# 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 Introduction to EELS (Duscher)

2:00-2:50 Remote and Smart Acquisition of spectra in STEM (Pratiush)

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 Microscopy(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)