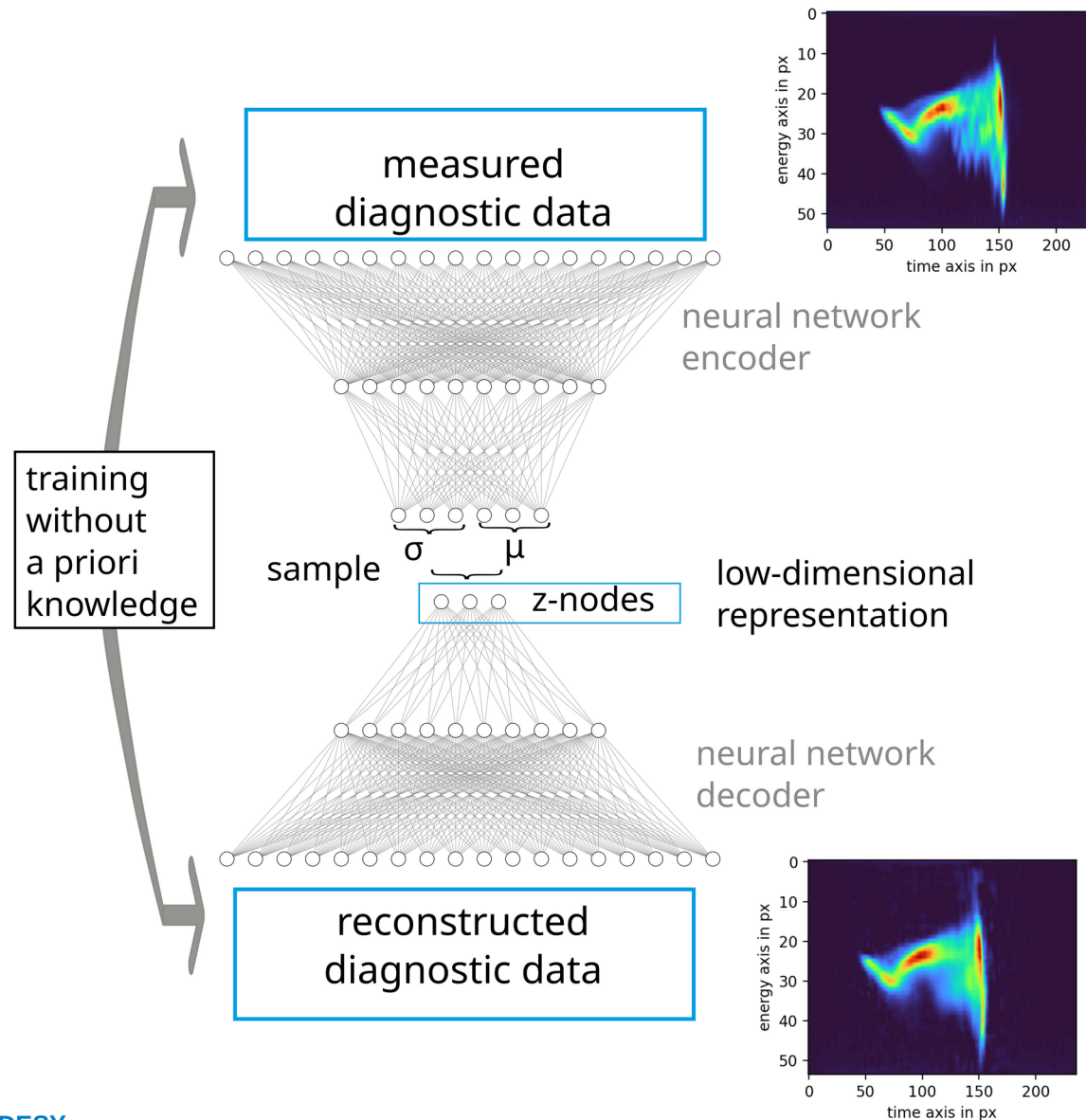
→ **Beta-Variational  
Convolutional Autoencoders**



# Autoencoder



# $\beta$ variational autoencoder



$\beta$ -VAE: LEARNING BASIC VISUAL CONCEPTS WITH A CONSTRAINED VARIATIONAL FRAMEWORK

Irina Higgins, Loic Matthey, Arka Pal, Christopher Burgess, Xavier Glorot, Matthew Botvinick, Shakir Mohamed, Alexander Lerchner  
Google DeepMind  
{irinah, lmatthey, arkap, cpburgess, glorotx, botvinick, shakir, lerchner}@google.com



Google DeepMind

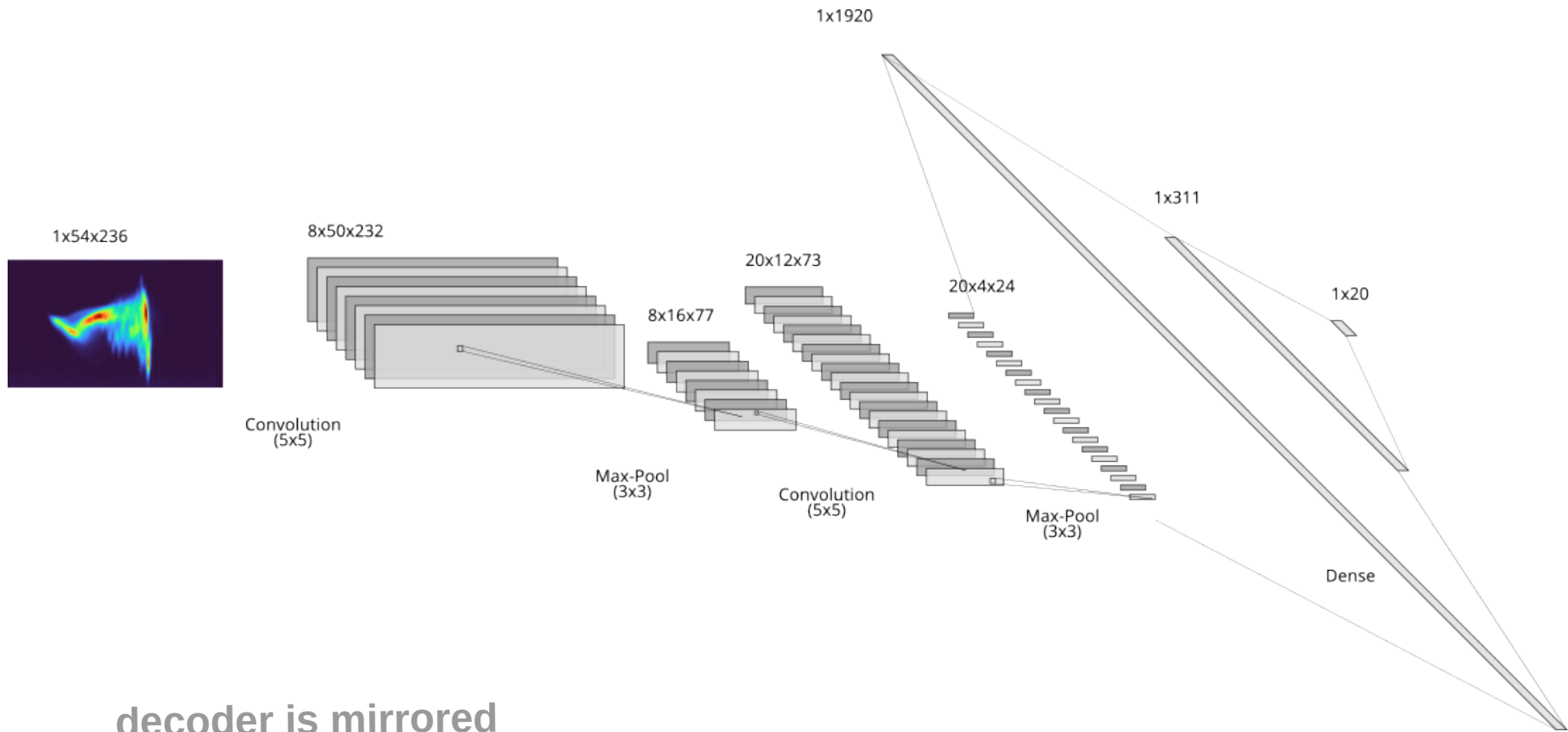
Unsupervised real-world knowledge extraction via disentangled variational autoencoders for photon diagnostics

Gregor Hartmann , Gesa Goetzke, Stefan Düsterer, Peter Feuer-Forsion, Fabiano Lever, David Meier, Felix Möller, Luis Vera Ramirez, Markus Guehr, Kai Tiedtke, Jens Viefhaus & Markus Braune

*Scientific Reports* 12, Article number: 20783 (2022) | [Site this article](#)

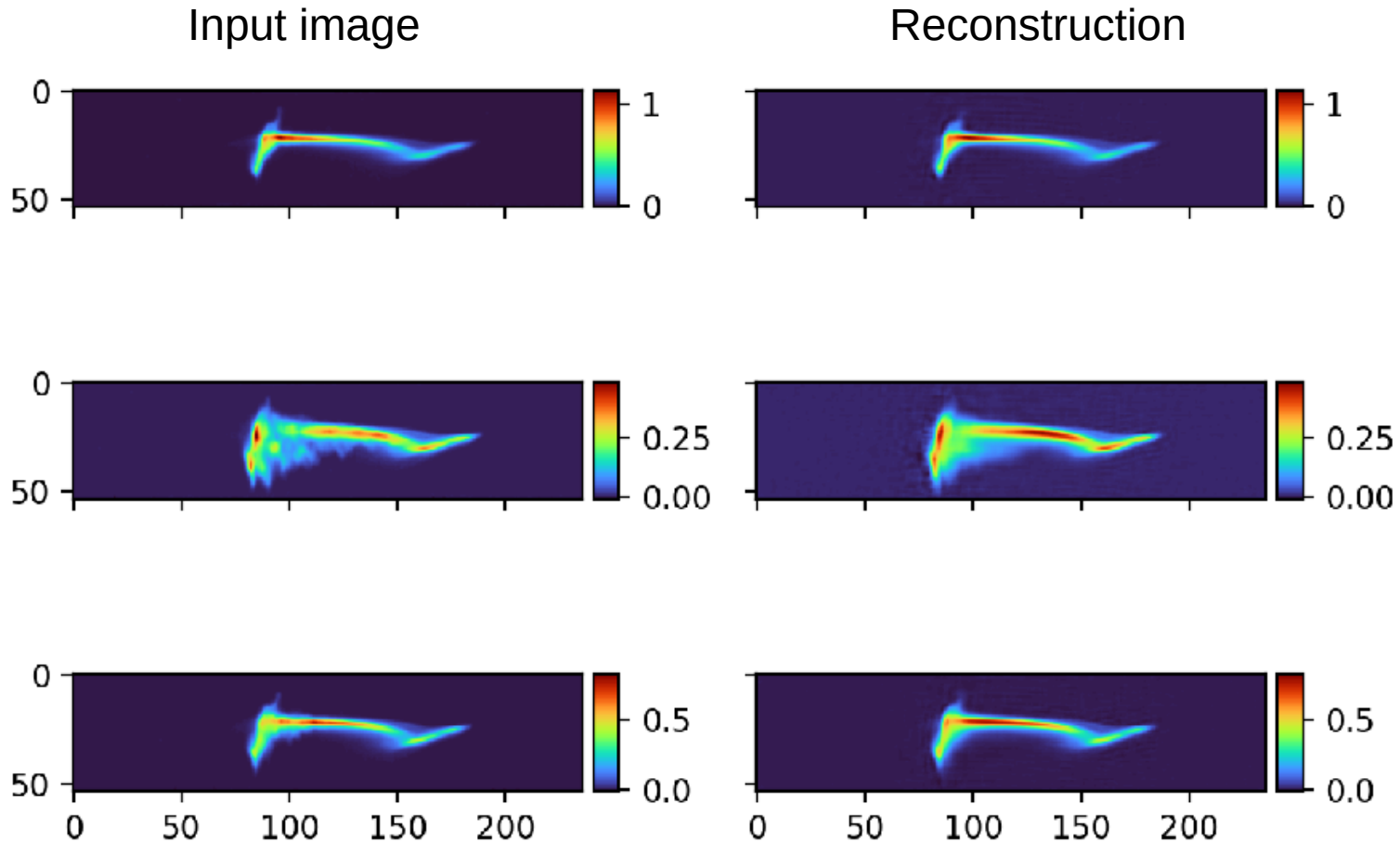


# Convolutional $\beta$ -Variational Autoencoder

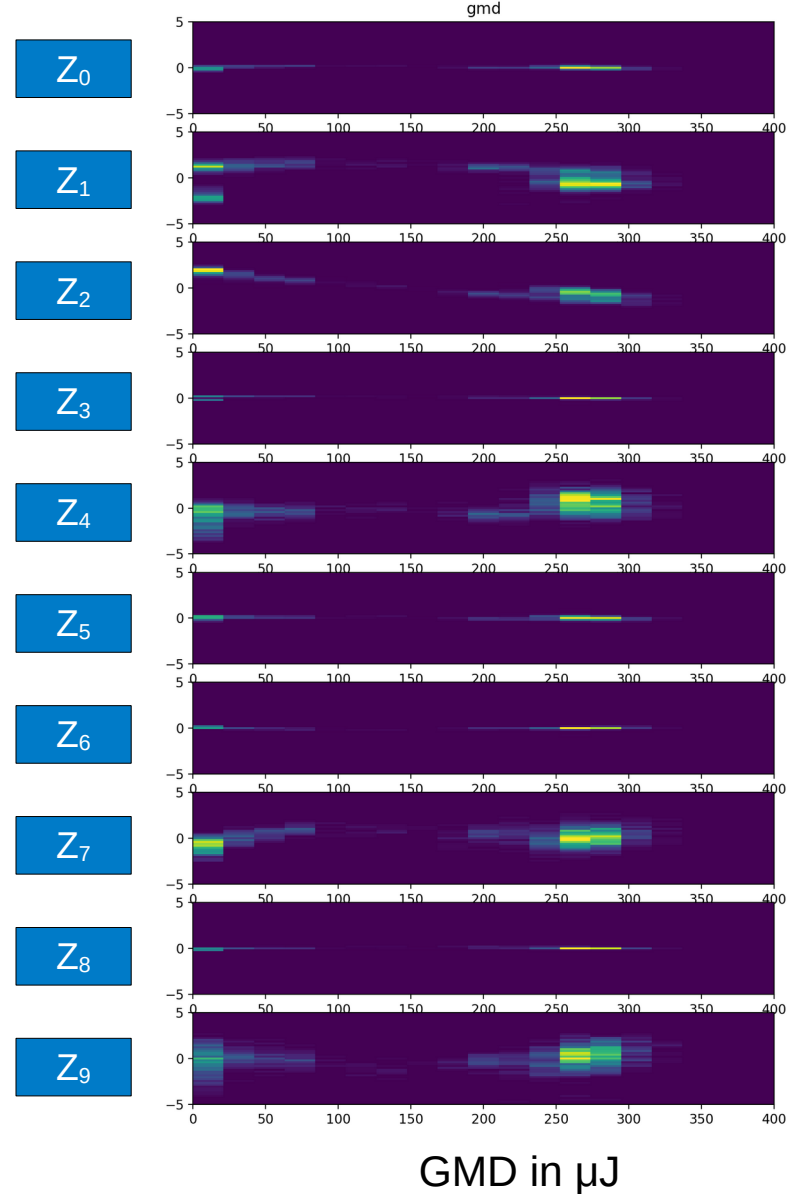
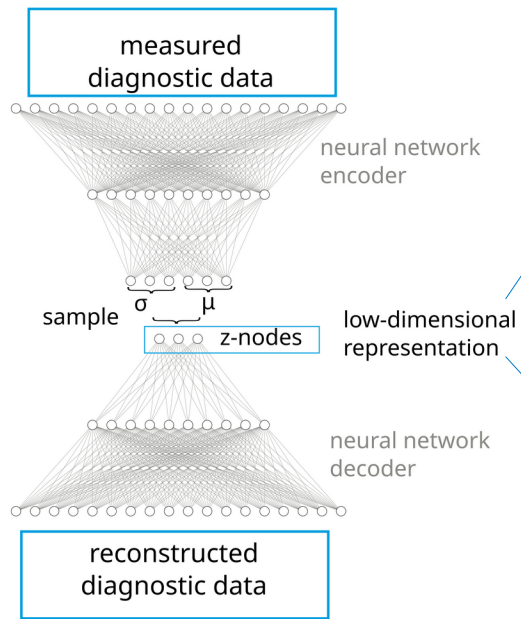


decoder is mirrored

# Some reconstructions

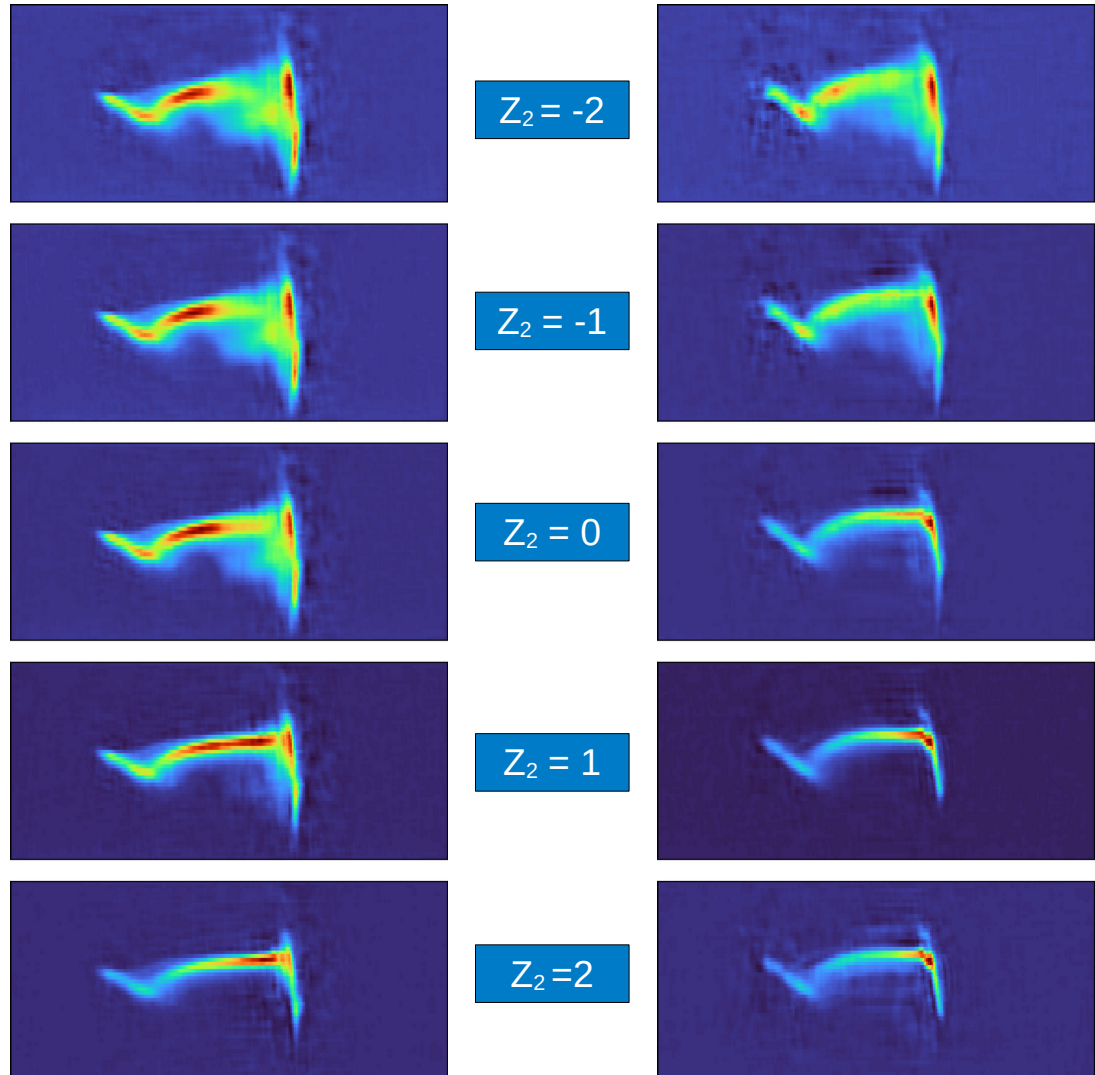
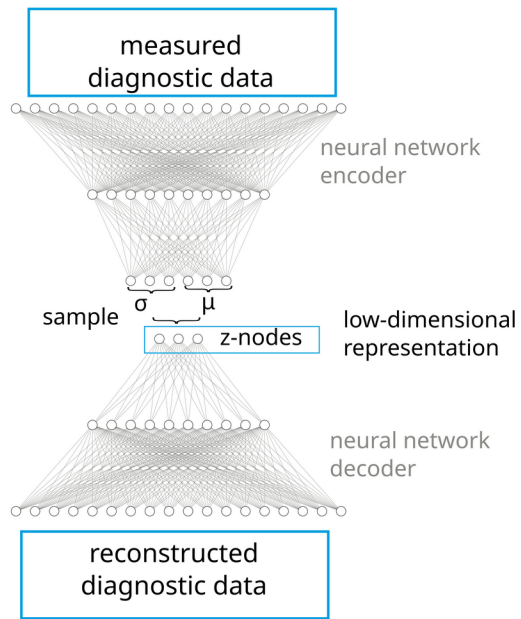


# Detect the lasing node

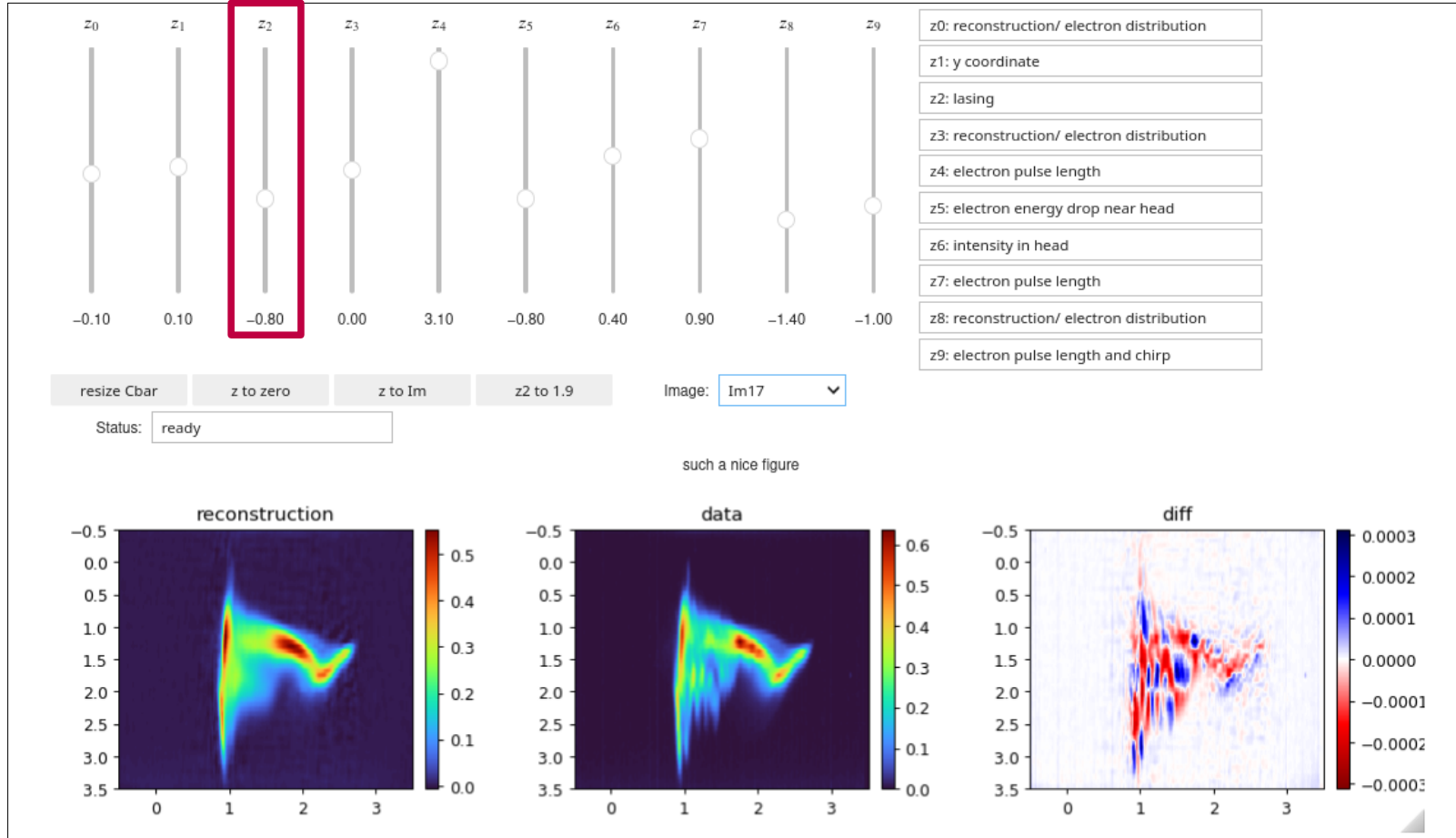




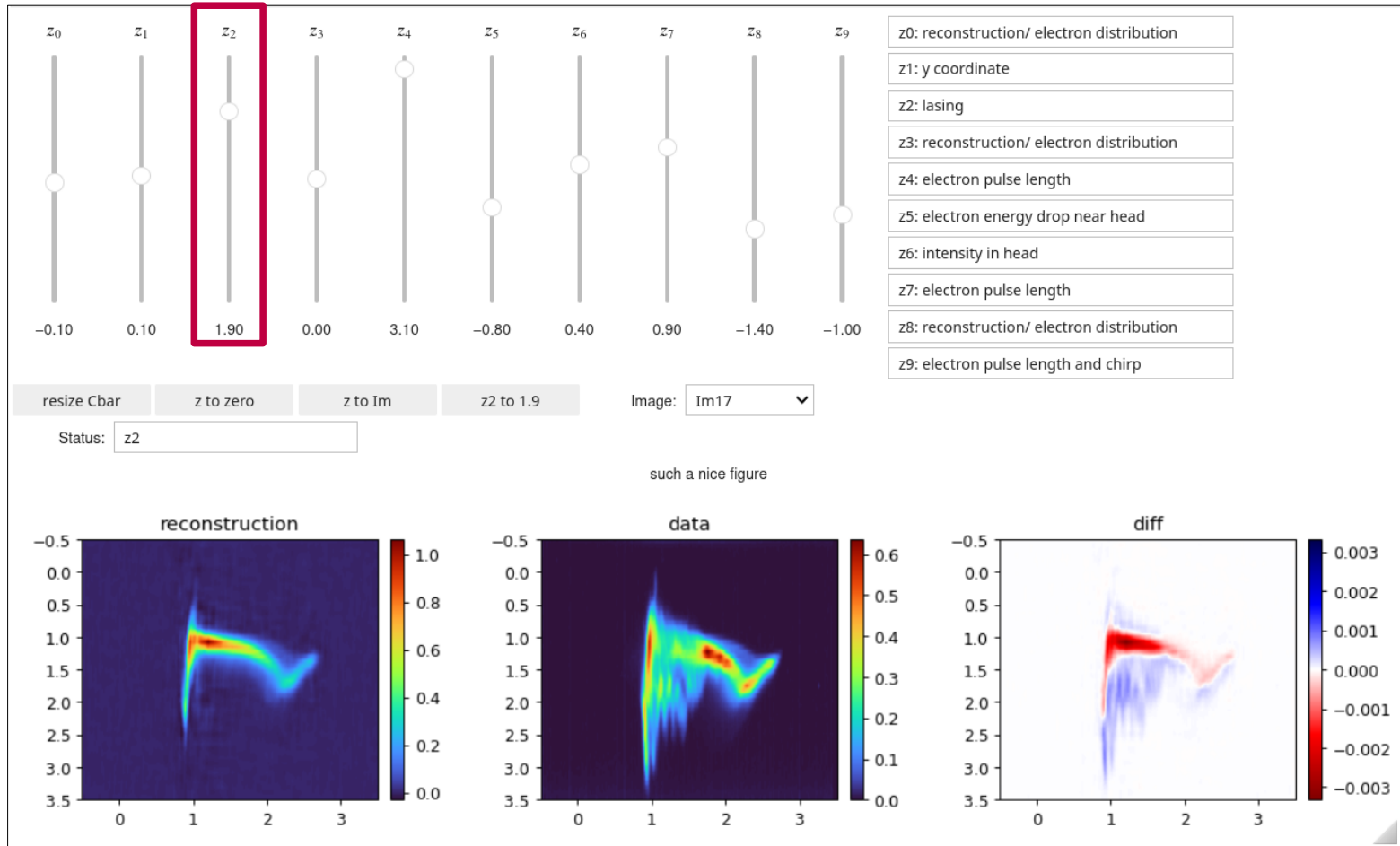
# POLARIX: Traversing the latent space



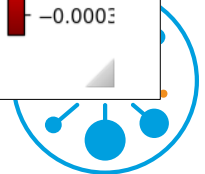
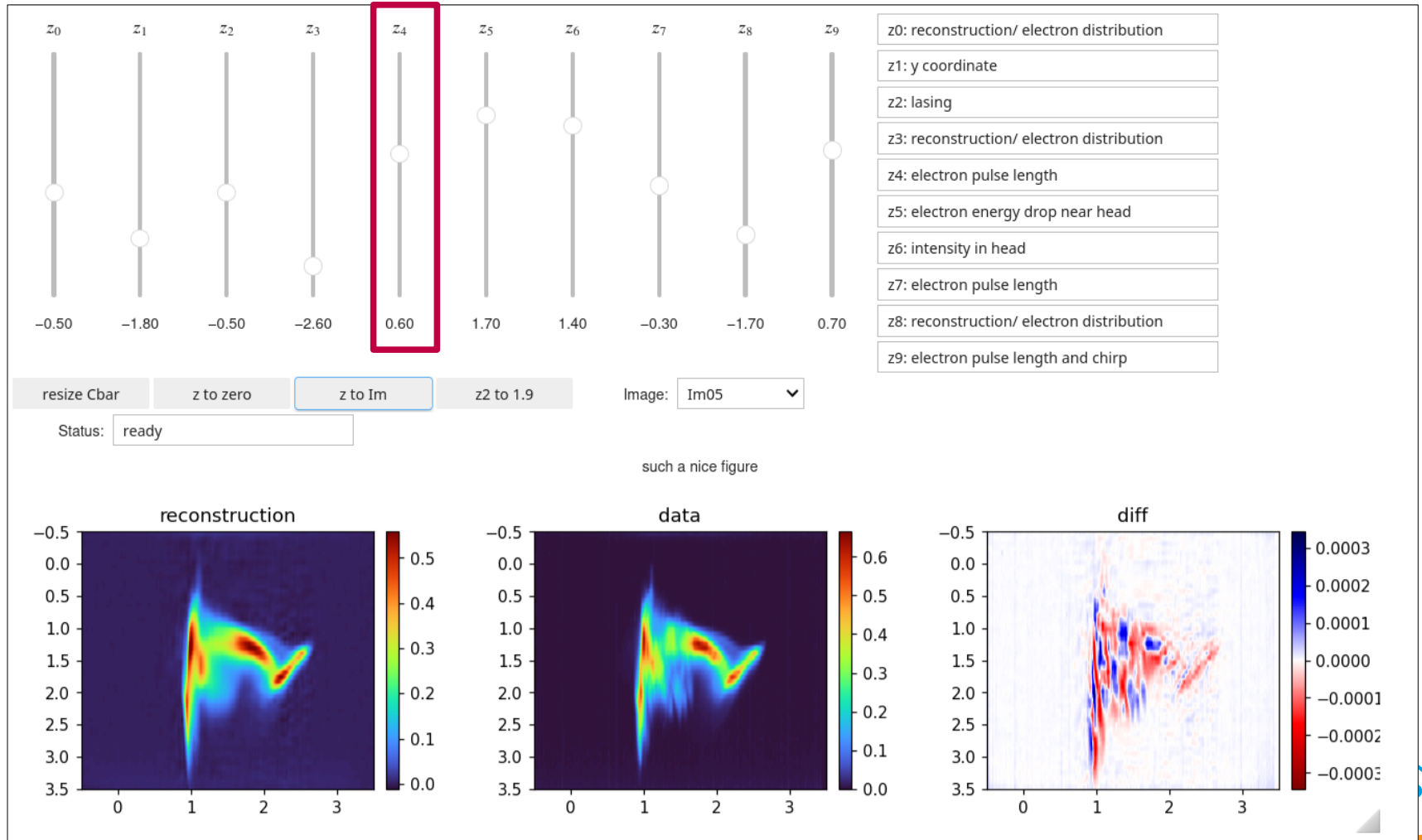
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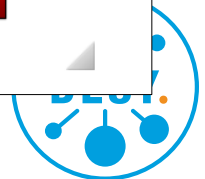
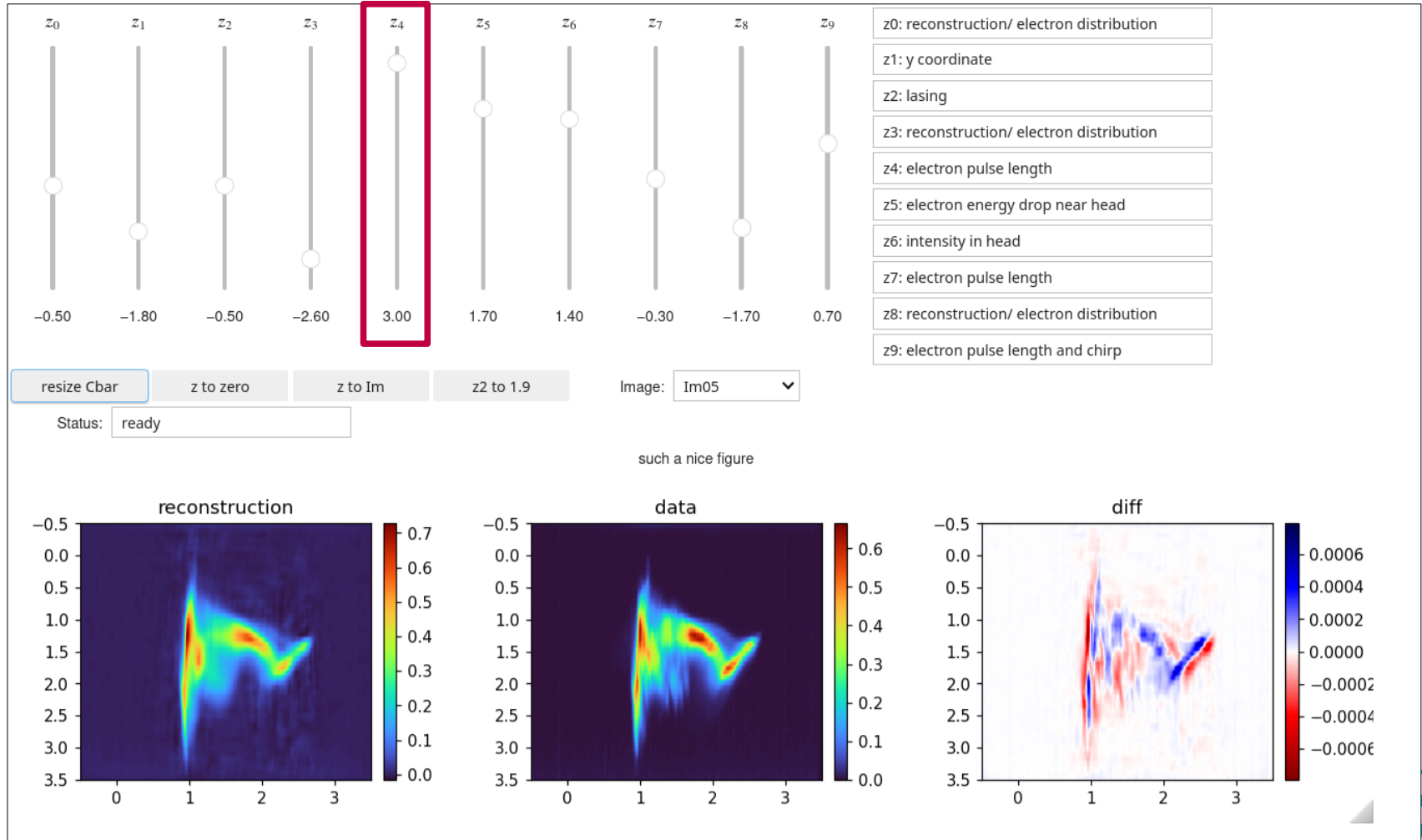
# POLARIX: Traversing the latent space



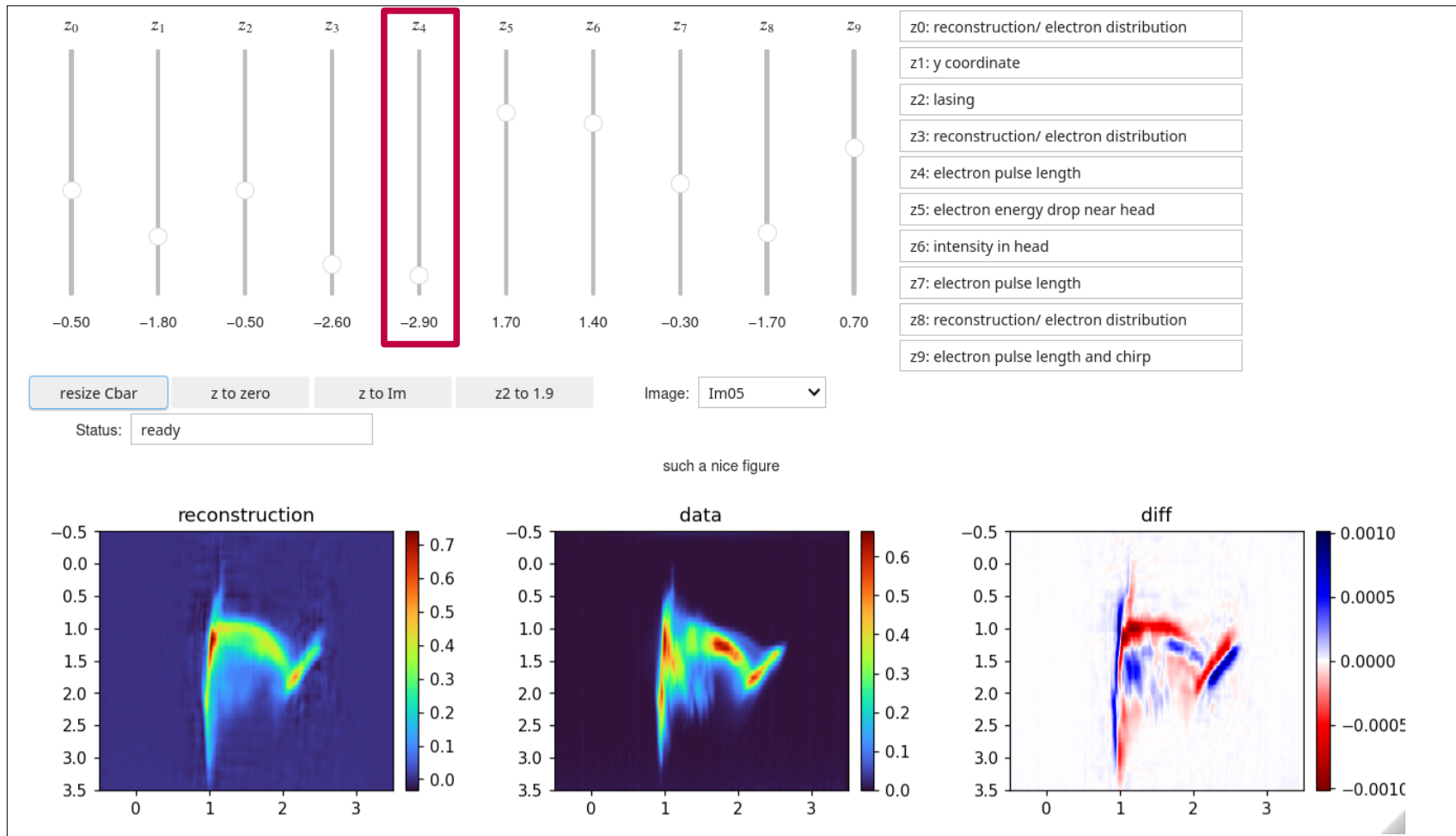
# POLARIX: Traversing the latent space



# POLARIX: Traversing the latent space



# POLARIX: Traversing the latent space



# Traversing the latent space: web app

1) Permanent link, start it and grab a coffee

```
https://mybinder.org/v2/gh/Goetzkeg/betaVAEDemo/HEAD?urlpath=voila%2Frender%2FvisLS_lowCompute.ipynb
```



update recons...

HELMHOLTZ

2) Just today, run it at my personal computer at home

```
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```



You are about to visit:

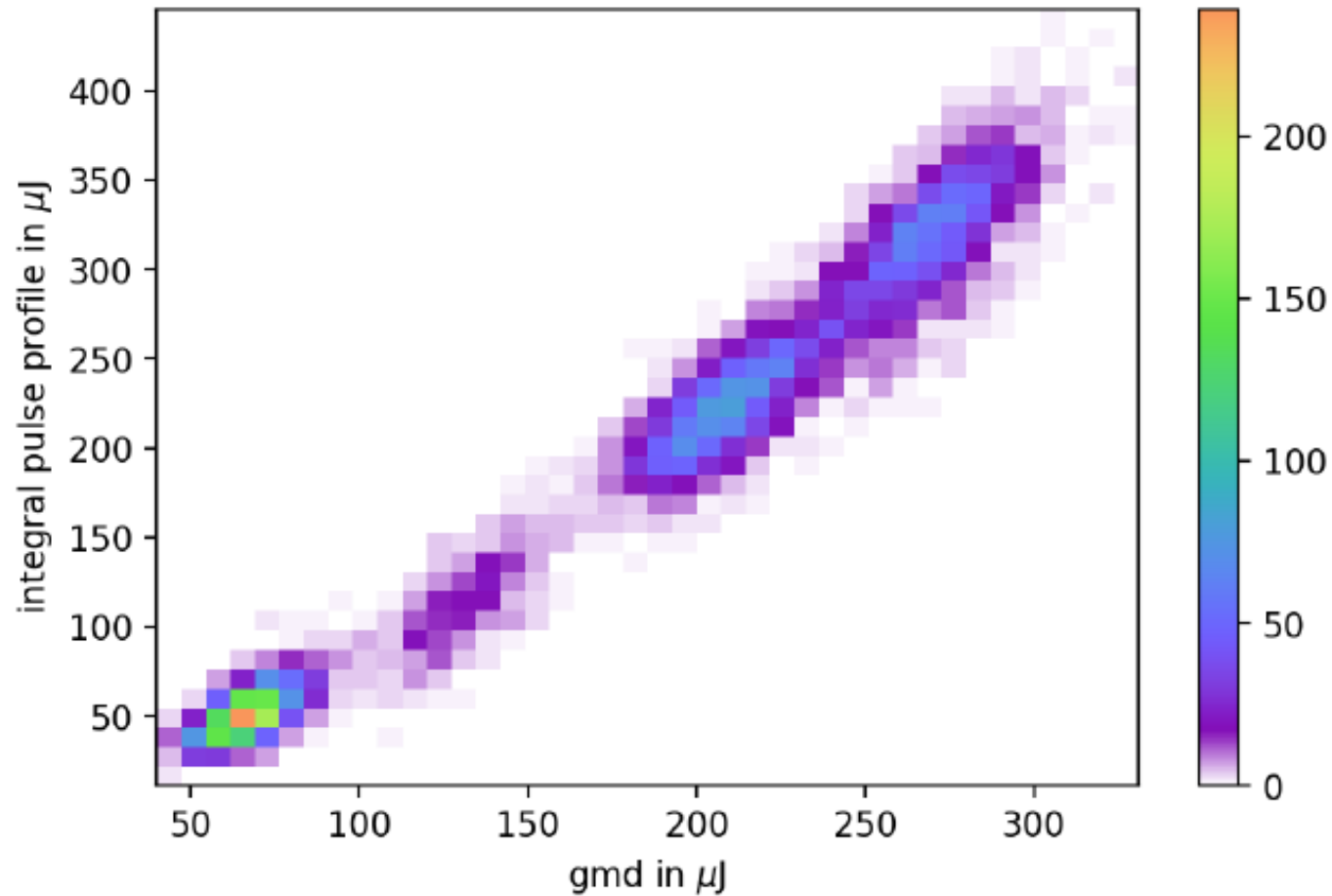
[8f7c-2a02-3100-8b01-8900-6611-aedc-7c73-d7f0.ngrok-free.app](https://8f7c-2a02-3100-8b01-8900-6611-aedc-7c73-d7f0.ngrok-free.app)

Website IP: 2a02:3100:8b01:8900::6611:aedc:7c73:d7f0

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# Correlation with the GMD



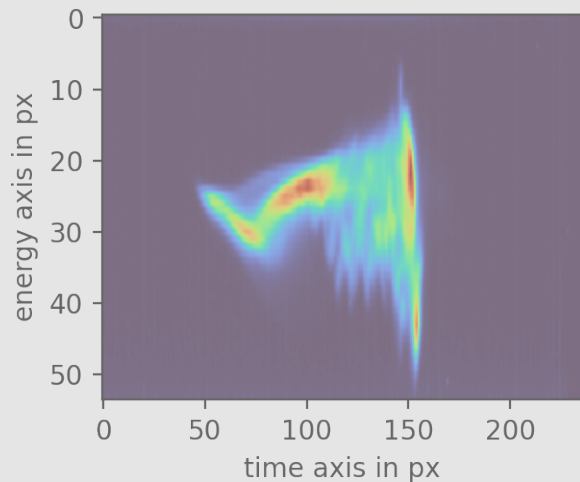


# Two projects with XTCAV and machine learning



## @FLASH (DESY)

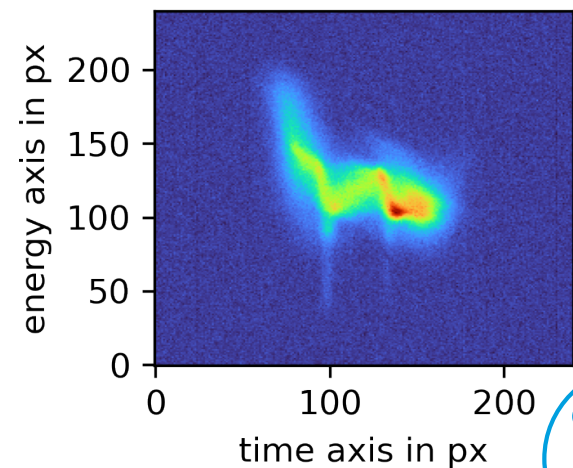
- SASE
- strong lasing signal



## @LCLS (SLAC)

With Rajan Plumley, Daniel Ratner, Joshua Turner

- self seeded
- emittance spoiling foil
- very weak lasing signal

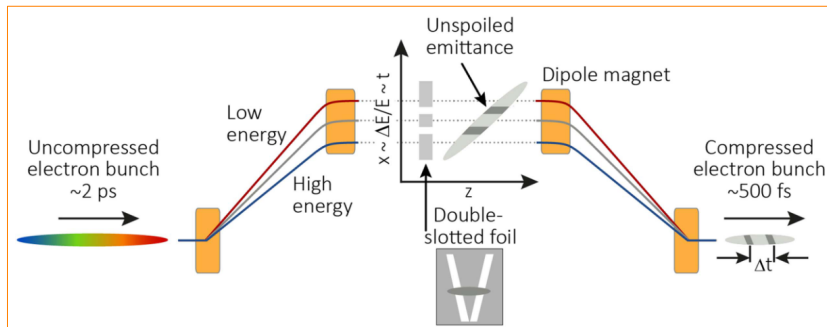


# Requirements and Setup

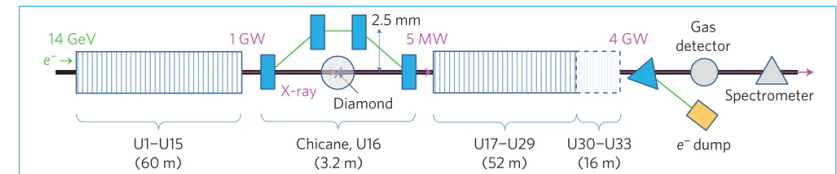
2 pulses with few fs distance, monochromatic (8.5 keV), known intensity ratio



## Emittance spoiling foil



## Self-seeding



### Femtosecond profiling of shaped x-ray pulses

M C Hoffmann<sup>16,1</sup>, I Grguraš<sup>16,2,3</sup>, C Behrens<sup>4</sup>, C Bostedt<sup>1,5</sup>, J Bozek<sup>1,6</sup>, H Bromberger<sup>2,3</sup>, R Coffee<sup>1</sup>, J T Costello<sup>7</sup>, L F DiMauro<sup>8</sup>, Y Ding<sup>1</sup> [+ Show full author list](#)

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[New Journal of Physics, Volume 20, March 2018](#)

Article | Published: 12 August 2012

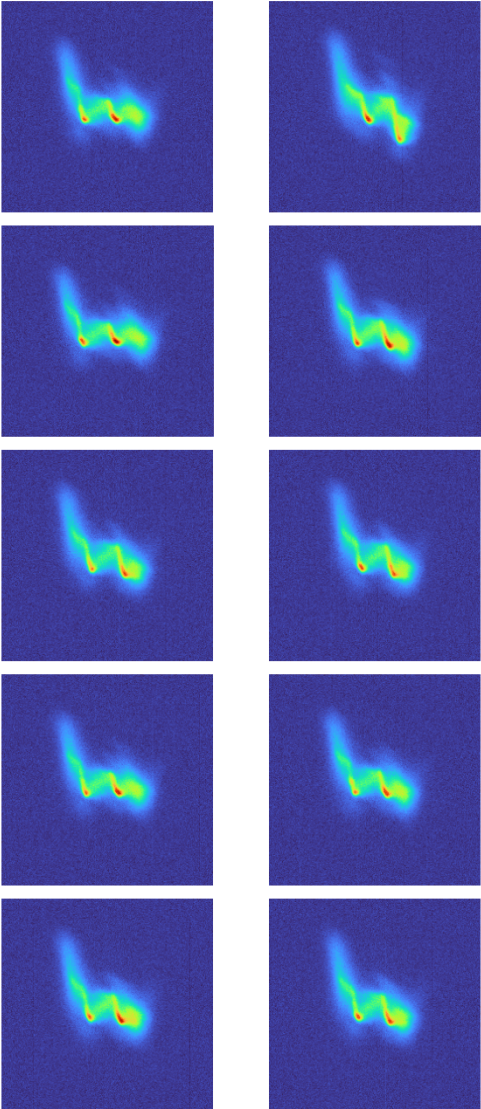
### Demonstration of self-seeding in a hard-X-ray free-electron laser

[J. Amann](#), [W. Berg](#), [V. Blank](#), [F.-J. Decker](#), [Y. Ding](#), [P. Emma](#), [Y. Feng](#), [J. Frisch](#), [D. Fritz](#), [J. Hastings](#), [Z. Huang](#), [J. Krzywinski](#), [R. Lindberg](#), [H. Loos](#), [A. Lutman](#), [H.-D. Nuhn](#), [D. Ratner](#), [J. Rzepiela](#), [D. Shu](#), [Yu. Shvyd'ko](#), [S. Spampinati](#), [S. Stoupin](#), [S. Terentyev](#), [E. Trakhtenberg](#), ... [D. Zhu](#) [+ Show authors](#)

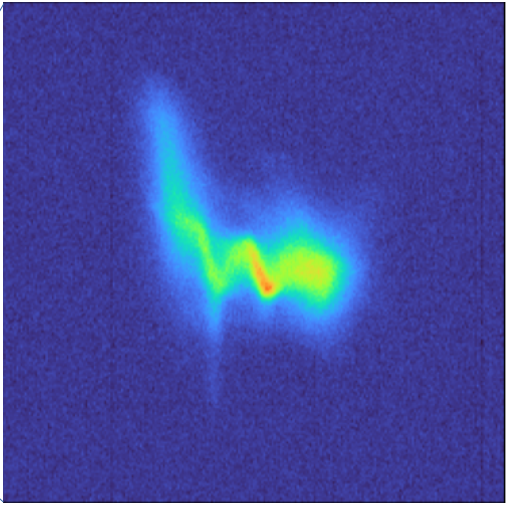
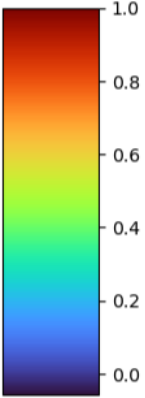
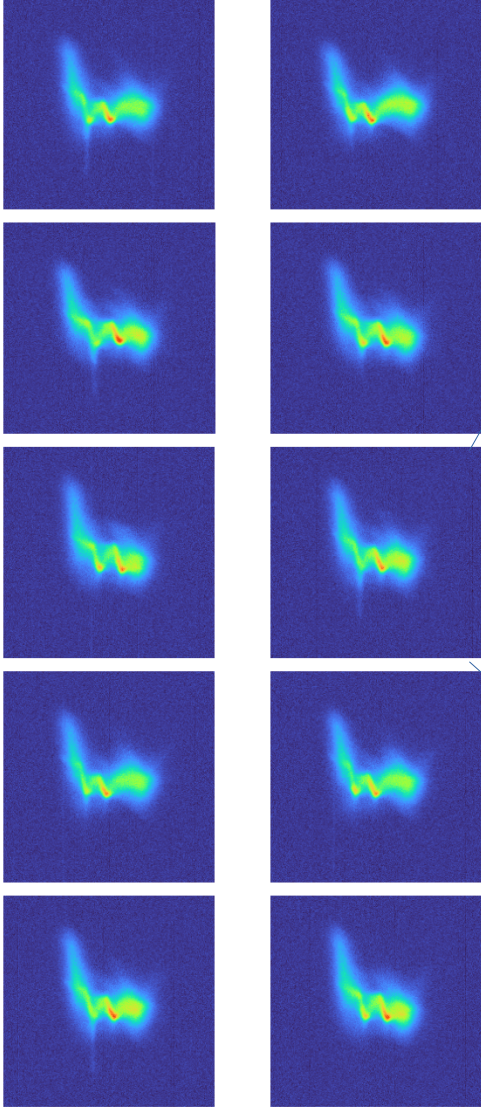
*Nature Photonics* **6**, 693–698 (2012) | [Cite this article](#)

# Lasing on and lasing off examples

Lasing off

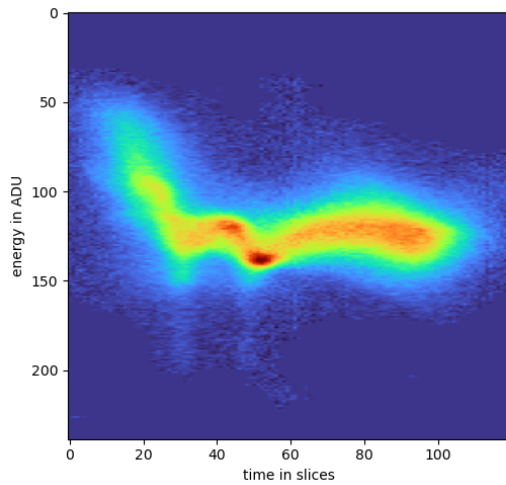


Lasing on

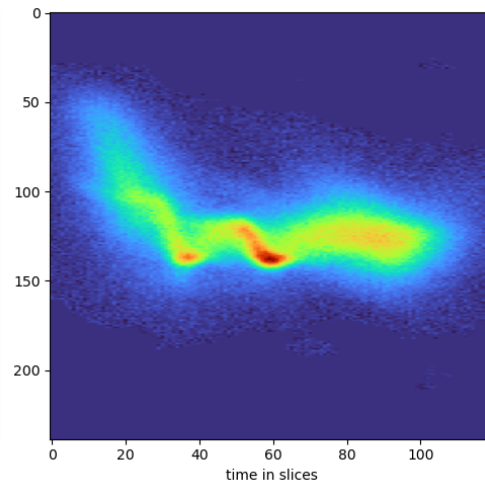


# Classical evaluation fails

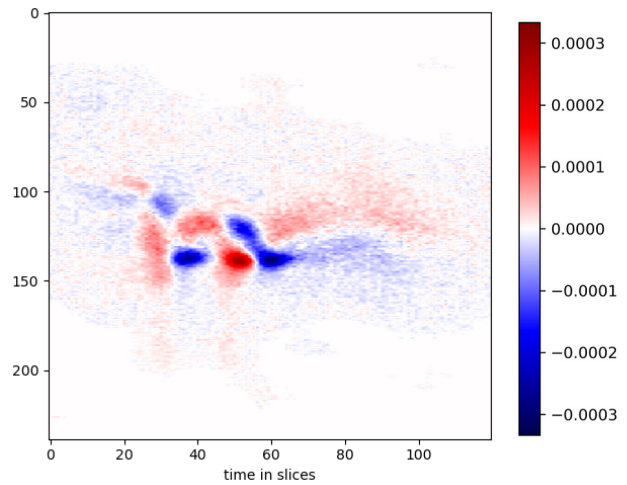
Lasing on



Lasing off

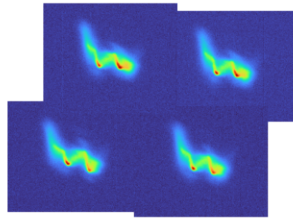


Lasing on – Lasing off

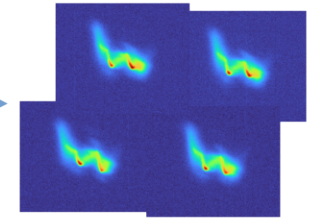
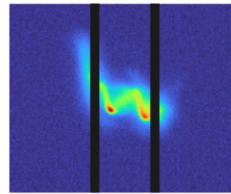


# Network approach: training phase

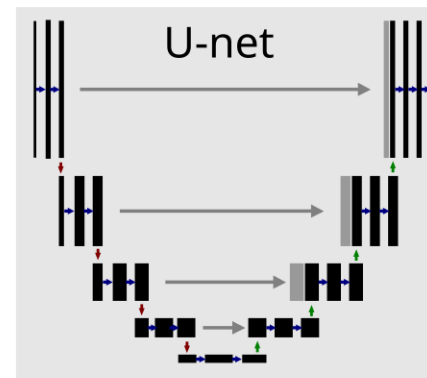
bunch of lasing off



two random masks



neural network  
reconstructs  
lasing off reference



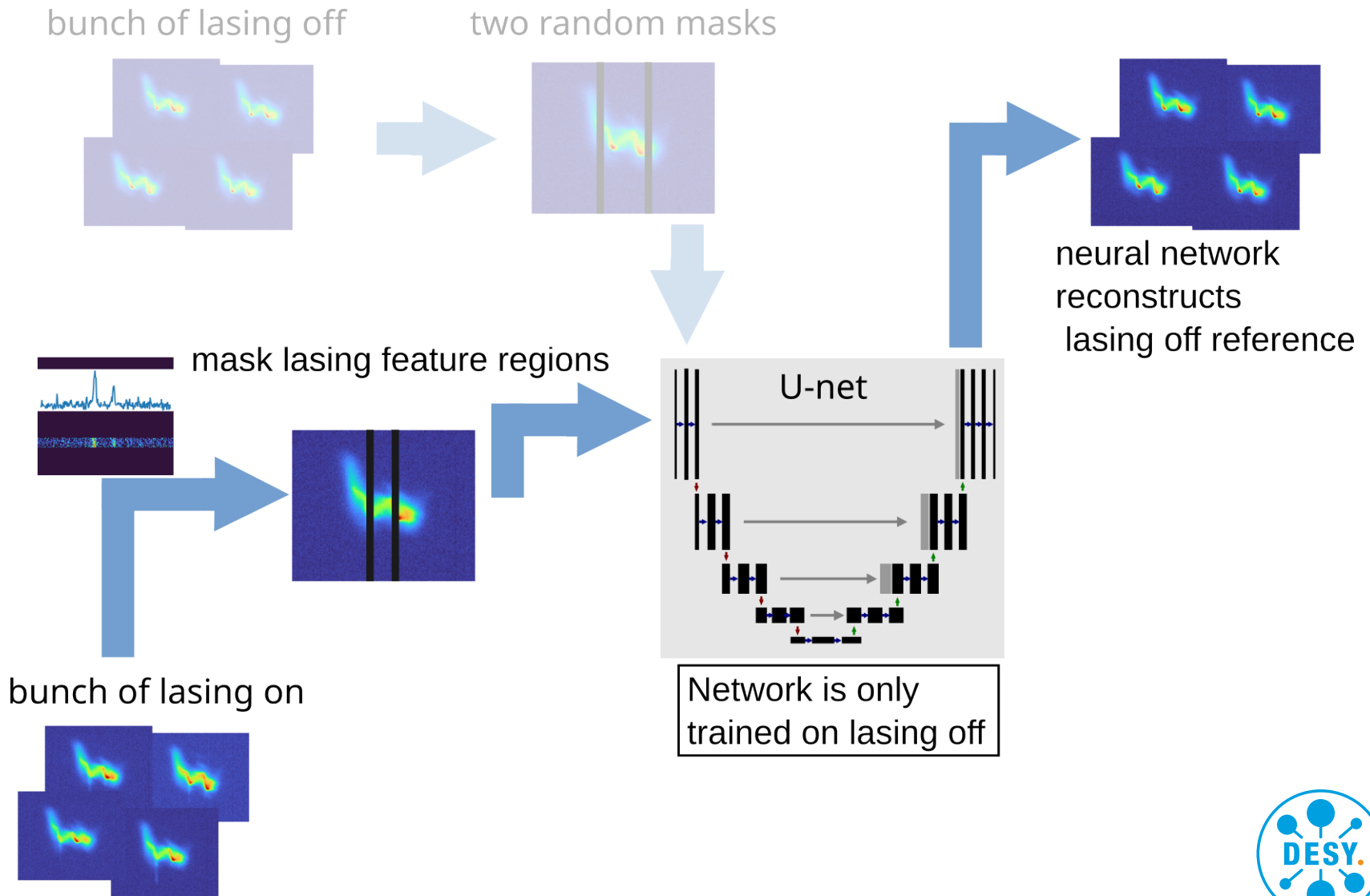
*[Submitted on 18 May 2015]*

**U-Net: Convolutional Networks for  
Biomedical Image Segmentation**

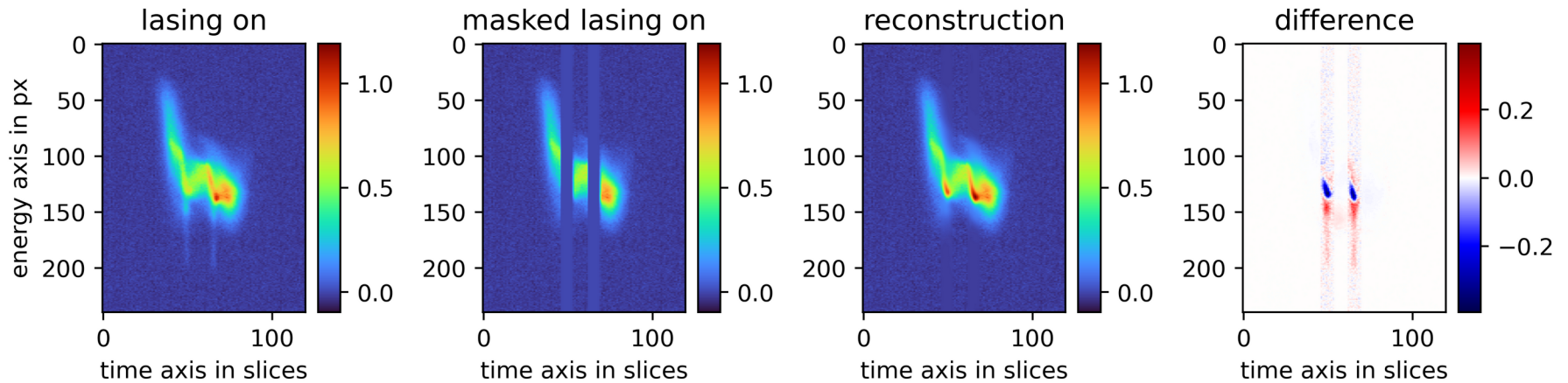
Olaf Ronneberger, Philipp Fischer, Thomas Brox



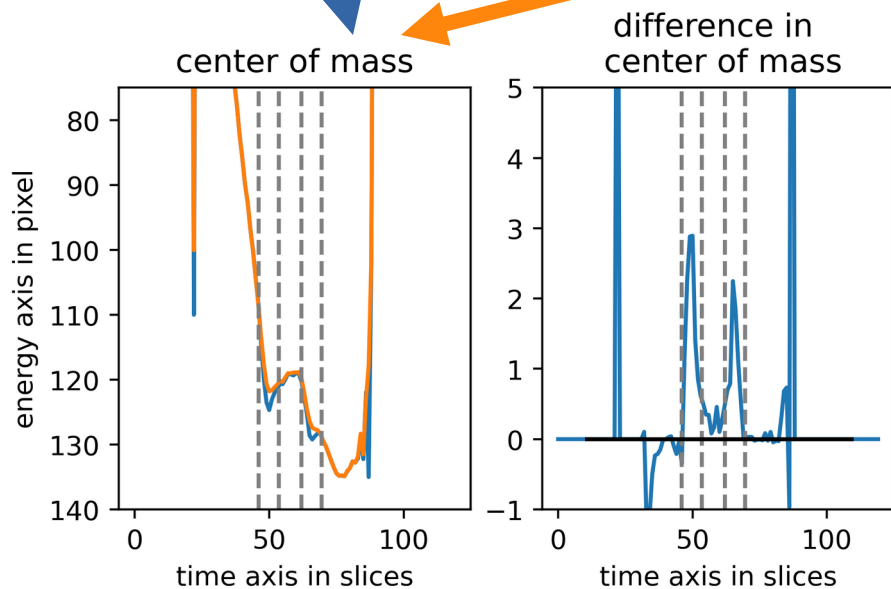
# Network approach: evaluation phase



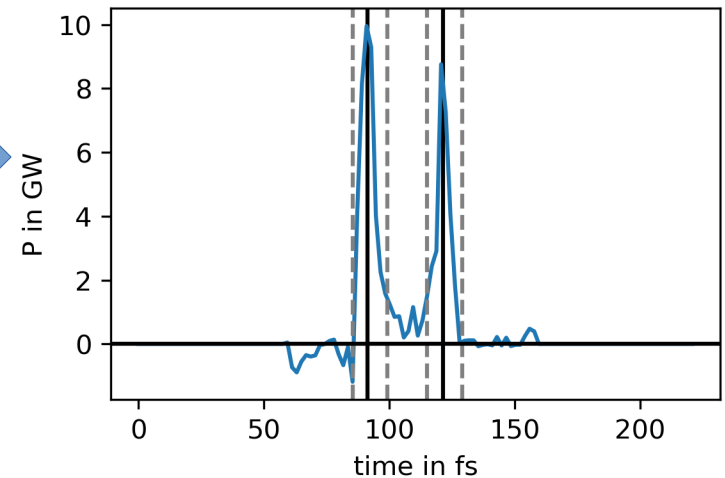
# Results: one reconstruction in detail



Calculate center of mass for each slice

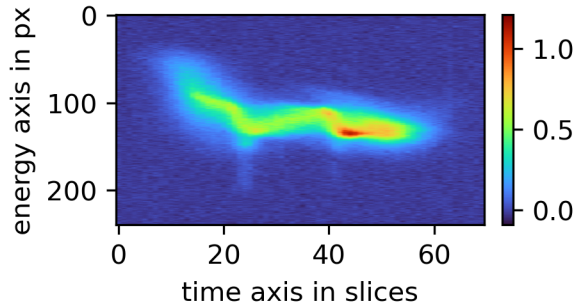


Power profile:  $P(t) = \Delta E(t)I(t)/e$

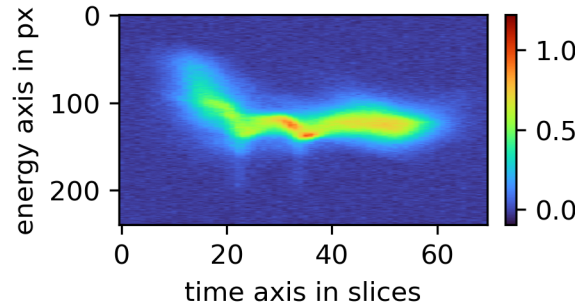


# Results: power profiles for different setups

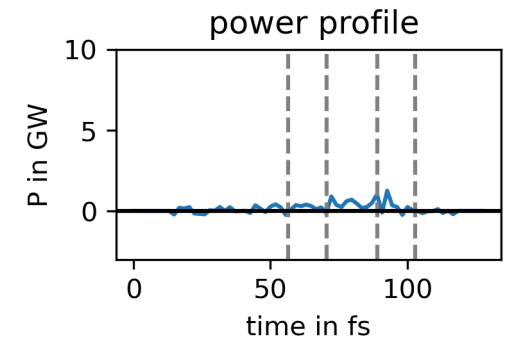
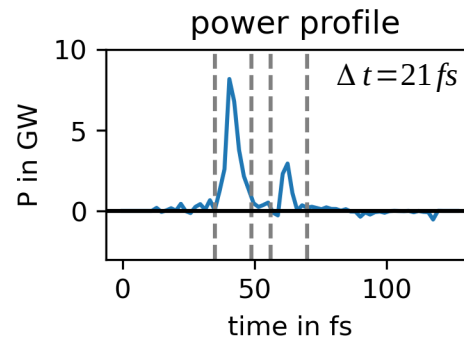
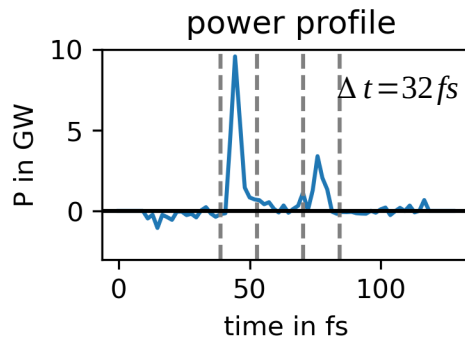
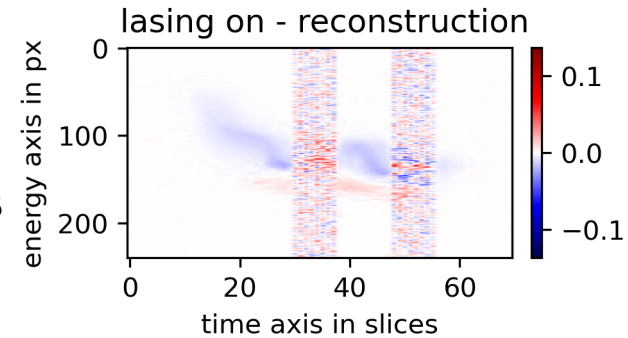
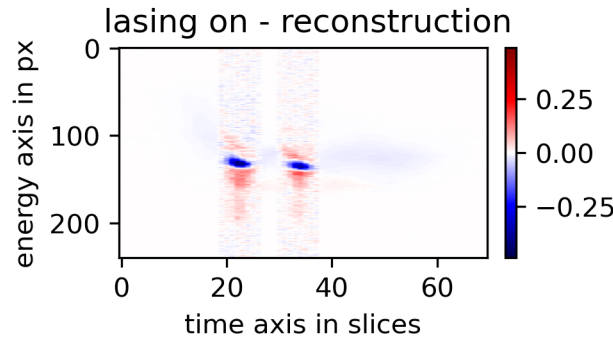
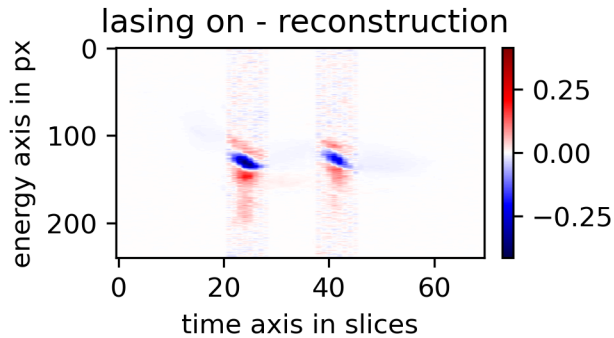
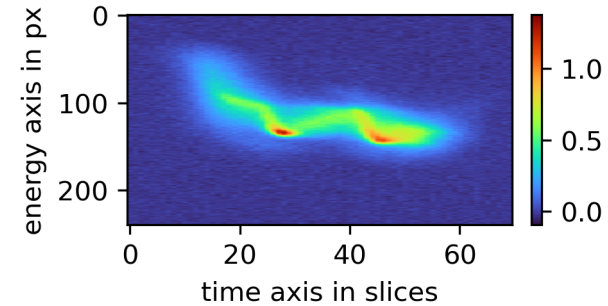
Setup 1:  
 $\Delta t \sim 33$  fs



Setup 2:  
 $\Delta t \sim 23$  fs



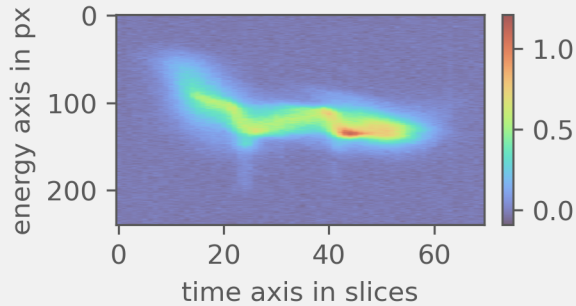
Lasing off:  
 $\Delta t \sim 33$  fs



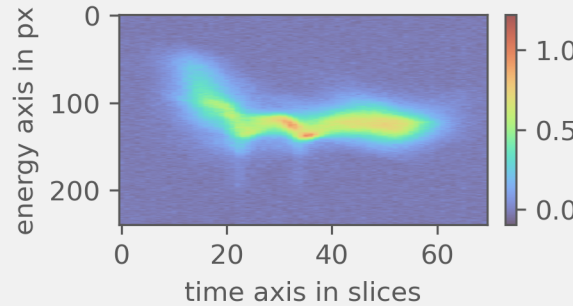


# Results: power profiles for different setups

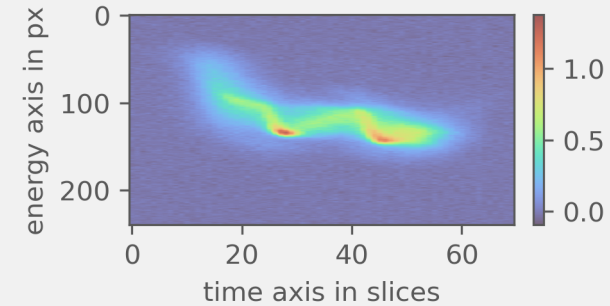
Setup 1:  
 $\Delta t \sim 33$  fs



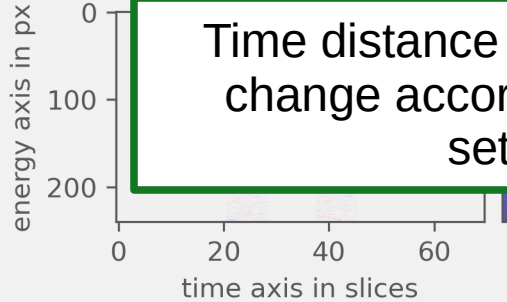
Setup 2:  
 $\Delta t \sim 23$  fs



Lasing off:  
 $\Delta t \sim 33$  fs

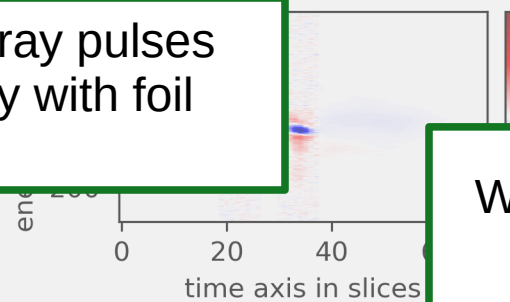


lasing on - reconstruction

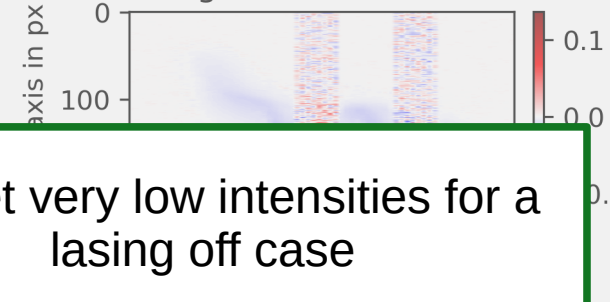


Time distance of X-ray pulses  
change accordingly with foil  
setting

lasing on - reconstruction

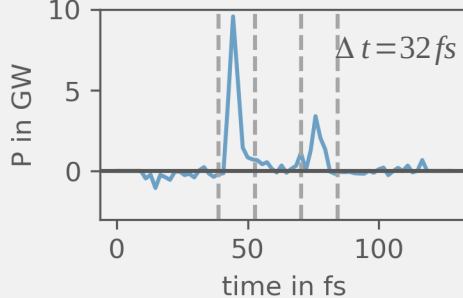


lasing on - reconstruction

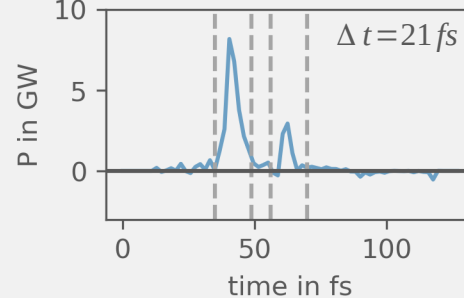


We get very low intensities for a  
lasing off case

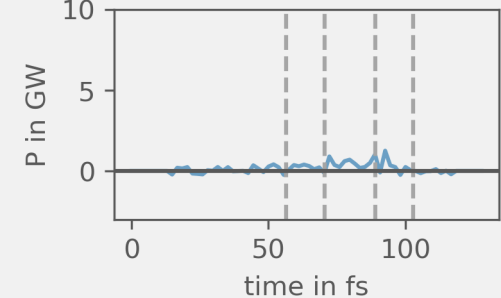
power profile



power profile

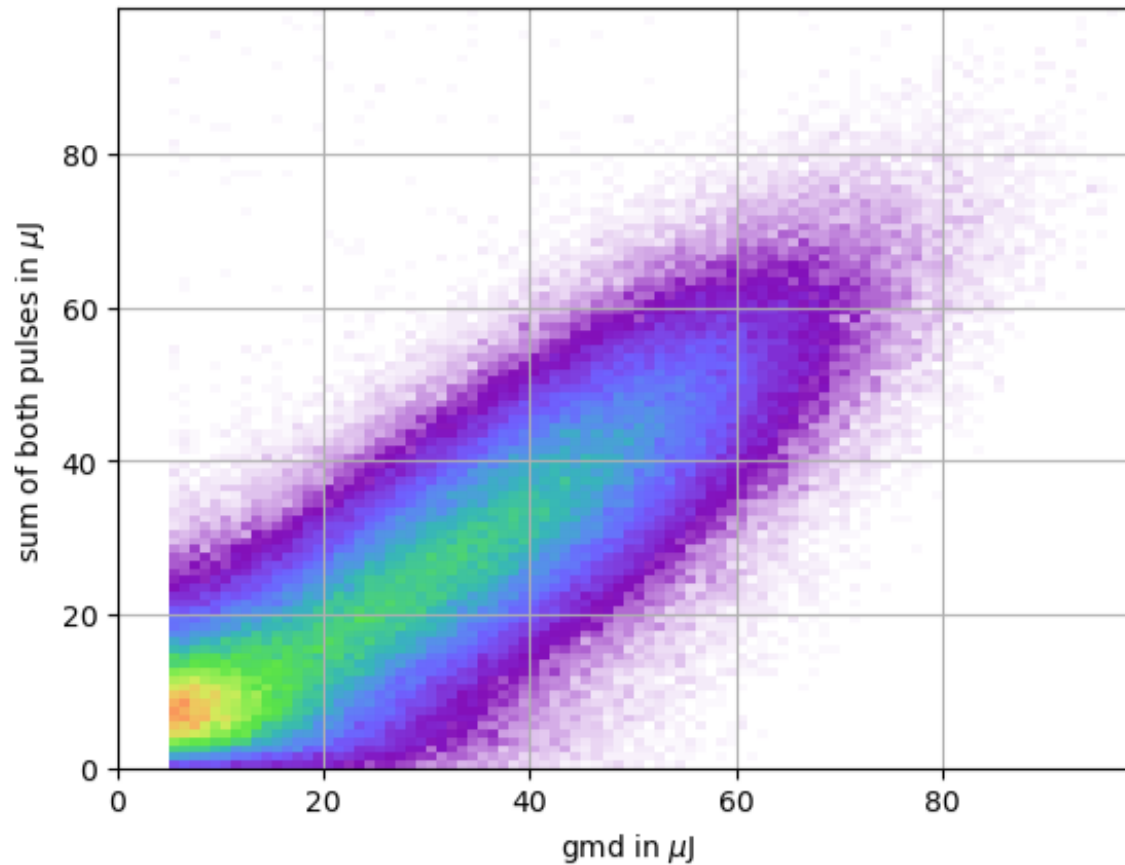


power profile

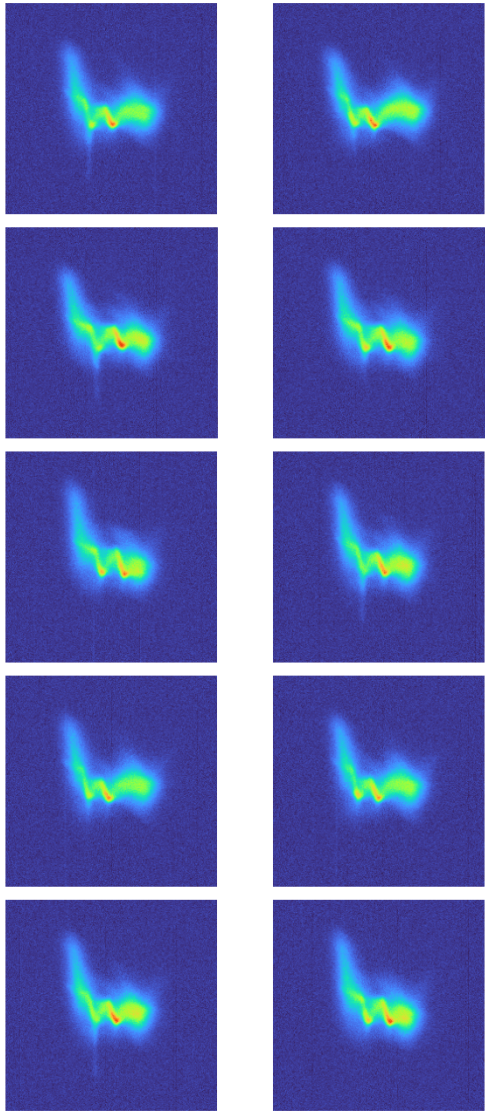
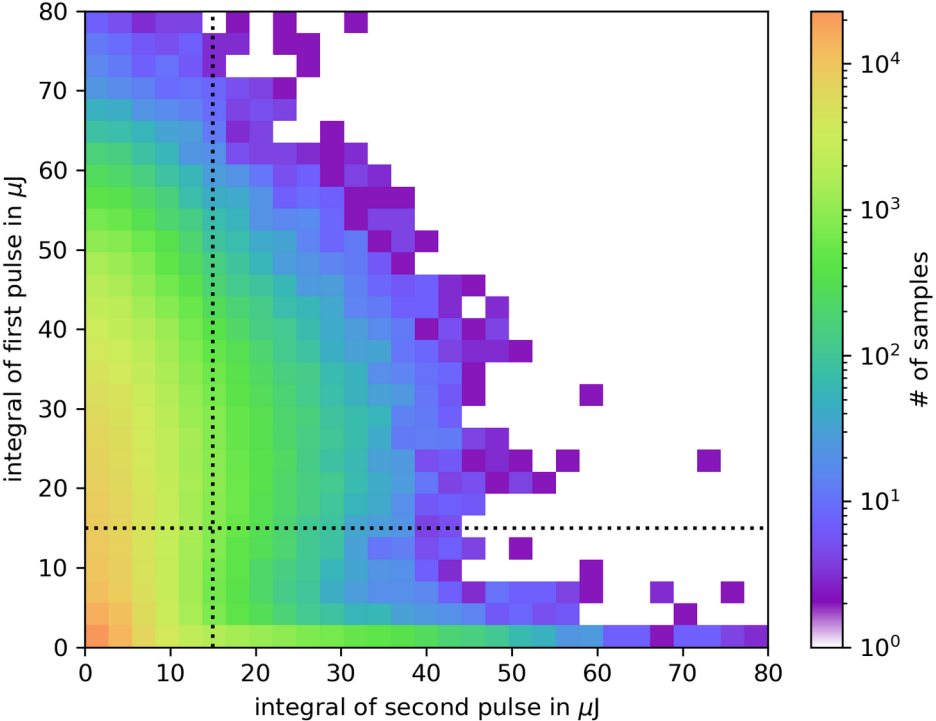


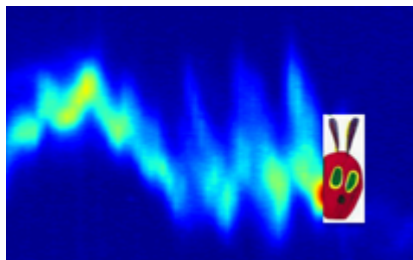
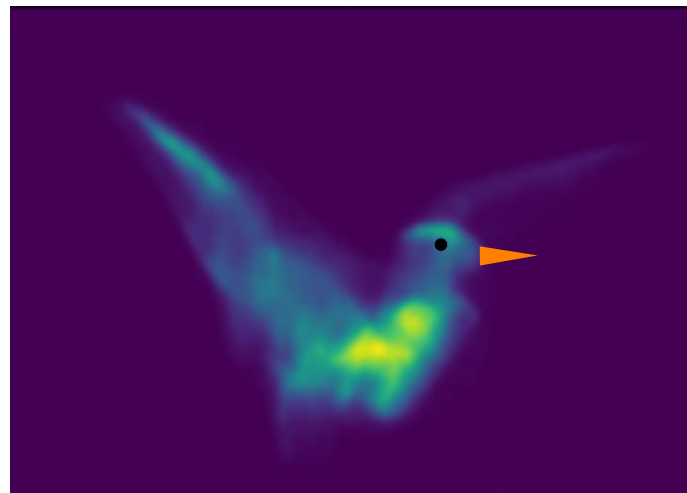
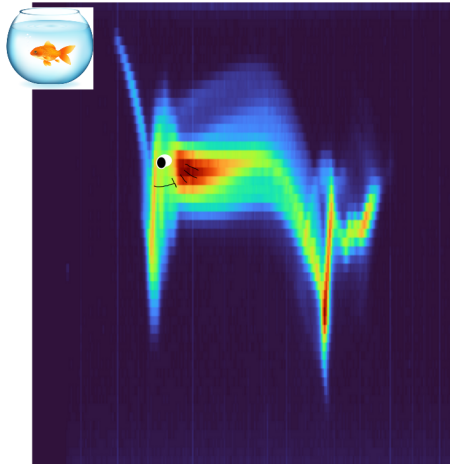
# Results: how to cross check

- Check if integral of both pulses match with GMD

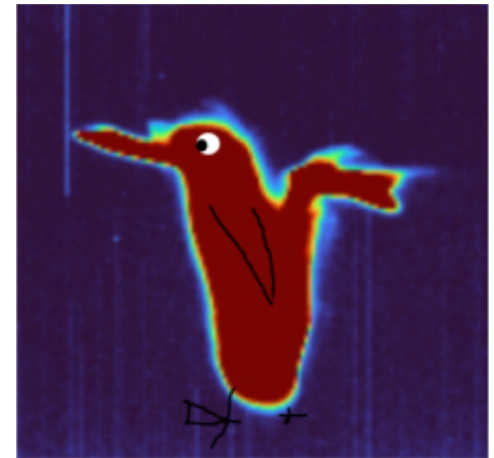
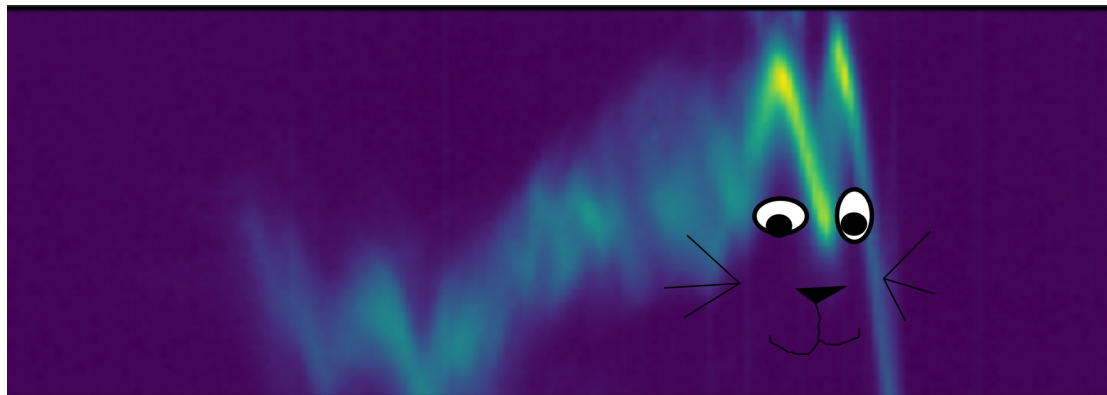


# Results: find the relevant pulses





Questions?



# Finding the right reference image

## 'classical approach'

- 1) clean lasing on/off images.
- 2) slice them in n slices.
- 3) calculate the x-Projection.
- 4) nr\_clusters manually or with gap\_statistics.
- 5) sklearn.cluster.AgglomerativeClustering with euclidean distance to cluster them in a group, calculate mean and spread of the group, average them.
- 6) use np.corrcoef to find the best reference group ( Pearson product-moment correlation coefficients).
- 7) compare com and spread of lasing on with the averaged con / spread of the best matching group.
- 8) use a different detector to find the matching total power / y offset.

$$R_{ij} = \frac{C_{ij}}{\sqrt{C_{ii}C_{jj}}}$$

# Beta-Variational Autoencoder

## Basic principle

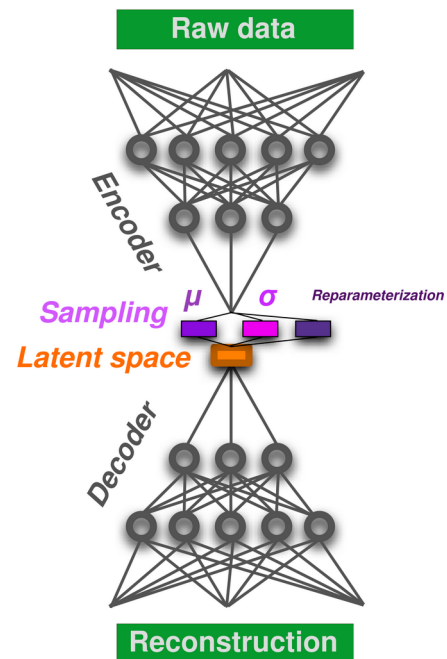
- Variational autoencoder: learn a distribution in the latent space
- Loss includes the deviation from a Gaussian normal distribution (KL divergence)

$$D_{KL} = \frac{1}{2} \sum_{i=1}^k (\sigma_i^2 + \mu_i^2 - 1 - \ln(\sigma_i^2))$$

- Reparameterization trick for backpropagation
- Beta controls the disentanglement

$\beta$ -VAE: LEARNING BASIC VISUAL CONCEPTS WITH A CONSTRAINED VARIATIONAL FRAMEWORK

Irina Higgins, Loic Matthey, Arka Pal, Christopher Burgess, Xavier Glorot, Matthew Botvinick, Shakir Mohamed, Alexander Lerchner  
Google DeepMind  
{irinah, lmatthey, arkap, cpburgess, glorotx, botvinick, shakir, lerchner}@google.com

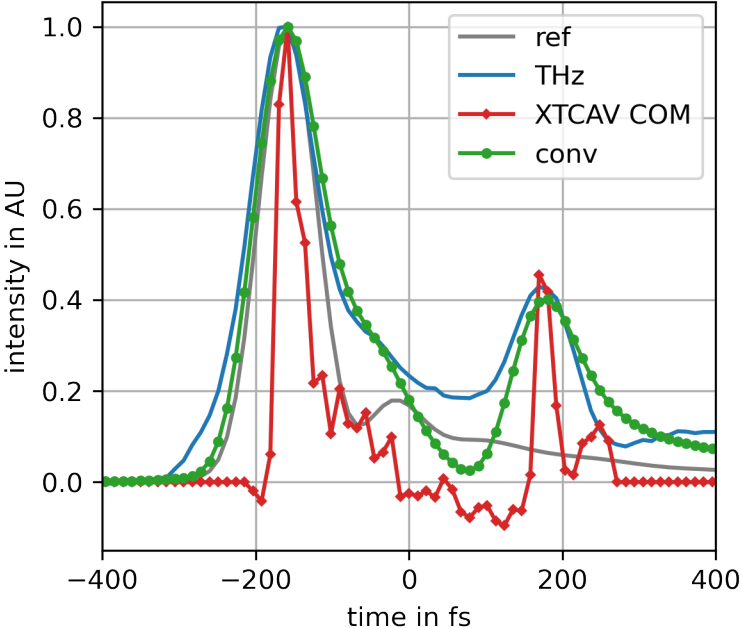
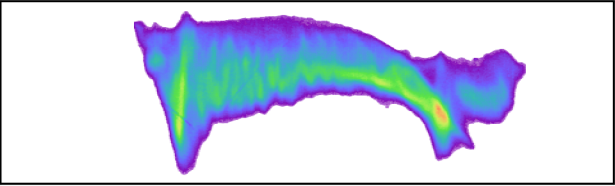


Loss =  
ReconstructionError +  $\beta$ \*DisentanglementError

# Polarix and THz streaking

## Two single shot examples

Good agreement



Different intensity ratios

