ML controlled acquisition : New opportunities

Supported by AI Tennessee initiative
IAMM, UTK

THE UNIVERSITY OF TENNESSEE KNOXVILLE

- Presented by Utkarsh Pratiush

Agenda

1. Go thorough last year survey
2. Our progress in AE-STEM(Hardware orchestration)
3. Hands on!
4. Summing up

We conducted a survey and what people want during our ML-STEM workshop(June 3rd to June 7th)

Q1. What type of automation would you like to see on the STEM that would be useful?

Q2. Which part of the microscope hardware do you think, if you had control using code, would be useful?

Q3. What kind of ML algorithms would you want to use to steer the data collection on the microscope?

Survey Question 1

Q: What type of automation would you like to see on the STEM that would be useful?

1. Automatic electron dose management for analysis of beam-sensitive materials.
    - Measure screen current, change screen current, HAADF
2. Automatic zone axis alignment.
    - Ceta camera for Diffraction acquisition, map the zone axis, stage tilt(alpha, beta)
3. Automated aberration correction.
    - Read aberration coefficient, Acquire HAADF, change aberration coefficient
4. Diffraction pattern matching.
    - part of Zone axis alignment
5. Automatic focusing on an SEM imaging tool.
    - Defocus – read and change, HAADF
6. Online/Offline segmentation of grains and particles.
    - HAADF detector, Field of view, stage movement
7. Automated image and spectroscopy acquisition in STEM based on reward functions.
    - Bayesian-optimization based workflow, Q. What rewards?
8. Defect segmentation.
    - HAADF , Stage movement
9. Automatic identification of sample regions with thickness below 0.5*mean free path.
    - thickness estimation from eels?
10. Automatic identification of specific structures and performing imaging/spectroscopy on them.
    - HAADF detector, stage movement(x, y, z), spectroscopy –EDX,EELS,
11. Fully automated alignment from the point of inserting a specimen to a crystal aligned on a specific zone axis.
    - Aberration coefficients, stigmation, defocus, diffraction, stage(x, y, x, alpha, beta)

Survey Question 2

Q: Which part of the microscope hardware do you think, if you had control using code, would be useful?

1. Ronchigram.- Flucam acquisition.
2. Stage position: x, y, z, alpha, and beta, also beam current and scanning positions in STEM. - stage, beam.
3. Sample tilt and rotation: alpha and beta angles, particularly useful in exploring and analyzing different grain orientations and boundaries. - stage, diffraction, haadf
4. Focus of EELS dispersion: automatically fix the low-order aberrations in EELS to make the ZLP sharp.
5. Besides the stage position, beam shifting is also important. To achieve ultra-high stability in experiments, sometimes we don't want to move the stage. - Beam shift
6. Aberration corrector: Appropriate aberration corrector tuning depending on the sample, such as in NCSI imaging in CTEM and six-fold astigmatism in STEM. - Control of aberration coefficients
7. Full stage control and all lenses.- stage, objective lens, condenser lens, aperture

Survey Question 3

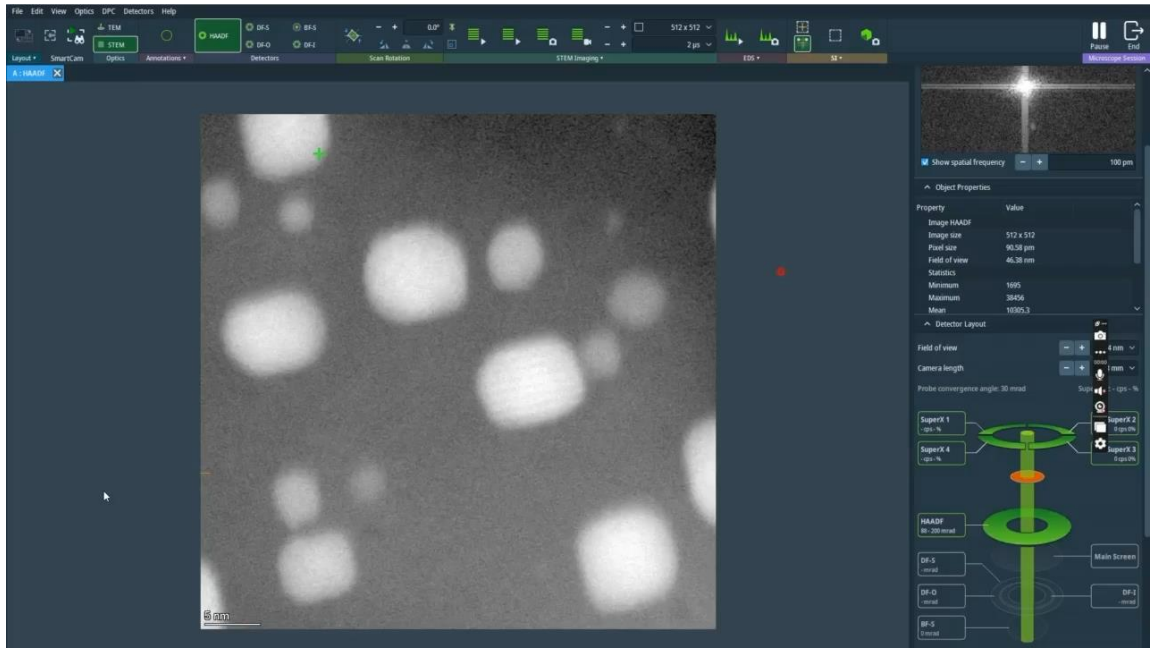
Q: What kind of ML algorithms would you want to use to steer the data collection on the microscope?

1. Deep learning will require many thousands of images
2. Reinforcement Learning (RL), Active Learning, Bayesian Optimization, Anomaly Detection, Physics-Informed Neural Networks (PINNs).
3. Reinforcement learning algorithms to steer the data collection process. Focus is to identify optimal scan parameters and adaptive scanning strategies based on real-time analysis of EBSD patterns.
4. Bayesian Optimization.
5. Automatically correct aberrations in imaging and EELS ZLP.
6. Clustering and Convolutional Neural Networks (CNN) algorithms.
7. I already use UNET and Gaussian processes to locate and determine specimen morphology.
8. I am very ambitious about direct ptychography for real-time phase reconstruction using ML.

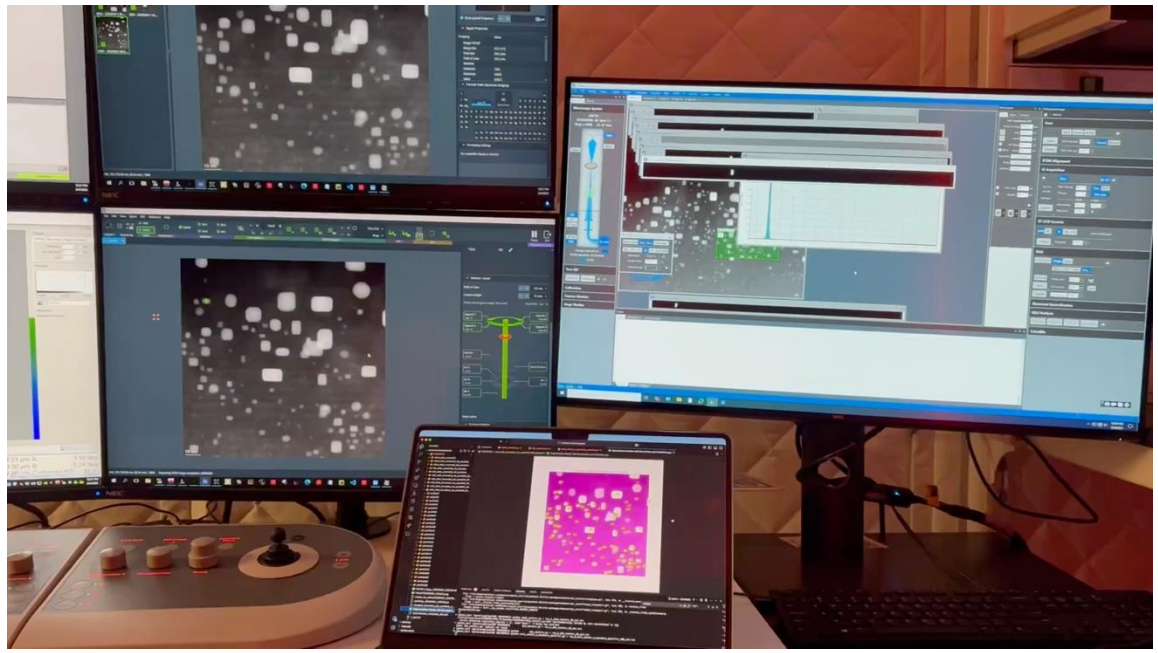
Some conclusions from the questions

- Hardware control is important – **co-orchestration**
- Benchmarks for performance(accuracy and time) of ML models
  - Denoising of images
  - Active learning
  - Particle segmentation
  - Instrument tuning
  - Drift correction
- Scientific questions and rewards
  - What sample?
  - Sample physics
- Scaling **can be** scientifically interesting
- Understanding how to deal with noisy/unreliable data from the detectors.

Next: I will go through some hardware orchestration we have accomplished here - thanks to our team & collaborators



Video - 1

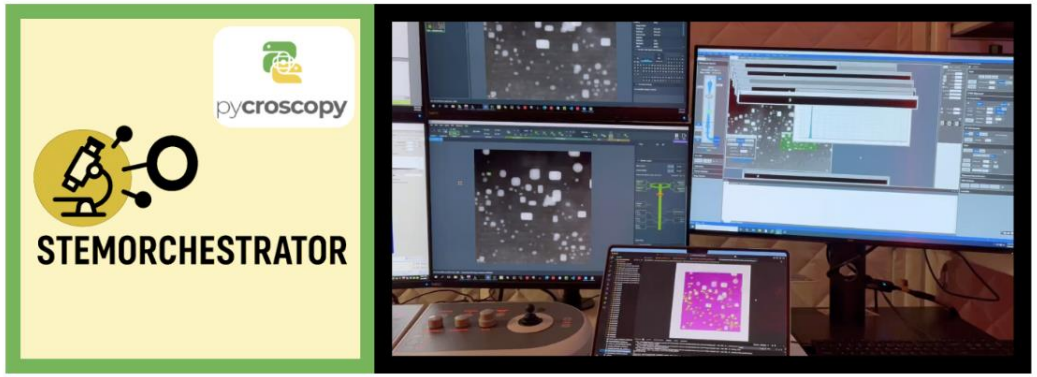


Video - 2

stemOrchestrator: Enabling Seamless Hardware Control and High-Throughput Workflows on Electron Microscopes.

Utkarsh Pratiush[1*], Austin Houston[1], Paolo Longo[2], Remco Geurts[2], Sergei V Kalinin[1,3], Gerd Duscher[1*]

[1]Department of Materials Science and Engineering, University of Tennessee, Knoxville, TN 37996, USA
[2]ThermoFisher Scientific, Eindhoven, the Netherlands
[3]Pacific Northwest National Laboratory, Richland, WA 99254, USA
*Corresponding author's: upratius@vols.utk.edu and gduscher@utk.edu



Preprint: Pratiush, U., Houston, A., Longo, P., Geurts, R., Kalinin, S., & Duscher, G. (2024). https://doi.org/10.31224/4645

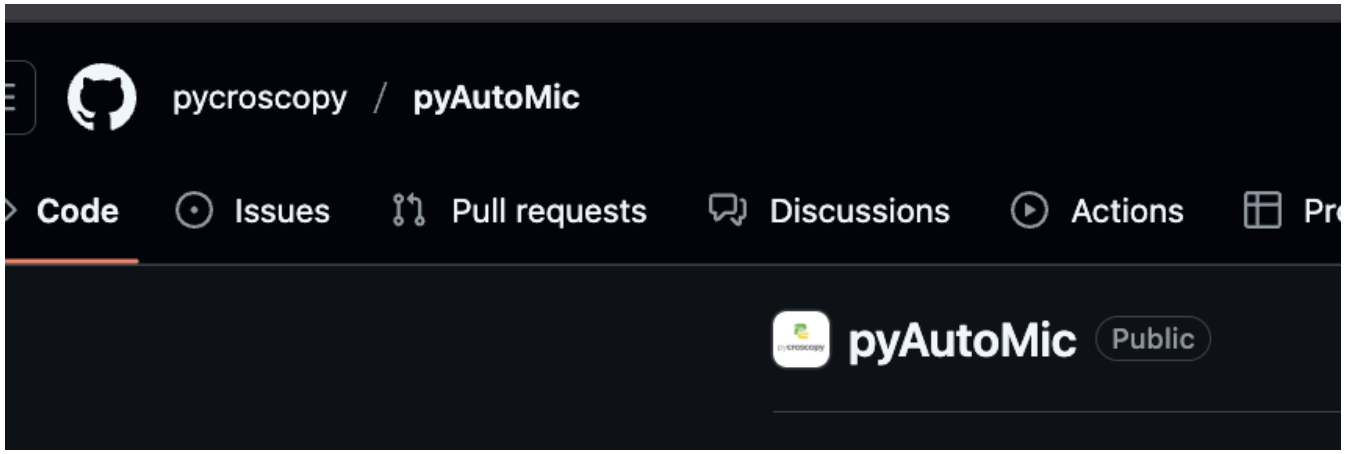
Let’s try Hands on!

- Link to offline server-client module – Thermofisher Autoscript

- Hardware control demonstration – **OFFLINE mode**
  - TF Auto-script control – beam, stage, HAADF, ceta, flucam …
  - Aberration corrector control
  - EELS control – we did Tutorial on 3rd day – link to notebook

- Hardware control – ONLINE mode
- Particle mapping workflow -

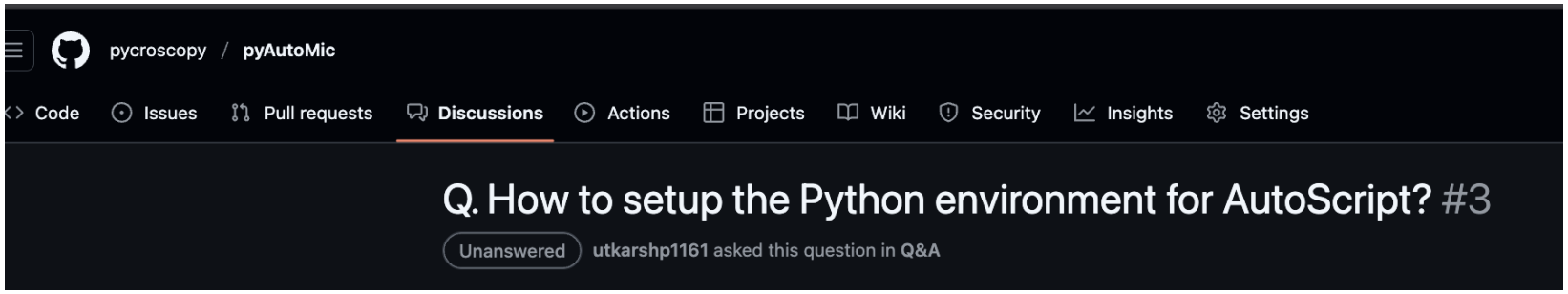
Please Contribute!



Raise:

- Issue's
- Discussion's

https://github.com/pycroscopy/pyAutoMic/tree/main/TEM/stemOrchestrator



Someone who wants to write for other manufacturer's (JEOL, Bruker etc) are more than welcome

Please join below slack channel to be updated

- AI + ML microscopy hackathon
- In general discussion and updates on AE in Microscopy

- Slack-link
- Google form link- AE stem Survey

Thank you for your attention!