Yes https://github.com/gduscher/MLSTEM2025/tree/mainAppalachian Regional Electron Microscopy Society Topical Conference

Third Summer School on ML for Electron Microscopy

University of Tennessee Knoxville, with Oak Ridge National Laboratory and Pacific Northwest National Laboratory (?), Thermo Fisher, AtomQ, Mat3ra

Organizers: Gerd Duscher, Sergei V. Kalinin, Tutorials by: Austin Houston, Utkarsh Pratiush, Elizabeth Heon, Kamyar Barakati, Kevin Roccapriore,

If you are working on machine learning for microscopy—whether it's for data analysis, real-time analytics, or running microscopes autonomously—keep your schedule open for the Third Summer School on ML for Electron and Scanning Probe Microscopy, hosted by <u>University of Tennessee</u>, <u>Knoxville</u> in collaboration with <u>Thermo Fisher Scientific</u>, ORNL, and PNNL.

- When? May 19-23, 2025
- Where? Hybrid format (join us in-person or online!)

The school will cover core ML topics, but the real focus will be on the latest advances in automated microscopy, including:

- ☑ Building Al-driven experimental workflows General principles of decision-making for autonomous instruments.
- Leveraging reward-driven workflows Transitioning from manual, biased image analysis to unsupervised, highly robust exploration.
- ✓ Making automation real Hands-on deep dive into AutoScript (<u>Paolo Longo</u>), exploring how to automate and control STEM and SPM instruments.

Participants will gain access to diverse STEM and SPM imaging, spectral, and structure-property datasets, as well as instrument digital twins, providing a unique opportunity to apply ML to real experimental challenges. A major focus of the course will be on engineering the transition from human-controlled to Al-augmented and fully autonomous workflows. Special emphasis will be placed on the AutoScript interface, which allows researchers to implement Python-based automation directly on Thermo Fisher electron microscopes, providing hands-on experience in running real-time data analytics, automated imaging optimization, and Al-driven decision-making workflows. Attendees will learn how to develop and deploy ML workflows on their own microscopes, tackling key challenges such as real-time API integration, stochastic optimization for decision-making, and adaptive Al models. Whether you are interested in microscopy data analysis, automated instrument control, or Al-enhanced materials discovery, this course will provide a comprehensive overview of the state-of-the-art and future directions in the field.

Fees:

The fees for participants will be \$150, AReMS members and UTK students have a reduced fee of \$75 UTK Undergraduate studnts are free of charge

Schedule

Monday May 19: Atomic Resolution STEM and Physics from Atomic Positions

8:30 - 9:00 Welcome

9:00-10:00 Principles of Electron Optics and Aberration Correction in STEM (Duscher)

10:00-10:50 Remote Aberration Correction in STEM (Duscher, Austin assist)

11:10-12:00 Simulation of Ronchigrams [Participant computer] (Duscher)

12:00-1:00 Lunch (provided for registered onsite participants)

1:00-2:00 Remote Atomic Resolution Imaging (Duscher, Austin assist)

2:00-2:50 Methods of Atom Position determination [Participant computer] (Barakati)

3:10 -4:00 First Machine Learning Algorithms for Atomically Resolved Images (Austin)

4:00-5:00 Introduction to Neural Networks (Heon)

Tuesday May 20: Electron Diffraction and 4D-STEM

9:00-10:00 Introduction to Diffraction (Duscher)

10:00-10:50 Remote Diffraction Acquisition in STEM (Duscher, Houston)

11:10-12:00 Simulation of Diffraction Pattern (Duscher)

12:00-1:00 Lunch (provided for registered onsite participants)

1:00-2:00 Analyzing Diffraction pattern [Participant computer] (Duscher, Houston)

2:00-2:50 Clustering Algorithms for 1 and 2D datasets (Barakati)

3:10-4:00 Conventional and Smart Acquisition of 4D STEM (Houston)

4:00-5:00 Processing of 4D Datasets [Participant computer] (Houston)

Wednesday May 21: Remote and Conventional Acquisition of Spectroscopic Data and ML-enabled analysis

9:00-10:00 Introduction to Spectroscopy (Duscher)

10:00-10:50 Remote Acquisition of EDS spectra in STEM (Duscher, Houston)

11:10-12:00 Analysis of EDS [Participant computer] (Duscher)

12:00-1:00 Lunch (provided for registered onsite participants)

1:00-2:00 Remote and Smart Acquisition of spectra in STEM (Duscher, Houston)

2:00-2:50 Conventional Analysis of EELS [Participant computer] (Duscher)

3:10-4:00 Machine Learning of Spectroscopic Datasets [Kalinin]

4:00- 5:00 ML-enhanced Analysis of EELS [Participant computer] (Kalinin)

Thursday May 22 ML for STEM: from post-acquisition to real time analytics

9:00-10:00 Introduction to Workflows in Machine Learning (Kalinin)

10:00-10:50 Convolutional Neural Network (Heon)

11:10-12:00 Neural Networks for Images II [Participant computer] (Pratiush)

12:00-1:00 Lunch (provided for onsite participants)

1:00-2:00 VAE for Image Analysis (Kalinin)

2:00-2:50 Autonomous Operation (TF Paolo)

3:10-4:00 Digital Twin Microscopy [participants computer] (Rama)

4:00-4:30 Streaming to Theory (Timur)

4:30-5:00 Automated JEOL (Spurgeon)

Friday May 23: Decision making in electron microscopy and human-in the loop automated experiment (hAE)

9:00-10:00 Decision Making in Microscopy (Kalinin)

10:00-10:50 Reward Functions for Decision Making (Kamyar)

11:10-12:00 Principles of Gaussian Processes and Bayesian Optimization (Kalinin)

12:00-1:00 Lunch (provided for onsite participants)

1:00-2:00 Deep Kernel Neural Learning and hAE (Kalinin)

2:00-2:50 New opportunities enabled by remote ML-controlled acquisition (Utkarsh)

3:20 -4:00 Atomic Fabrication with STEM (Kevin)

4:00-4:30 AE STEM at CNMS (Lupini)

4:30-5:00 Conclusion (Kalinin and Duscher, hackathon)