UE117 Advanced Control of the ATF MUED Electron Beam Using Automation, Artificial Intelligence, and High-Performance Computing
UE110-Baseline materials for characterizing the MUED configuration, their role verifying daily alignment and in operation and implementation of a non-destructive real-time machine learning diagnostic for ensuring beam stability

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Funding secured through DOE EPSCoR program

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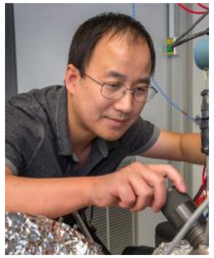

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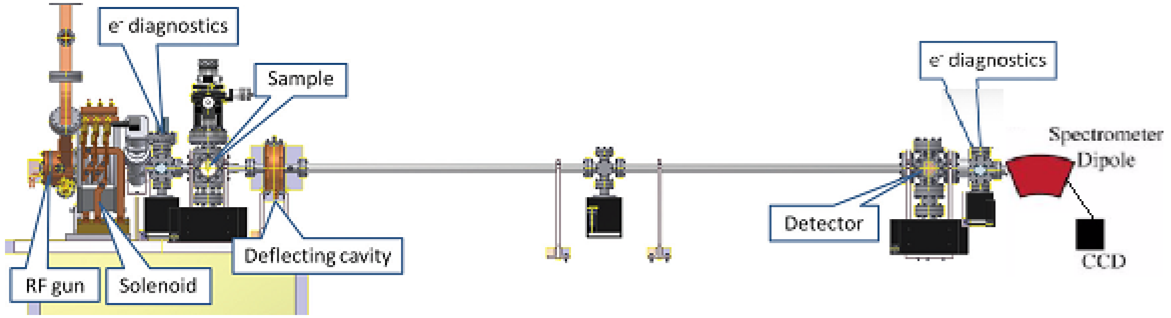
Outline

– Experiment Goals & Overview
– Summary of major results and/or critical experimental preparations to date
– Experimental plans for the next year
– Summary of products delivered from the work to date (presentations, publications, other)

- MeV ultrafast electron diffraction (MUED)
- Autonomous identification of anomalous patterns (Preprocessing is key)
- Convolutional autoencoder for pattern reconstruction



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MeV ultrafast electron diffraction (MUED)

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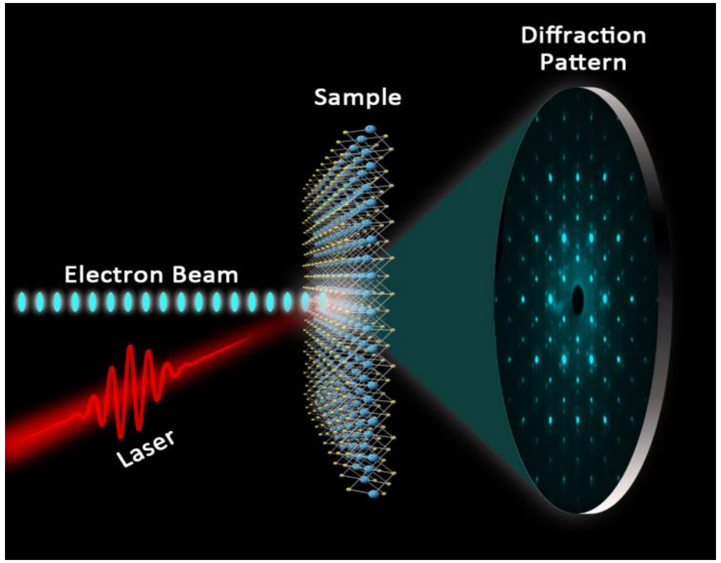
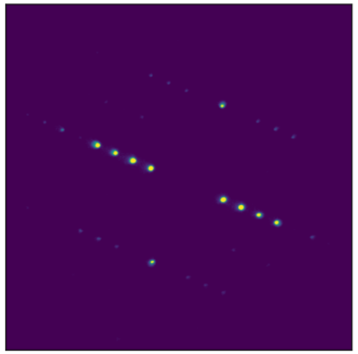
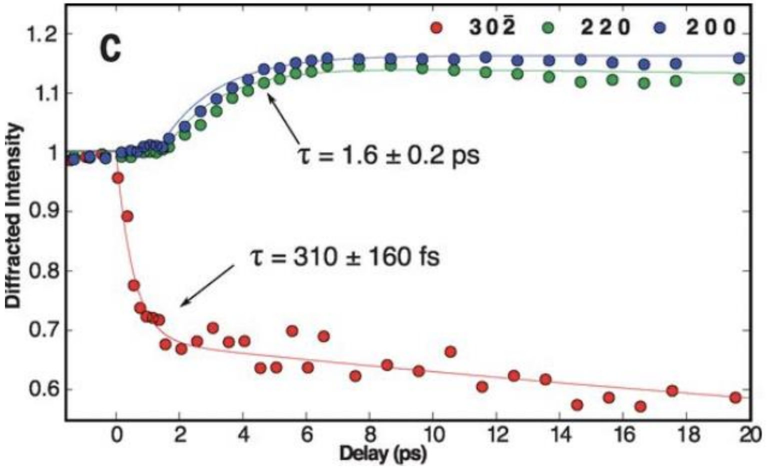
A powerful structural measurement technique for exploring time-resolved, ultrafast processes in different material systems.



- ✓ Diffraction measurements made at time scales ~100 fs
- ✓ High scattering cross-section
- ✓ Extremely short wavelength (diffraction patterns contain many reflections)
- ✓ Reduced space charge effects (peak broadening and displacement)
- ✓ Less multiple scattering effects (structural reconstruction sometimes possible)



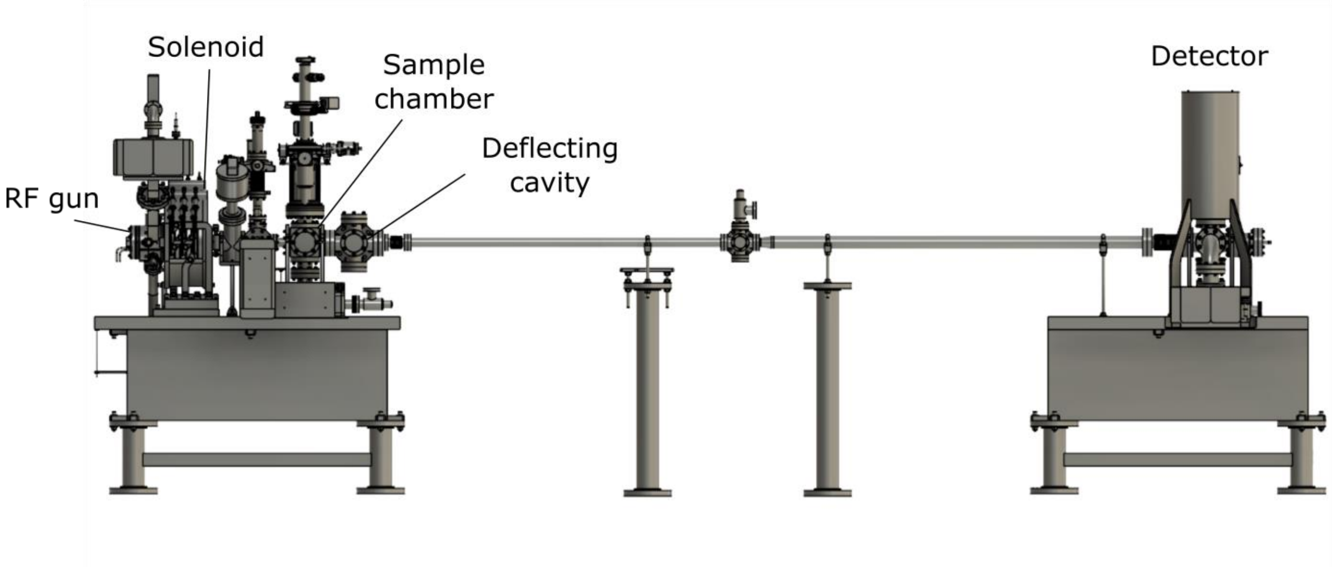
Ta_2NiSe_5
2D material



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	1.25×10^6
Temporal resolution	180 fs
Beam diameter	300 (100 best) µm
Max repetition rate	5 – 48 Hz
N e- per sec per µm²	88-880

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

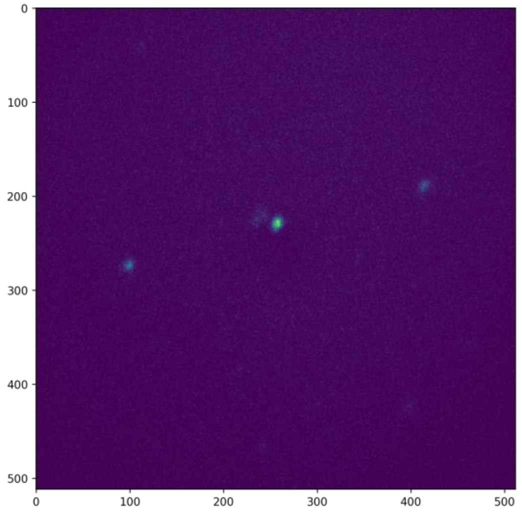
Why do we need machine learning for analysis?

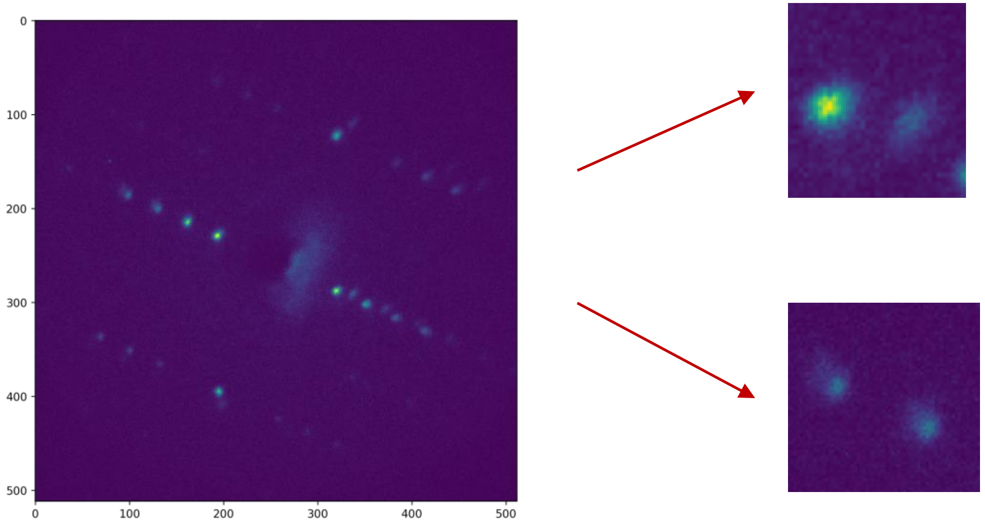
- Due to instabilities in the electron beam, **anomalous** patterns are usually observed in single shot mode.

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

- Some examples:

Ta_2NiSe_5





- 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

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

- Different types of anomalies and would like to also recognize unseen types.
- Limit analysis to Ta_2NiSe_5 as it is single crystal.
- The anomalies are under sampled, can't employ a classification model.

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

Preprocessing is key for good ML performance

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Input: images of 512 x 512 pixels.

1. Split each image in 80 x 80 pixels tiles, using a sliding window with overlap.
2. Filter out the tiles that are background, devised a simple algorithm to decide if a tile contains white noise:

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

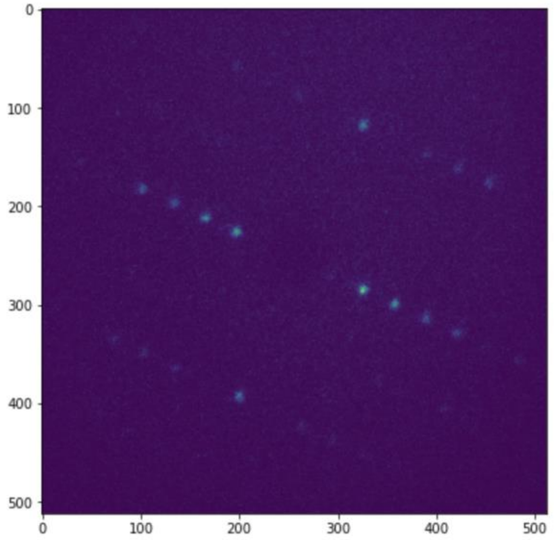
$$IPR = \sum_{i=1}^{N} f(x)^2$$

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

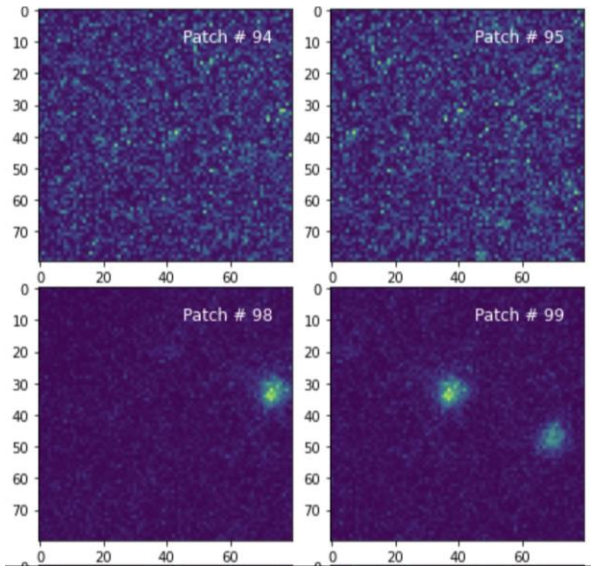
$$f_i(x) = 1/N \Rightarrow IPR = \sum_{i=1}^{N} 1/N^2 = 1/N$$

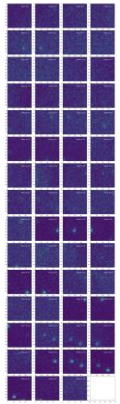
Do the FFT of the tile, calculate the IPR and if it is equal to 1/N the tile is not included in the dataset for the autoencoder.

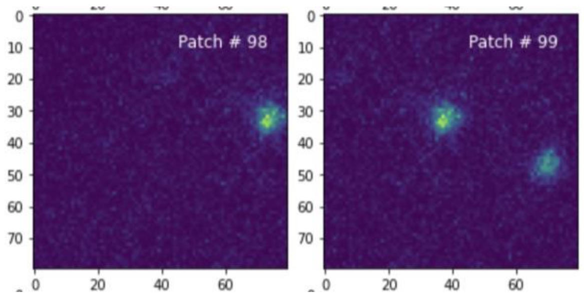
Preprocessing is key for good ML performance



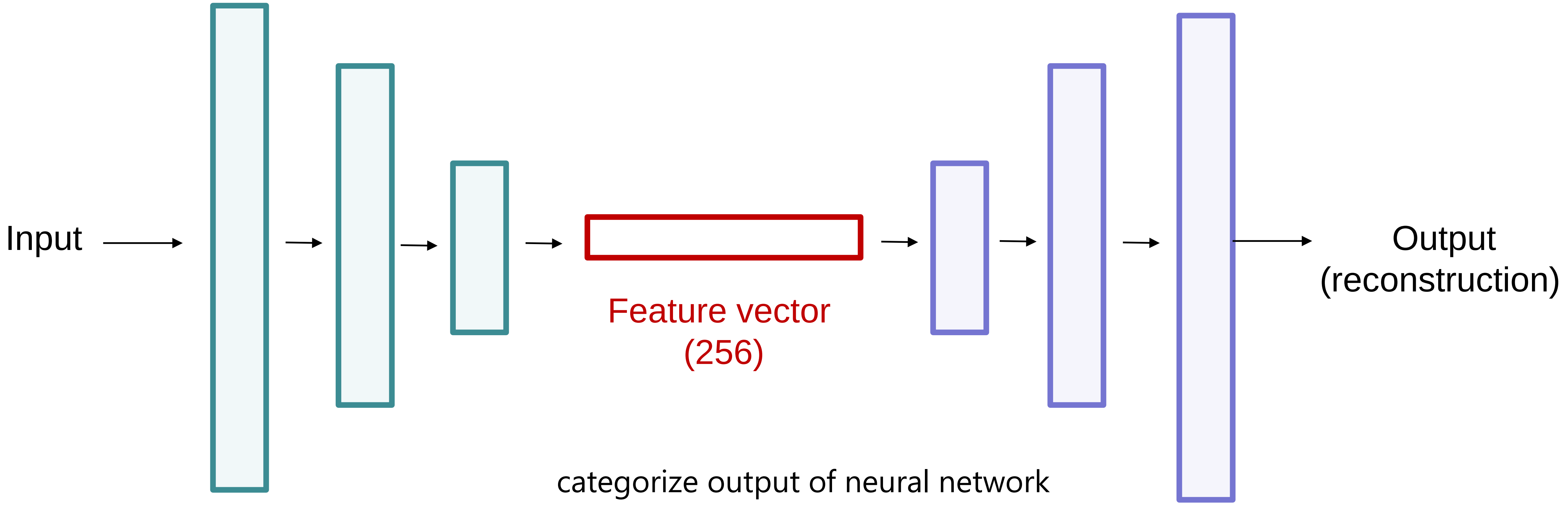
Ta_2NiSe_5







Convolutional autoencoder for pattern reconstruction



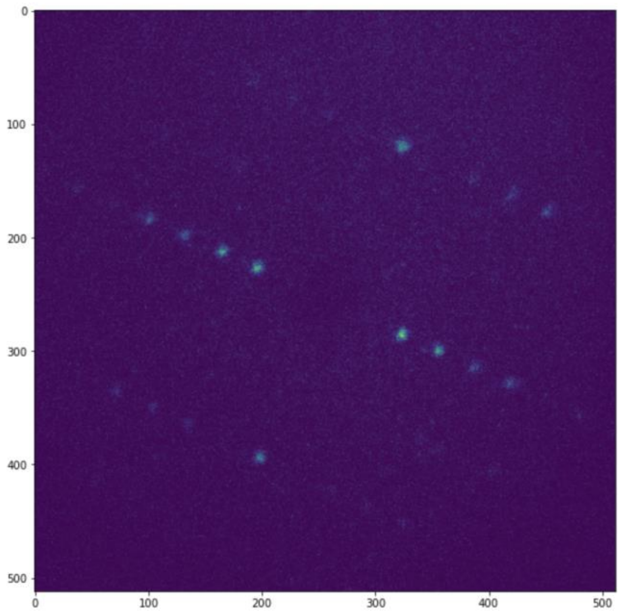
categorize output of neural network

- 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.

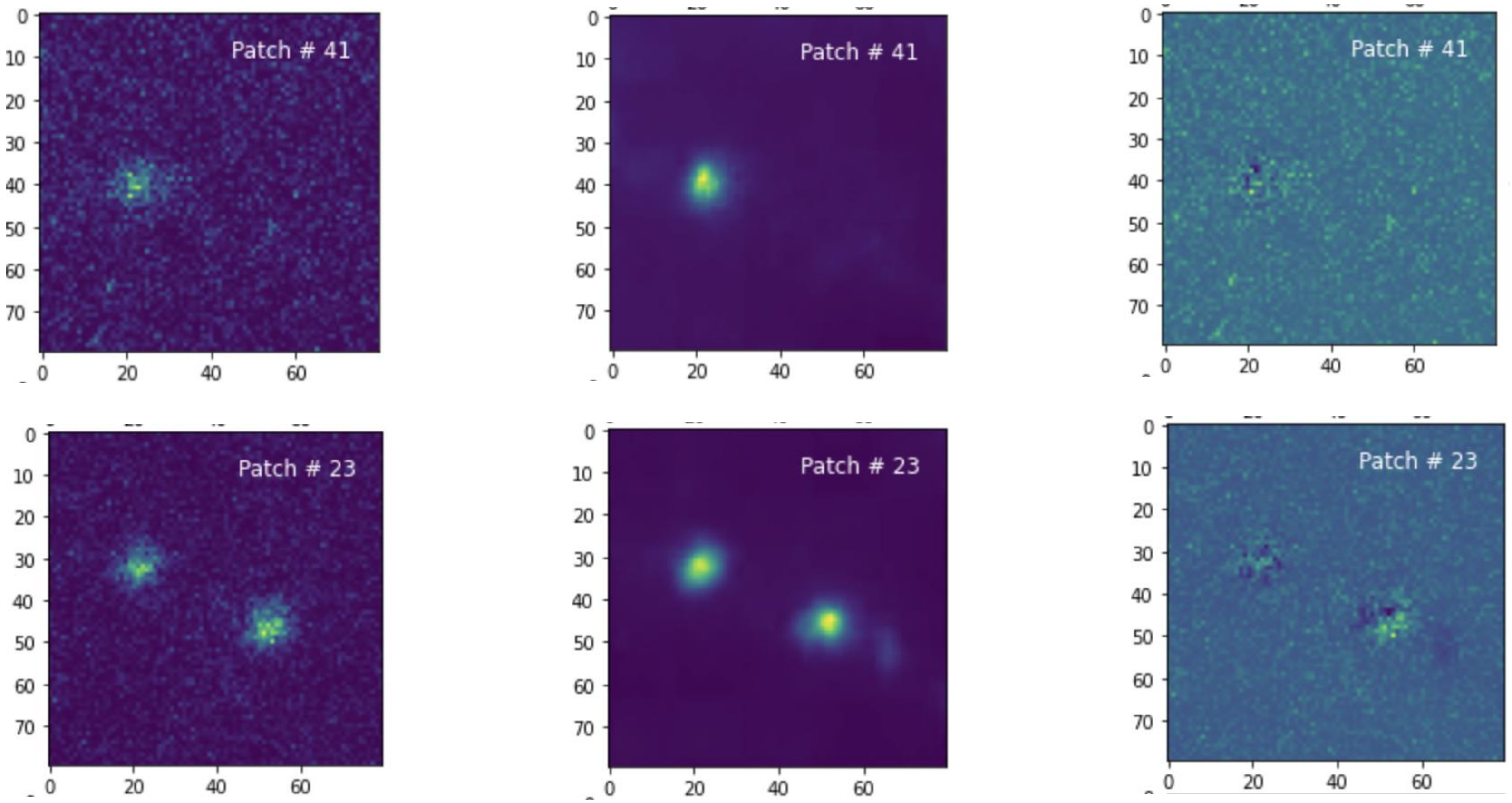
discretization process

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)



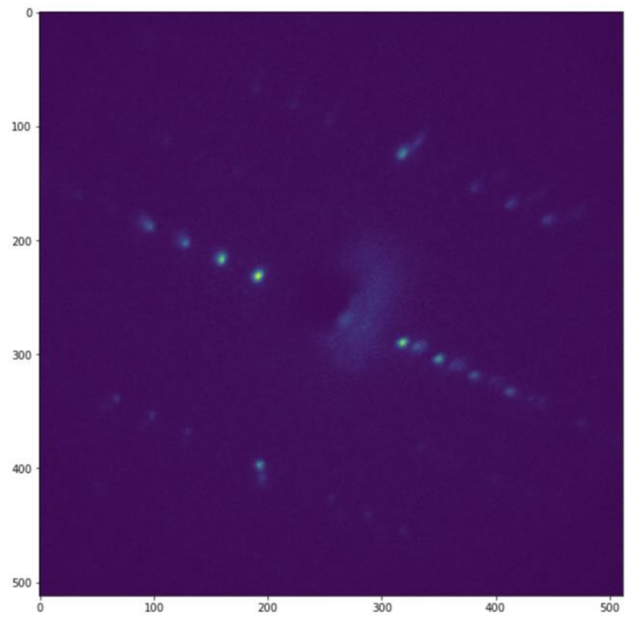
Original *Reconstruction* *Error*

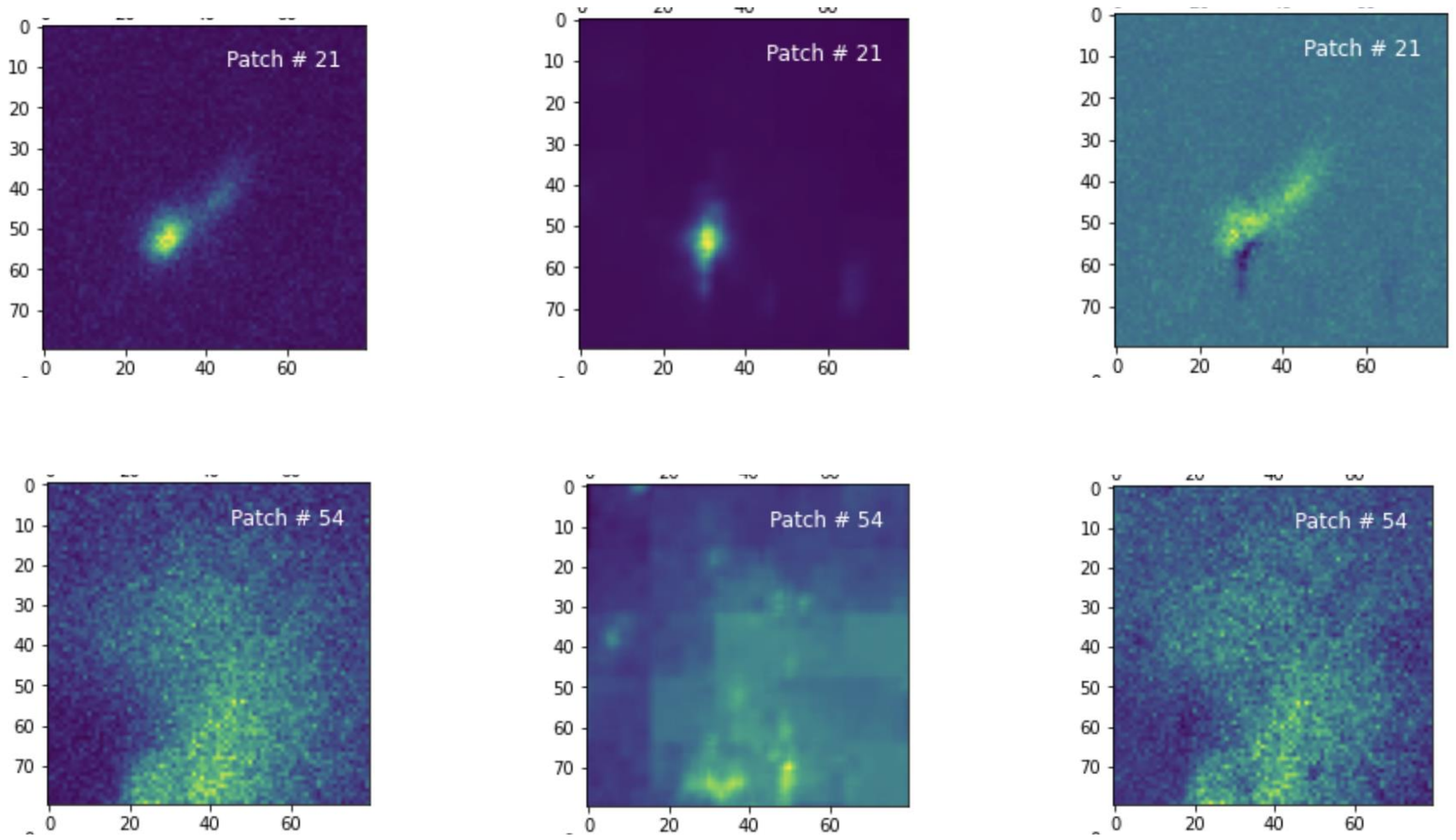


Our autoencoder performs poorly for anomalies

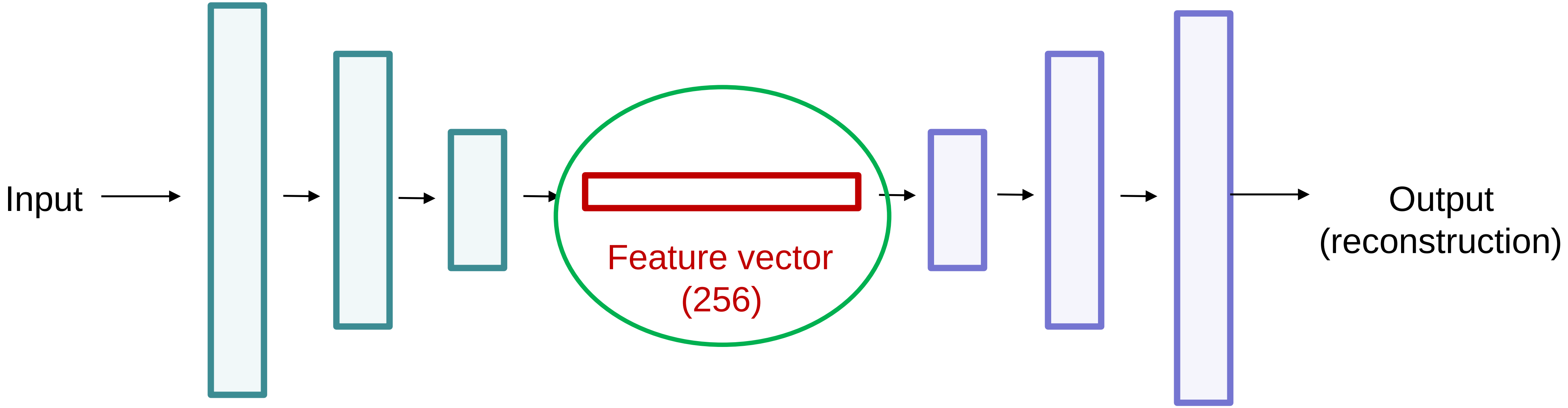
- Recognizable features of anomalies are not well reconstructed:

Original *Reconstruction* *Error*





Anomaly detection: one-class support vector machine



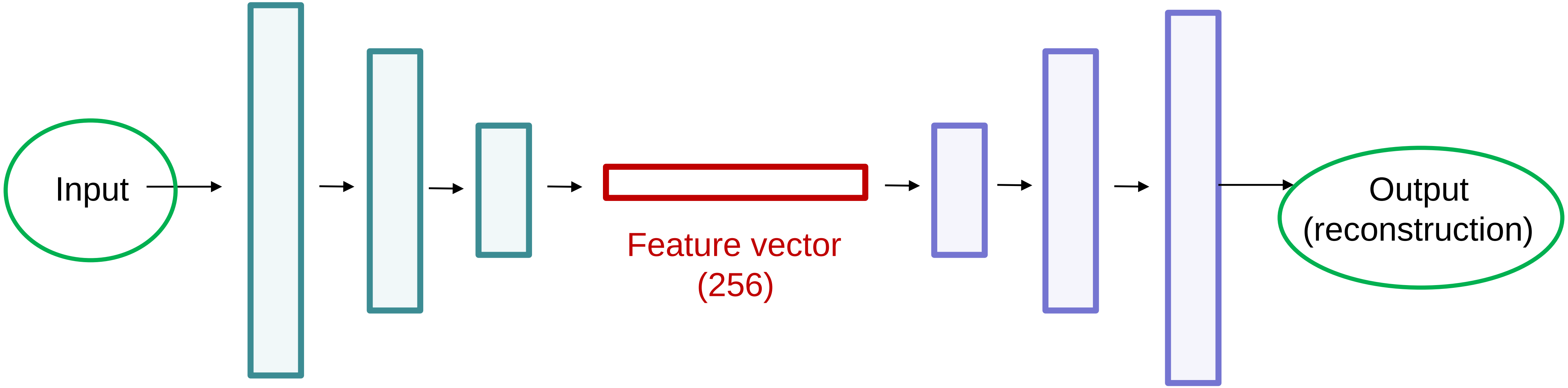
- We implemented a **one-class support vector machine** with Gaussian kernel.

- 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.

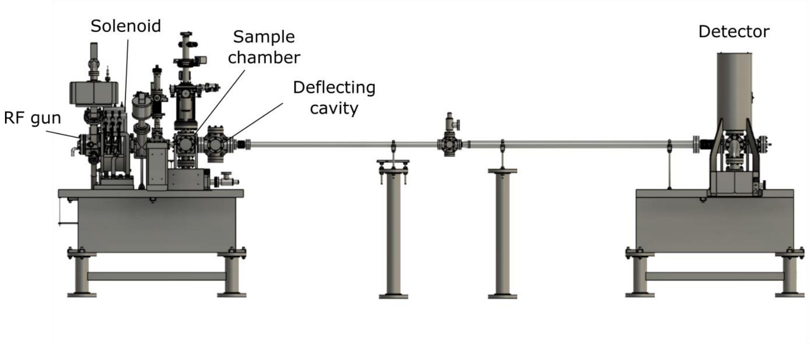
- We proved that this fits a **Skellam distribution** (only significant source of noise is Poisson)

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)

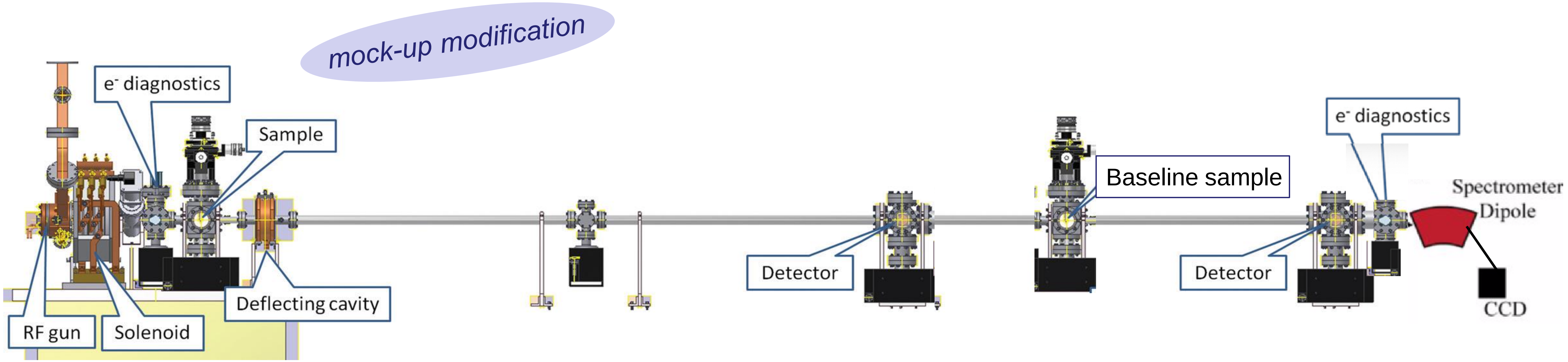


Argonne Leadership Computing Facility (ALCF)

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

- We have allocation at Theta and ThetaGPU 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

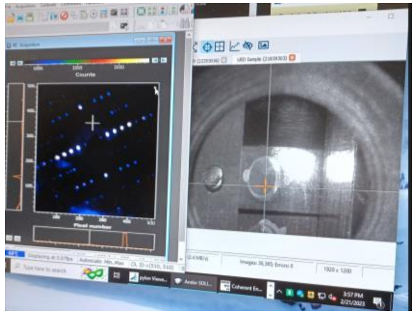
- ✓ We applied a convolutional autoencoder for reconstruction of electron diffraction patterns.
- ✓ The machine performs well and also denoises (great plus!).
- ✓ Both pixel-wise reconstruction error and OCSVM applied to feature vector are good detectors of anomalies.

  One-class support vector machine, unsupervised

- ✓ 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**

Recent Beamline Activities

- Two main tracks for February, 2023
  - **Beamline Operations** (w/M. Fedurin and W. Li and M. Babzien)
    - Trained on beamline operations in order to get diffraction data (J. Li has accepted another position so I had to come up to speed quickly)
      - Beamline Alignment and procedure development; “start-to-finish” training
      - Learning how to perform tasks such as energy calibration
      - Identifying factors that affect data quality
      - Etc…



  - **Software/computer operations development** (w/B. Malone) For example:
    - Identified a method for remote operation
    - Implemented python to call camera library functions
    - Script development such as “sanity checks” for establishing meaningful detector communication
    - Communicated directly with the Andor camera in preparation for image export t ALCF
    - Initialized camera API environment
    - Next phase is to develop a stand-alone code using functions outside of solis

Details of future plans…

- A significant opportunity for a more “self-driving” beamline
- A lot of details…
  - What are the “knobs” that we can adjust to optimize the beamline performance?
    - I’ve been collecting data for preliminary examination
    - Additional diagnostics?
  - How is data going to be prepared for transfer over to the ALCF?
  - How is it fed back to the beamline?
  - Etc…
  - ***Going to involve significant teamwork!***

Publications, etc.

As of 2022…

Publication

Updates in Efforts to Data Science Enabled MeV Ultrafast Electron Diffraction System, S. Biedron, T.B. Bolin, M. Martínez-Ramón, S.I. Sosa Guitron, M. Babzien, M.G. Fedurin, J.J. Li, M.A. Palmer, D. Martin, M.E. Papka, in *Proc. IPAC'22*, Bangkok, Thailand, pp. 397-399. doi:10.18429/JACoW-IPAC2022-MOPOPT057 (2022)

Design of a Surrogate Model for MUED at BNL Using VSim, Elegant and HPC Salvador Sosa Guitron, Sandra Biedron, Trudy Bolin (Oct 20, 2022) Published in: JACoW NAPAC2022 (2022)

Data Analysis and Control of an MeV Ultrafast Electron Diffraction System using Machine Learning Trudy Bolin, Marcus Babzien, Sandra Biedro, Mariana Fazio, Mikhail Fedurin, et al. (Oct 19, 2022) Published in: JACoW LINAC2022 (2022)

Presentations & Posters

3rd ICFA Beam Dynamics Mini-Workshop on Machine Learning Applications for Particle Accelerators Hosted by Brookhaven National Laboratory, Chicago, IL November 1-4, 2022
Data Analysis and Control of a MeV Ultrafast Electron Diffraction System using Machine Learning, Trudy Bolin, Salvador Sosa Guitron, Junjie Li, Marcus Babzien, Mikhail Fedurin, Mark A. Palmer, Manel Martínez-Ramón, Sandra G. Biedron

APS March Meeting 2023, Las Vegas, Nevada (March 5-10) (upcoming)
Updates to an MeV Ultrafast Electron Diffraction (MUED) System for Data Analysis and Control using Machine Learning, Trudy B Bolin, (UNM), Salvador Sosa Guitron (UNM), Aasma Aaslam (UNM) Sandra G Biedron(UNM)

CoDA 2023, Santa Fe, New Mexico, (March 7-9) (upcoming)
Data Analysis and Control of an MeV Ultrafast Electron Diffraction System using Machine Learning Trudy Bolin, Salvador Sosa, Aasma Aslam, Sandra Biedron

Two more papers in preparation on the beamline surrogate model and data analysis….

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 contributions to this project.

Very Special Thanks to ATF people…

- Mark Palmer
- Mikhail Fedurin
- Junjie Li
- William Li
- Marcus Babzien
- Bob Malone
- Karl Kusche
- MJ Ilardi

Thank You!