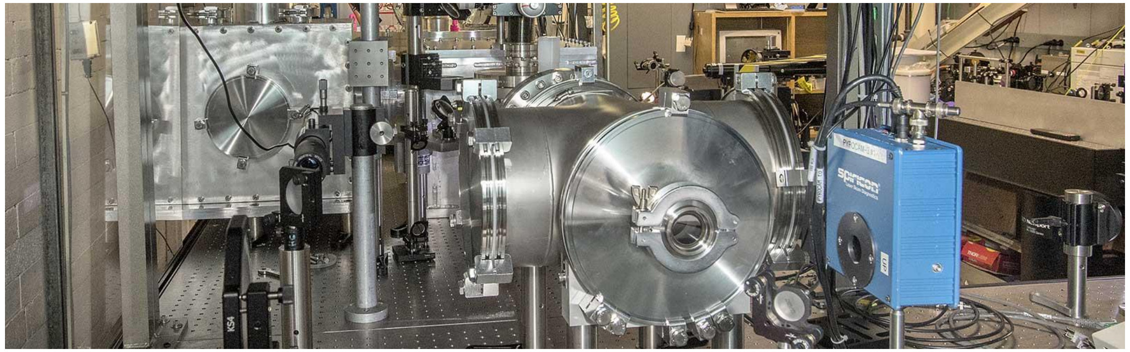
Data Analysis and Control of a MeV Ultrafast Electron Diffraction System using Machine Learning

Trudy Bolin[1], Salvador Sosa Guitron [1], Junjie Li [3], Marcus Babzien [3], Mikhail Fedurin [3], Mark A. Palmer [3], Manel Martínez-Ramón [1], Sandra G. Biedron [1,4]

[1] Department of Electrical and Computer Engineering, University of New Mexico, New Mexico, USA
[2] Department of Biomedical Engineering, University of Strathclyde, Glasgow, UK
[3] Brookhaven National Laboratory, Upton, New York, USA
[4] Department of Mechanical Engineering, University of New Mexico, New Mexico, USA

Outline

- MeV ultrafast electron diffraction (MUED)
  - Why?
  - Where?
  - How?
- Why do we need machine learning for analysis?
  - Autonomous identification of anomalous patterns
  - Preprocessing is key
- Convolutional autoencoder for pattern reconstruction



https://www.bnl.gov/atf/

Funding secured through DOE EPSCoR program


Sandra Biedron *(PI)*

Manel Martínez-Ramón *(Co-PI)*



Trudy Bolin


Salvador Sosa


Mariana Fazio


David Martin

Michael Papka

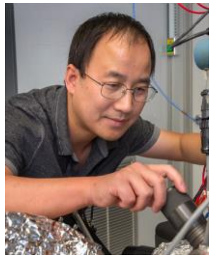


Thomas Uram

Marcus Babzien


Kevin Brown


Mark Palmer


Junjie Li



Mikhail Fedurin


Robert Malone


Christine Sweeney


Alan Hurd

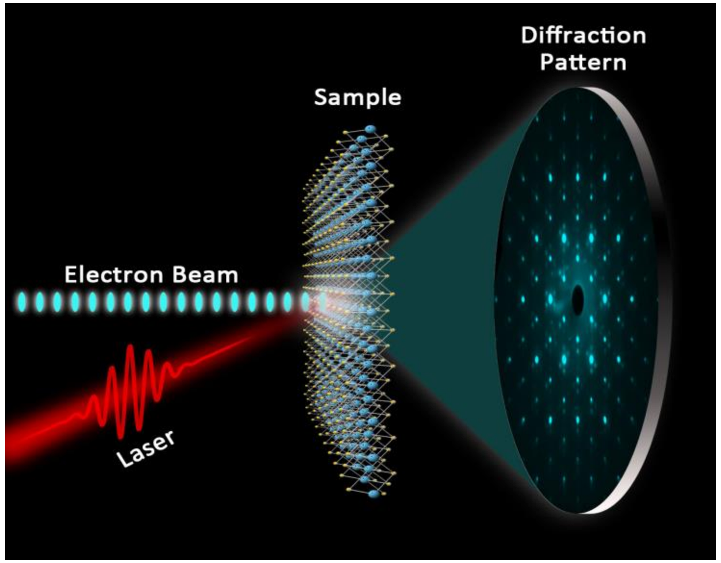

John Sarrao


Julian Chen

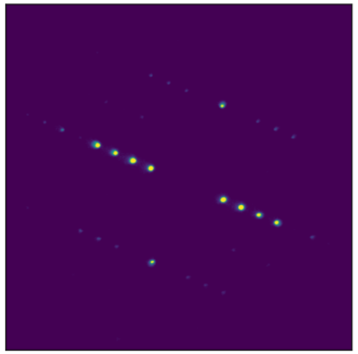

Rohit Prasankumar

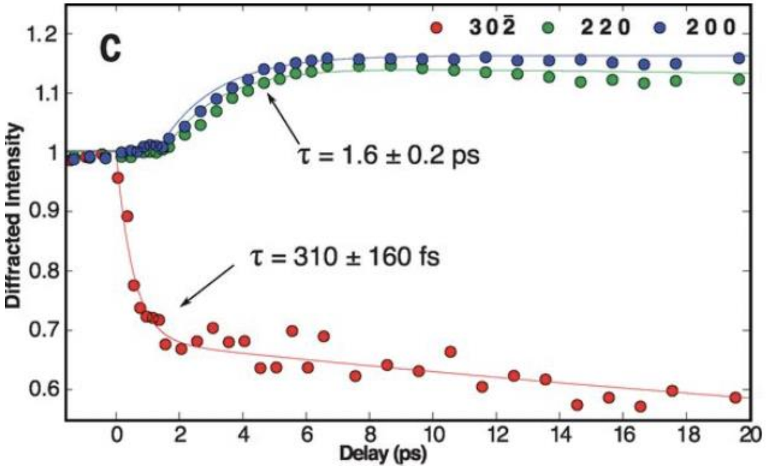
MeV ultrafast electron diffraction (MUED)

It is a powerful structural measurement technique for exploring time-resolved, ultrafast processes in different material systems.



- ✓ Diffraction measurements made at time scales below ~10 fs
- ✓ High scattering cross-section
- ✓ Extremely short wavelength (diffraction patterns contain many reflections)
- ✓ Reduced space charge effects
- ✓ Less multiple scattering effects (structural reconstruction sometimes possible)

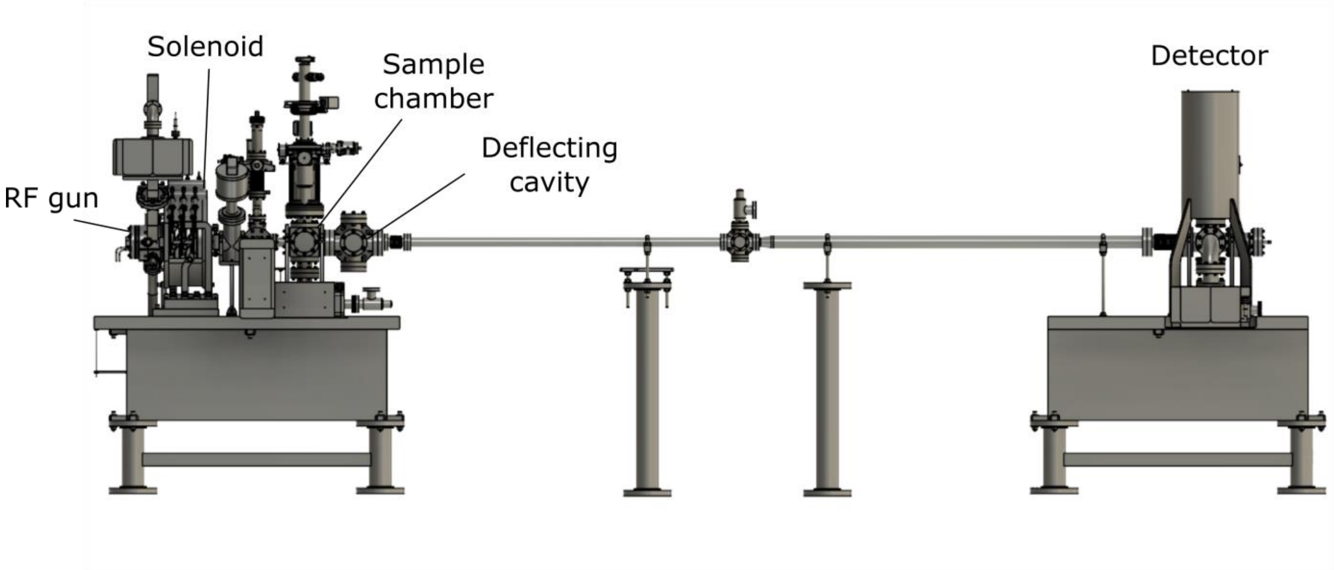




MeV ultrafast electron diffraction (MUED)

It is a powerful structural measurement technique for exploring time-resolved, ultrafast processes in different material systems.

Accelerator Test Facility (ATF @ BNL)



Beam energy	3 MeV
N e- per pulse	1.25 x 10^6
Temporal resolution	180 fs
Beam diameter	300 (100 best) µm
Max repetition rate	5 – 48 Hz
N e- per sec per µm^2	88-880

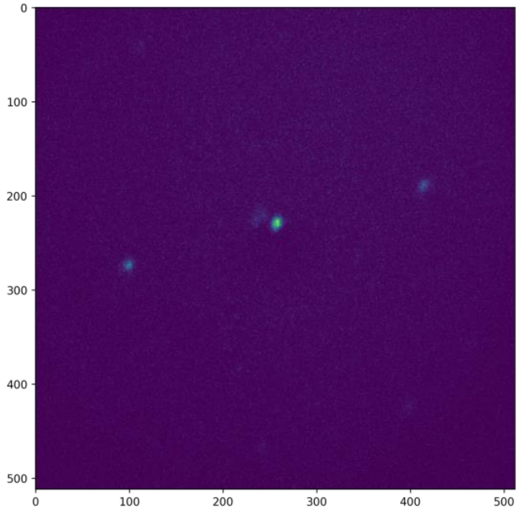
- Ti:Sapph pump (but OPA available, up to 9 um)
- Liquid N_2 or liquid He cooling
- Strict sample requirements (electron transparent, lateral size > 300 nm)

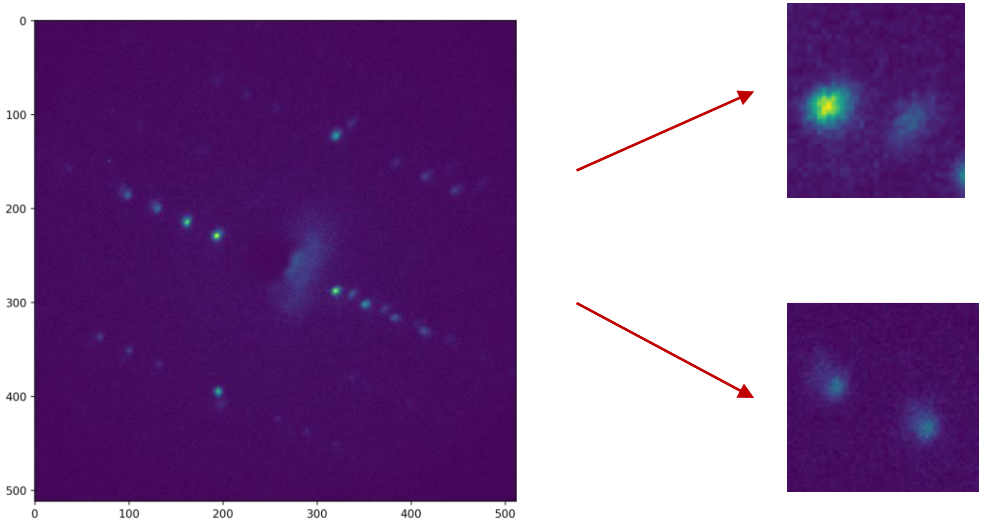
Why do we need machine learning for analysis?

- Due to instabilities in the electron beam, **anomalous** patterns are usually observed in single shot mode.

- These anomalies are integrated when accumulating several patterns (typically 70) and will be detrimental for the accuracy of the experiment.

- Some examples:





- The rate of anomalies is about 10% but can vary largely with experimental conditions (eg: 38% anomaly rate in a pump-probe experiment).

Autonomous anomaly detection

We want to be able to find anomalous patterns in the large datasets with no user input (autonomous)

- We have different types of anomalies and would like to also recognize unseen types.
- We will limit our analysis to Ta_2NiSe_5 as it is single crystal.
- The anomalies are under sampled, we can't employ a classification model.

- We developed a **convolutional autoencoder** model to reconstruct the diffraction patterns.
- Our model trains on all data (unsupervised).
- An anomaly will have a large reconstruction error or different feature vector values.
- We tested different strategies to detect anomalies.

Preprocessing is key for good ML performance

Input: images of 512 x 512 pixels.

1. We split each image in 80 x 80 pixels tiles, using a sliding window with overlap.

2. Filter out the tiles that are background, for this we devised a simple algorithm to decide if a tile contains white noise:

For f(x) a discreet distribution of N samples that is normalized, we define the inverse participation ratio (IPR) as:

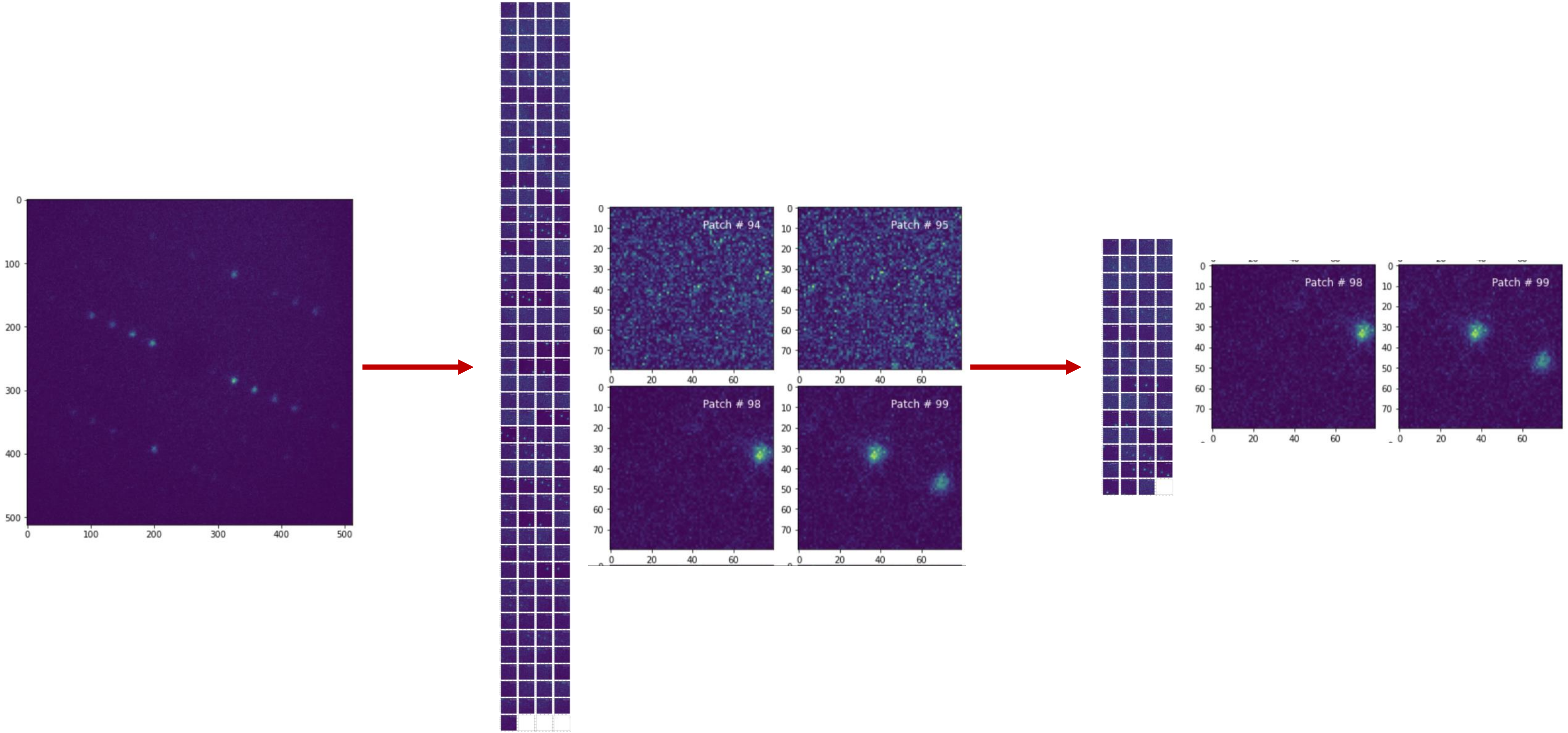
$$IPR = \sum_{i=1}^{N} f(x)^2$$

For white noise, all frequencies contribute equally so f(x) has the same value for all x then:

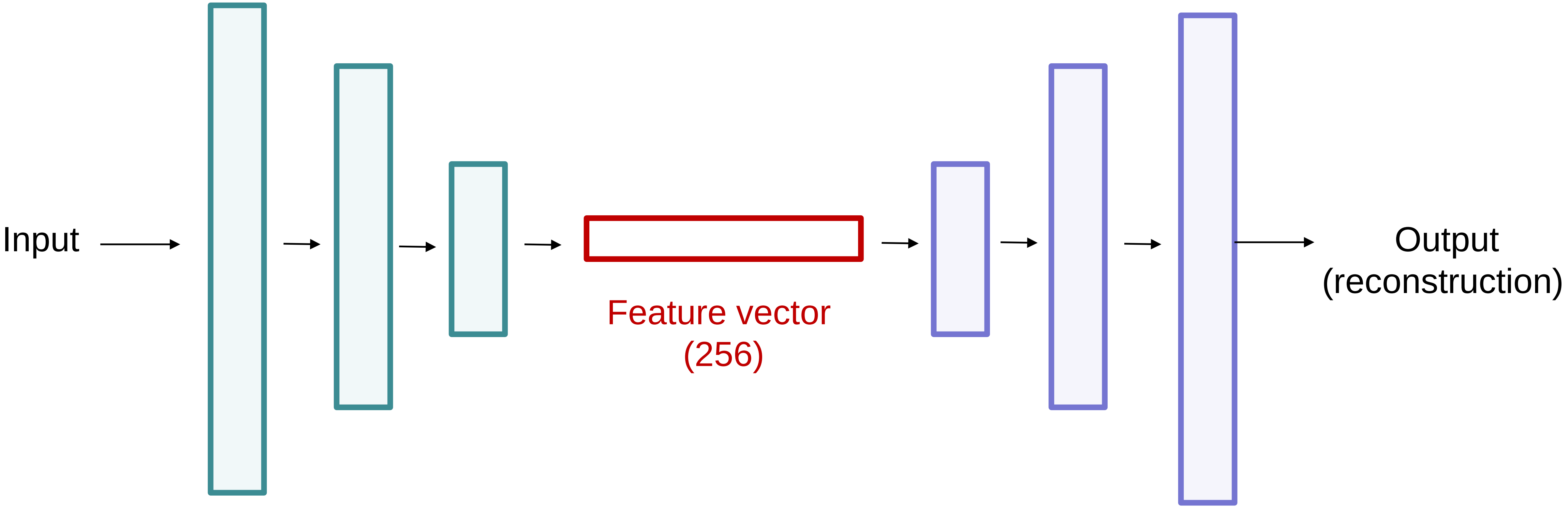
$$f_i(x) = 1/N \Rightarrow IPR = \sum_{i=1}^{N} 1/N^2 = 1/N$$

We do the FFT of the tile, calculate the IPR and if it is equal to 1/N the tile is not included in the dataset for the autoencoder.

Preprocessing is key for good ML performance



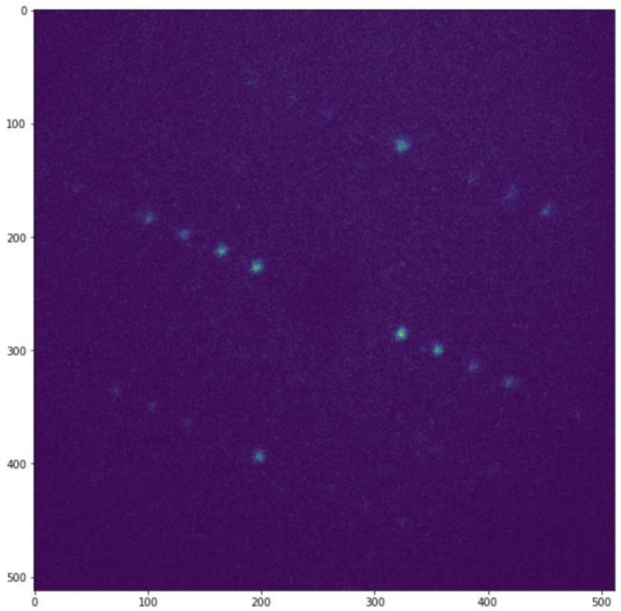
Convolutional autoencoder for pattern reconstruction



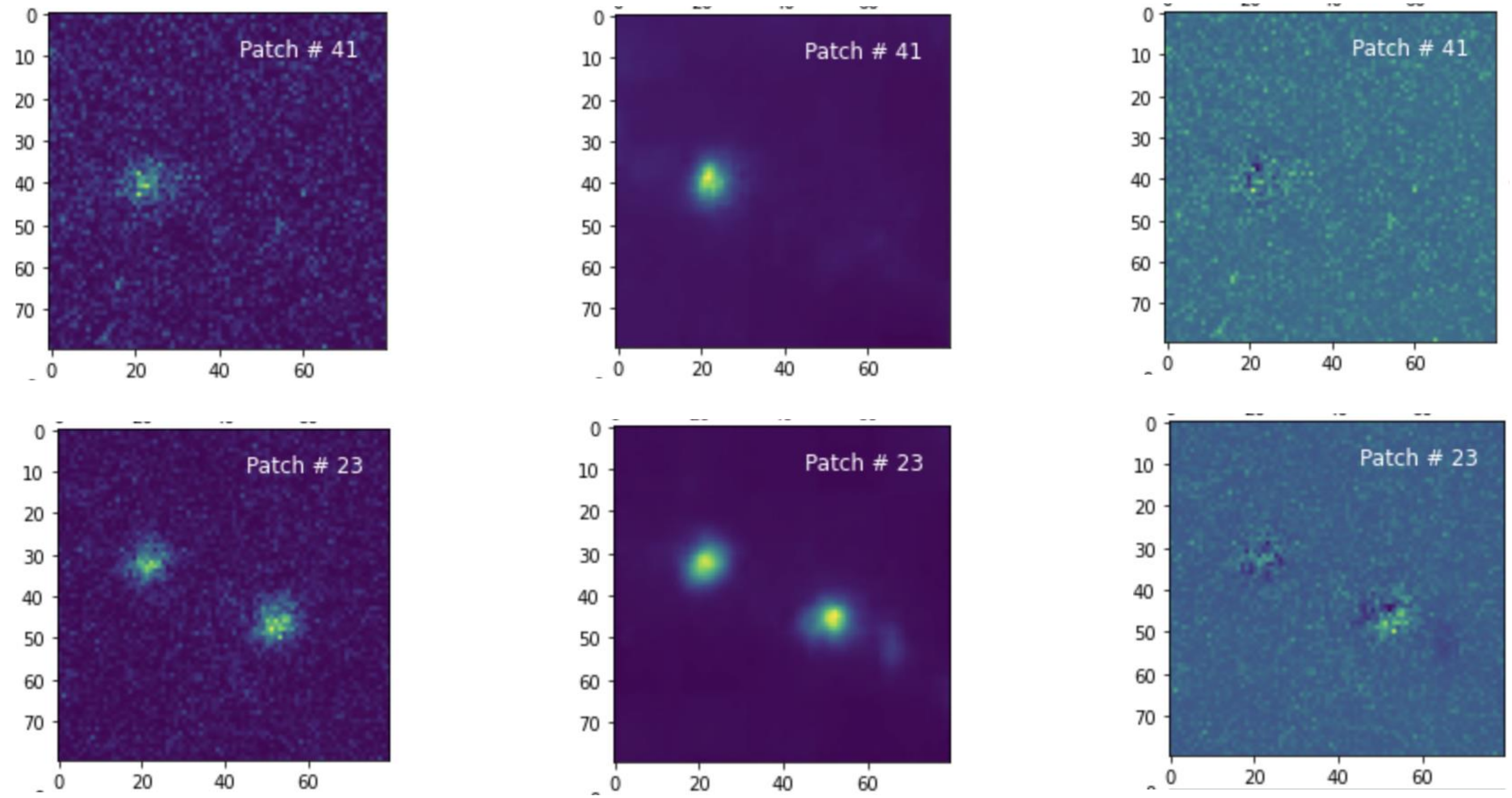
- Each layer of the encoder: Conv2d with relu activation followed by MaxPool.
- MSE loss is used, model trained with 3789 diffraction patterns.
- Dataset is split 10-10-80 for test-validation-training.

Our autoencoder reproduces and denoises patterns

- The autoencoder performs very well and is trained in 100 epochs.
- It also served to denoised the images (which we plan to explore further)



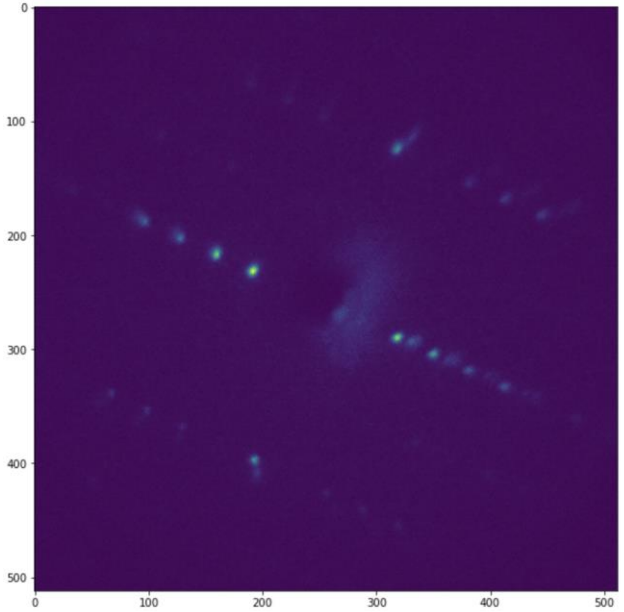
Original *Reconstruction* *Error*

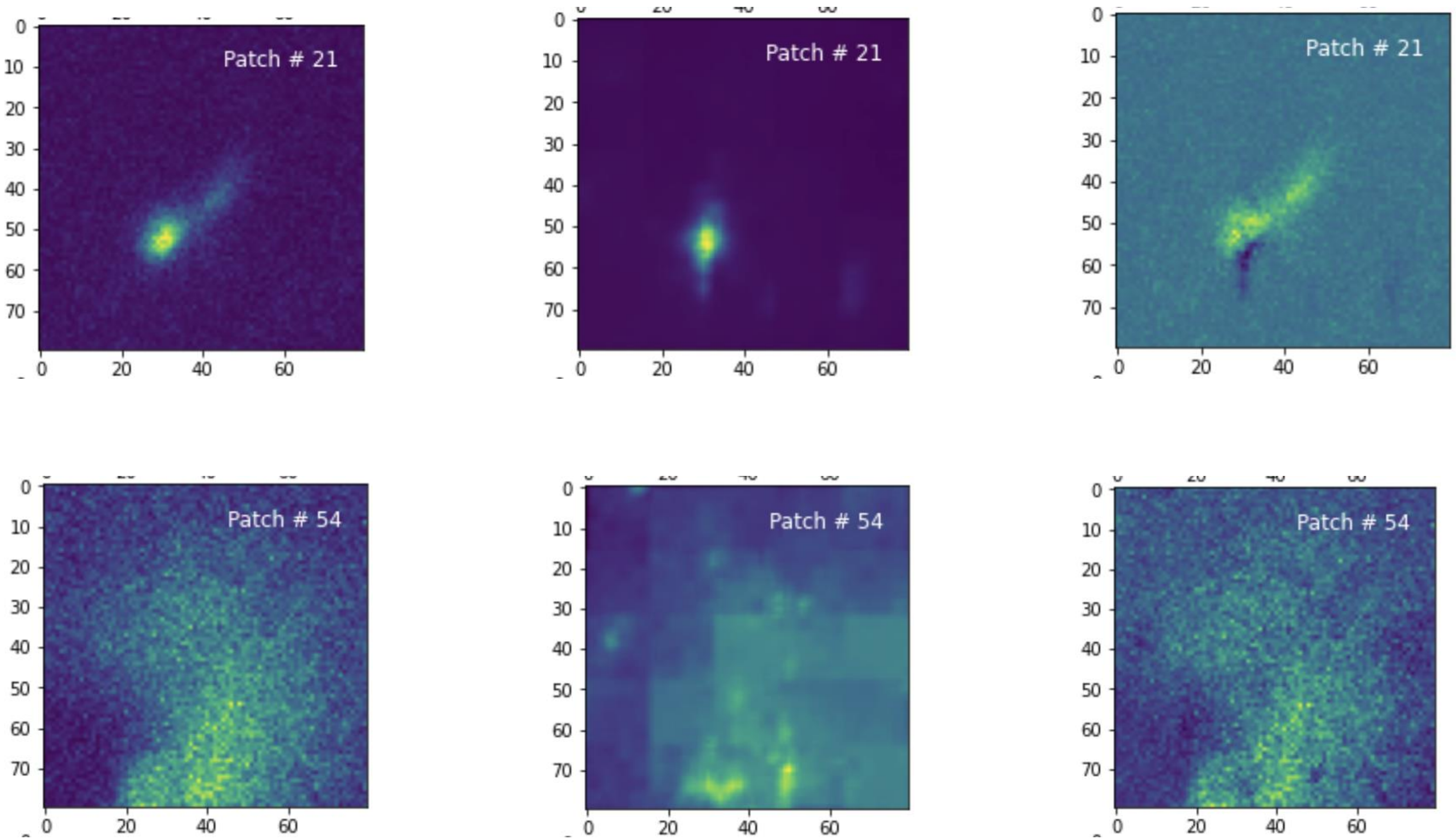


Our autoencoder performs poorly for anomalies

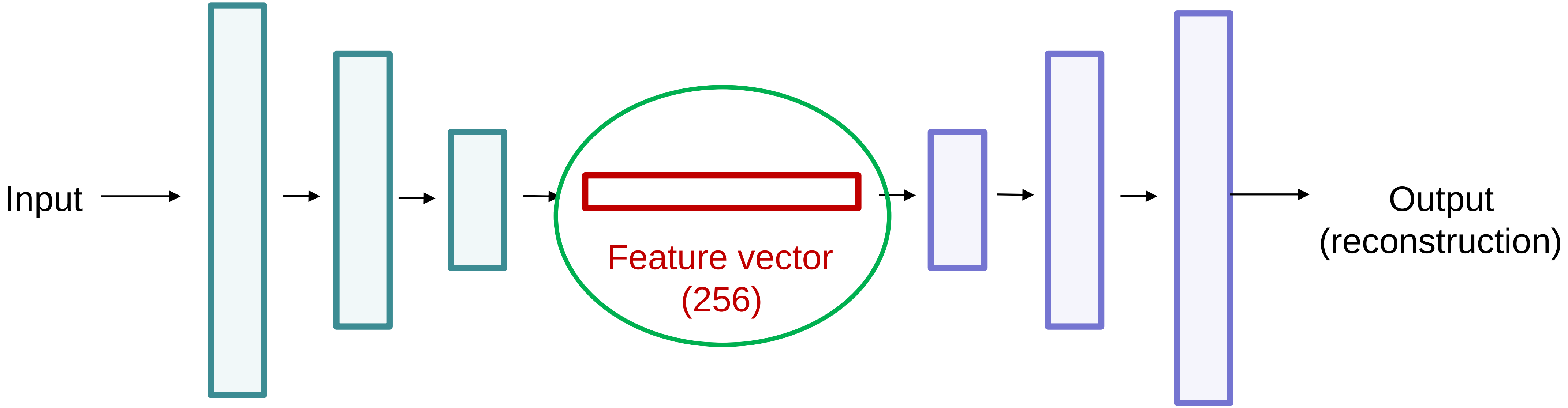
- Recognizable features of anomalies are not well reconstructed:

Original *Reconstruction* *Error*





Anomaly detection: one-class support vector machine



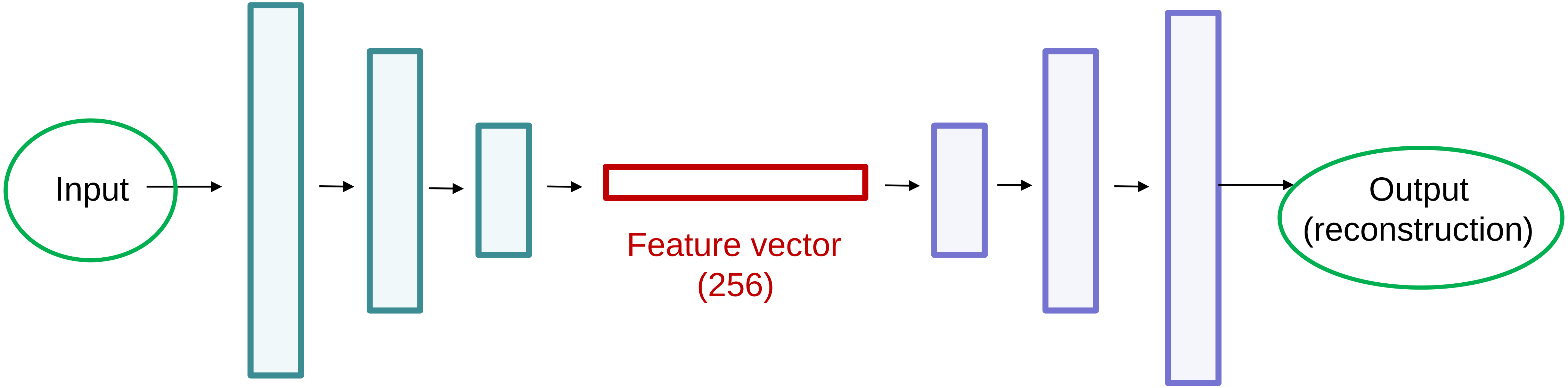
- We implemented a **one-class support vector machine** with Gaussian kernel.

- We estimated the parameters in an **unsupervised** way.

However, we still have much to do:

- We want to use OCSVM in a probabilistic approach.
- We are having issues detecting a class of anomalies related to large energy variations.

Anomaly detection: pixel-wise error distribution



- We can use the **pixel wise error** between input and output.

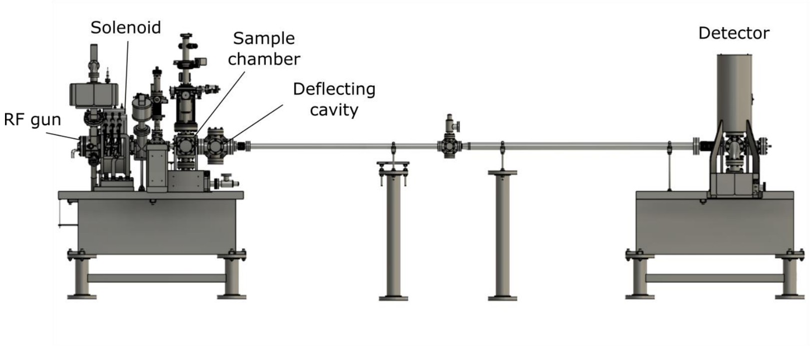
- We proved that this fits a **Skellam distribution** (only significant source of noise is Poisson)

However, we still have much to do:

- We want to combine both anomaly detection approach for increased confidence.
- We want to set thresholds defined by users needs and tolerances.

Connection to ALCF: two DOE facilities

Accelerator Test Facility (ATF @ BNL)

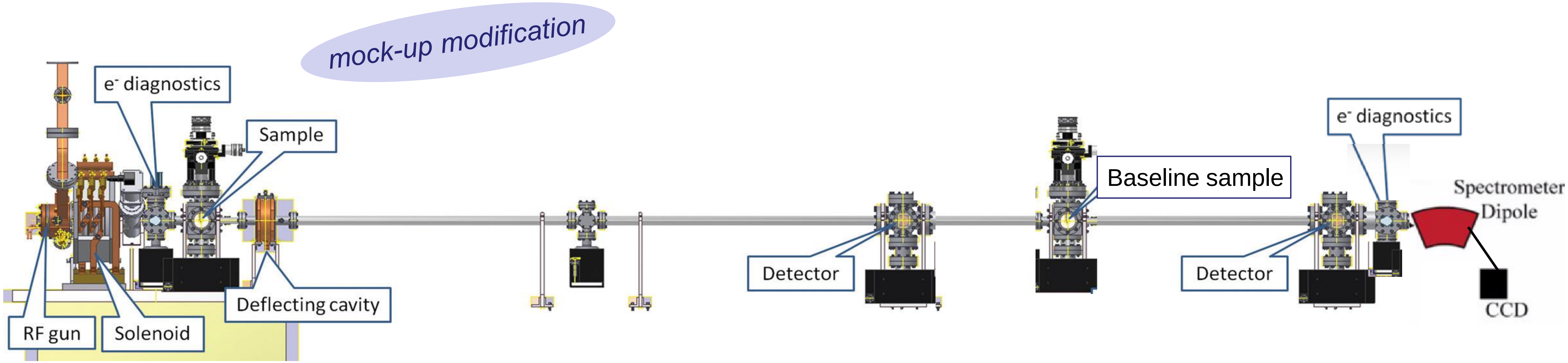


Argonne Leadership Computing Facility (ALCF)

https://www.alcf.anl.gov/

- ➢ We have allocation at Theta and <u>ThetaGPU</u> for this experiment.
- ➢ We are establishing a connection from a computer in the control room at BNL to ALCF.
- ➢ We plan to allow users to train / do inference with the model using ALCF resources for near-real time results (training on single GPU ~ 12 sec/epoch).
- ➢ This would be as simple as running a Jupyter notebook (for inference) and we already have custom built code for analysis and instrumental diagnostics.

Future Plans: enabling shot-to-shot with ML



- ➢ Add beamline extension to measure concurrent diffraction patterns of a baseline sample. We will use this as a shot-to-shot nondestructive diagnostic tool.
- ➢ We plan to employ ML/AI techniques for control of the instrument.
- ➢ Simulations of the beamline underway to use a surrogate model for control.

Conclusions

- ✓ We applied a convolutional autoencoder for reconstruction of electron diffraction patterns.
- ✓ The machine performs well and also denoises (great plus!).
- ✓ Both pixel-wise reconstruction error and OCSVM applied to feature vector are good detectors of anomalies.
- ✓ Next step: combining both approaches for more robust (and tunable) anomaly detection.
- ✓ We stablished a workflow for data originating from ATF to stream to ALCF.
- ✓ Upcoming: applying the machine to other materials. Interested in MUED? If so, **biedron@unm.edu**

Thank you for your attention

This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, Program of Electron and Scanning Probe Microscopies, under award number DE-SC0021365. This funding was made available through the Department of Energy's Established Program to Stimulate Competitive Research (EPSCoR) State-National Laboratory Partnerships program in the Office of Basic Energy Sciences. This research used resources of the Brookhaven National Laboratory's Accelerator Test Facility, which is a DOE Office of Science User Facility. This research used resources of the Argonne Leadership Computing Facility, which is a DOE Office of Science User Facility.

We wish to extend our heartfelt thanks to Mariana Fazio for her valuable contributions to this project!