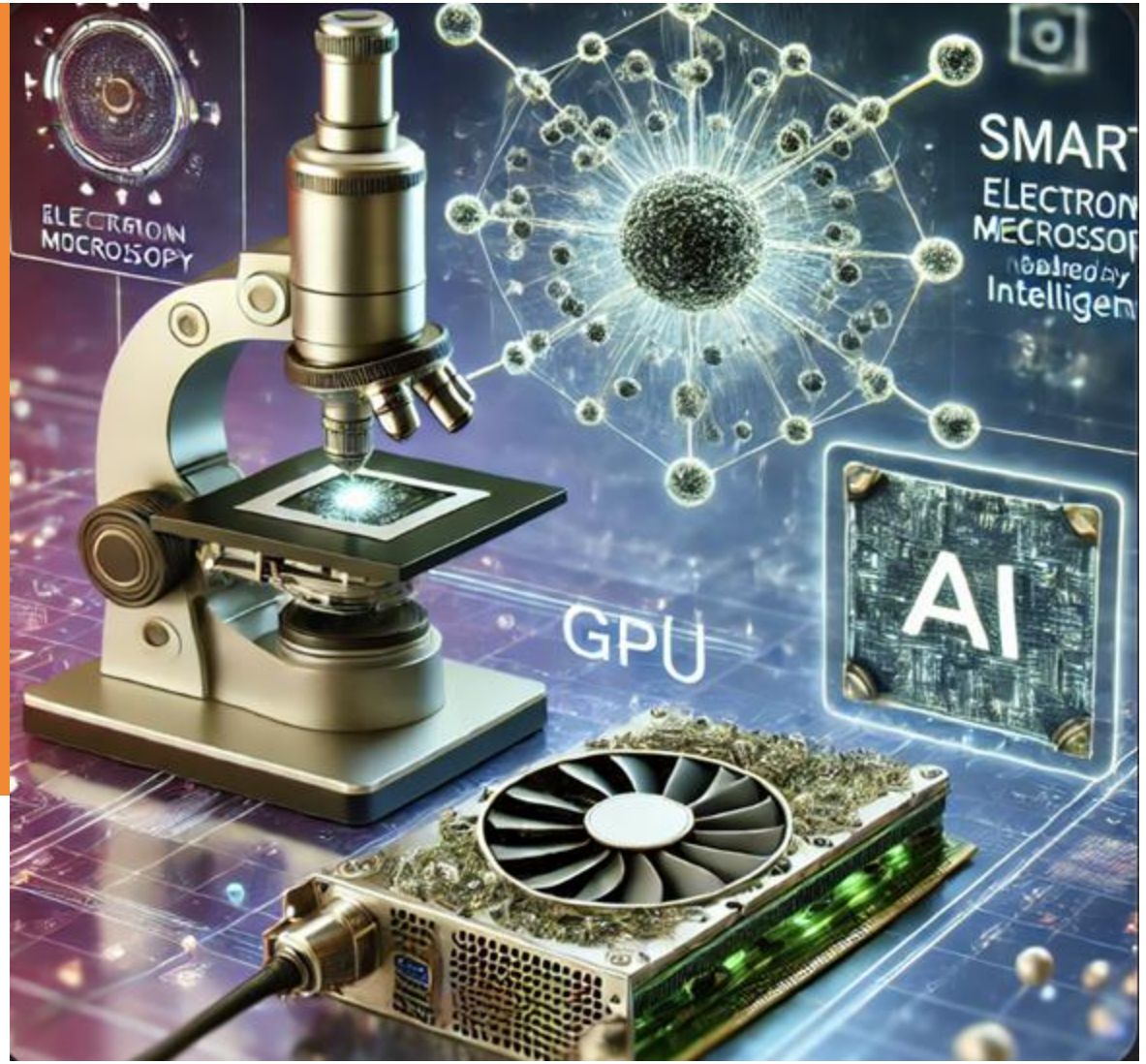
Remote and smart acquisition of spectra in STEM

Supported by AI Tennessee initiative
IAMM, UTK

THE UNIVERSITY OF TENNESSEE KNOXVILLE

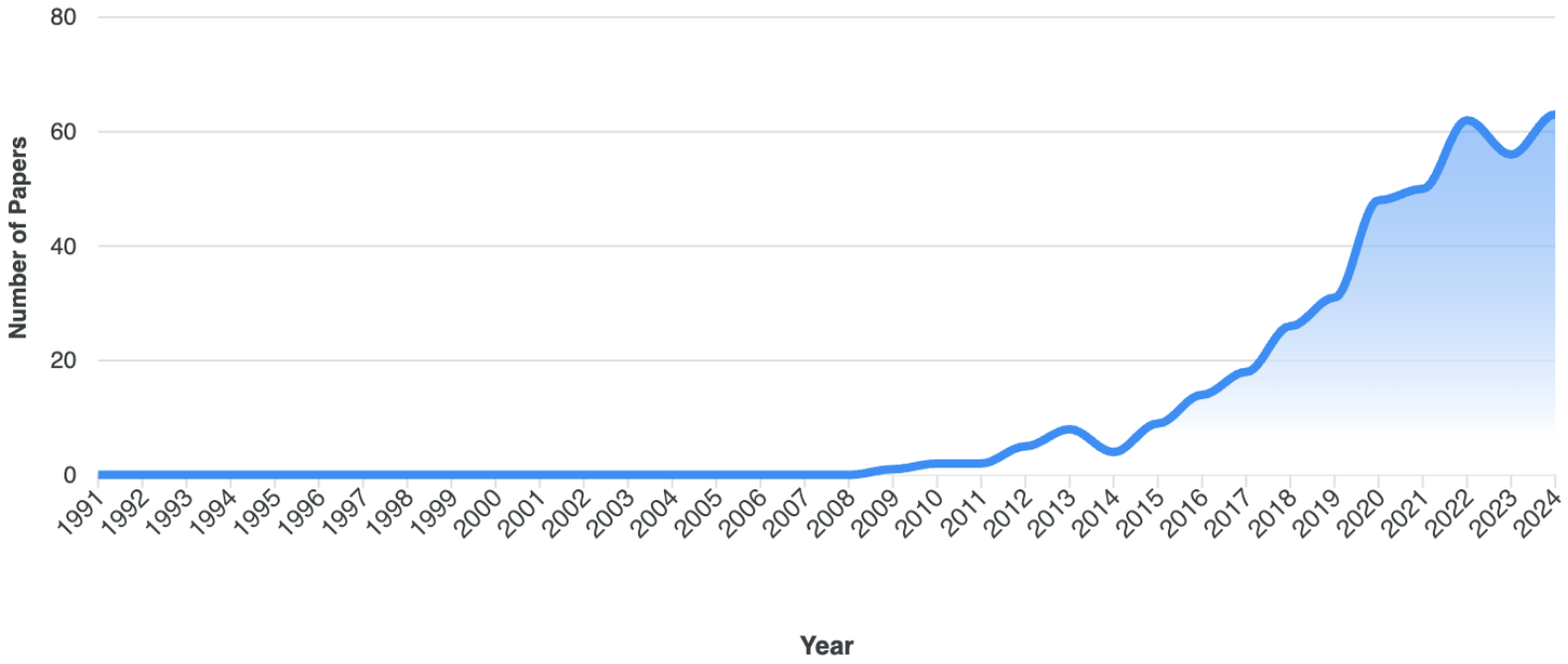


- Presented by Utkarsh Pratiush

Agenda


Motivation
Microscope setup
Remote connection
Workflows enabled
Future workflow
Hands on!

Keyword search for “Automated microscopy” on arxiv



Q. What do we mean by ”Automated Microscopy”?

Created using: https://arxiv-trends.com/

Automated Microscopy ≠ Smart Microscopy

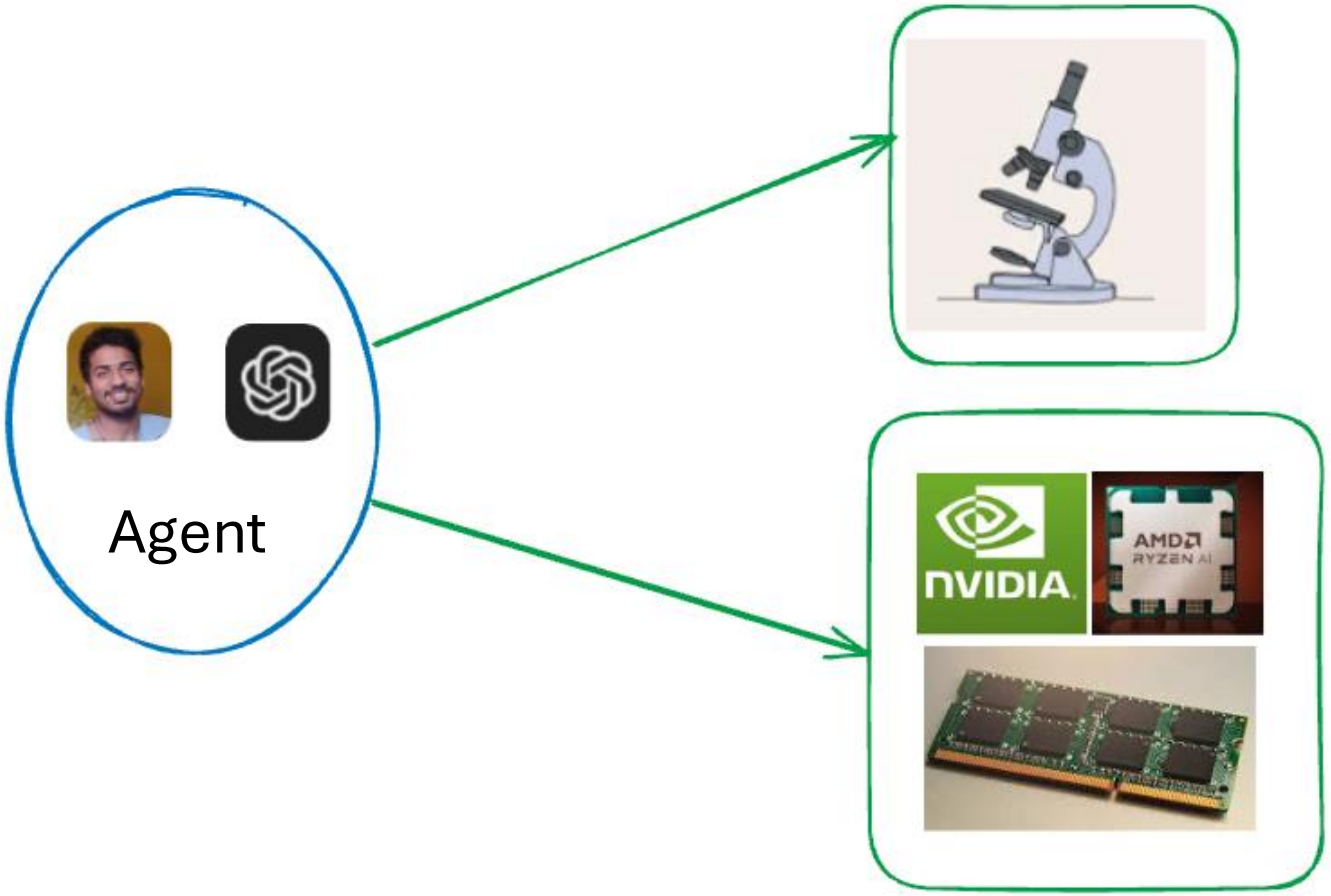
Too much time and resources wasted on

- Acquiring grid data
- Post acquisition analyzing the data
- Handling the unimportant data

Can we with the help of AI agent make data acquisition smart at source?

Q. What is this agent? Human, AI or both?

Human AI collaboration:



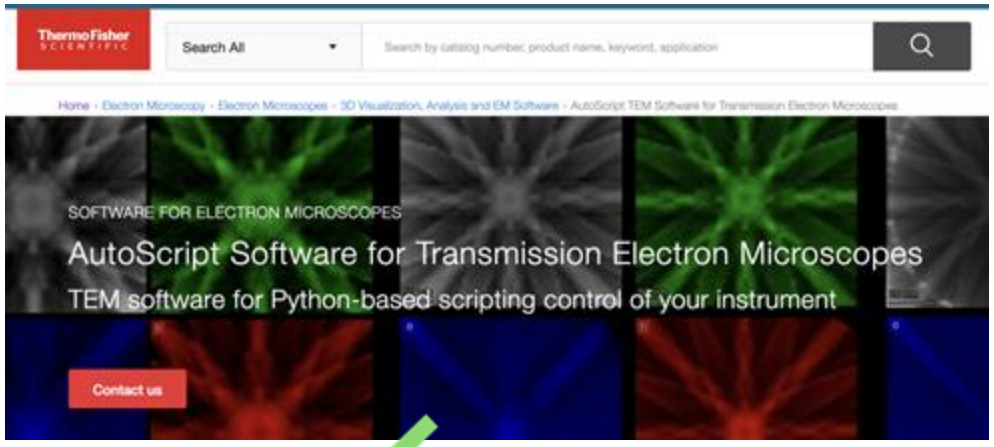
Most of the organization have their hpc capabilities:

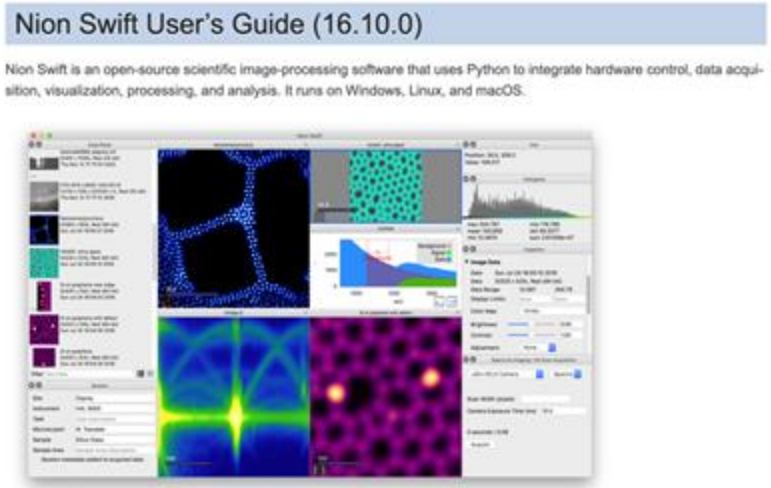
We have exclusive compute access(Thanks to AI TENNESSEE funding) spread across 5 nodes

- 960 CPU cores
- 4 Nvidia H100's gpu (80 GB memory) - Can run SOTA AI models (LLM's etc)
- Around 5 TB of ram
- Can run jobs till 720 hours(30 days)

Need to build a "hyper-language" so that Agent can talk to microscope and also access compute!

Examples of Electron microscopy software's





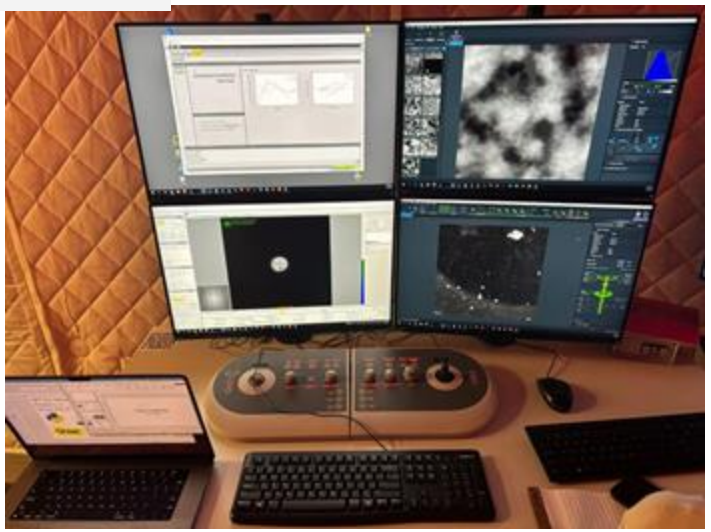
DigitalMicrograph Software

DigitalMicrograph, also known as Gatan Microscopy Suite, drives your digital cameras and surrounding components to support key applications including tomography, *in-situ*, spectrum and diffraction imaging, plus more.

GATAN
AMETEK

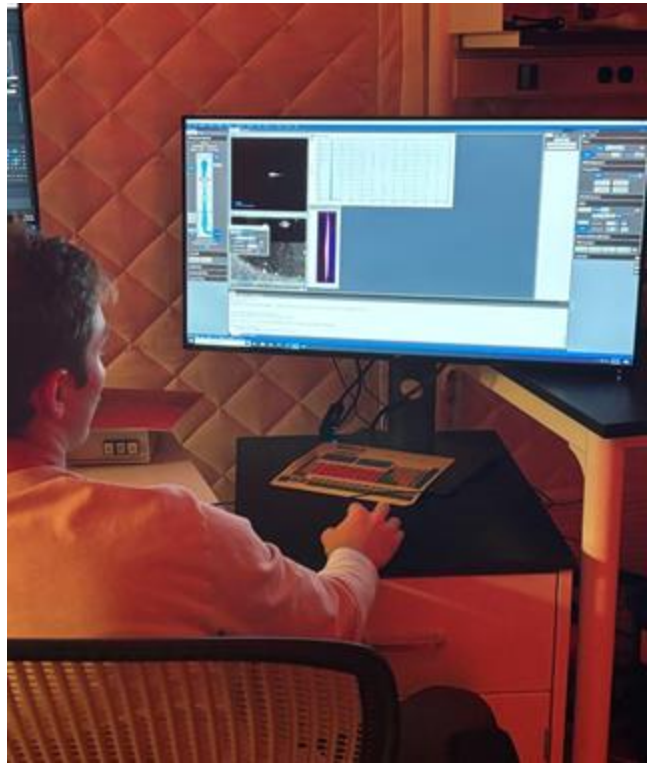
Spectra 300 by Thermofisher

Microscope



Microscope-control 1

Velox



Microscope-control 2

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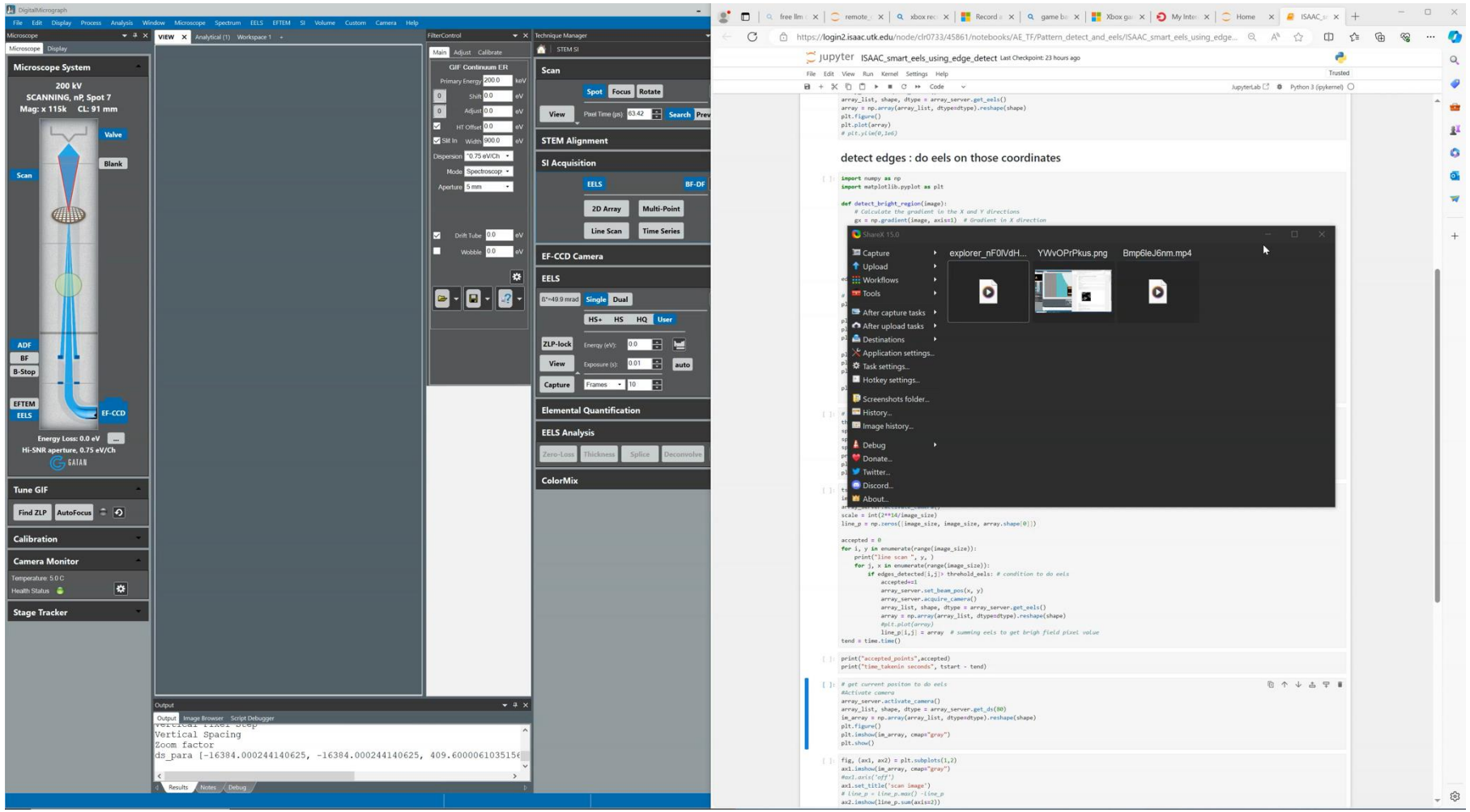
Building a remote window through DigitalMicrograph

Let’s see what it looks like:

VIDEO →



For more demos from our group see: https://aespm.utk.edu/about/

What is our minimal need from the connection?

- Get survey image
- Query Beam position
- Set beam position at desired pixel
- Acquire live EELS

Brief overview of connection

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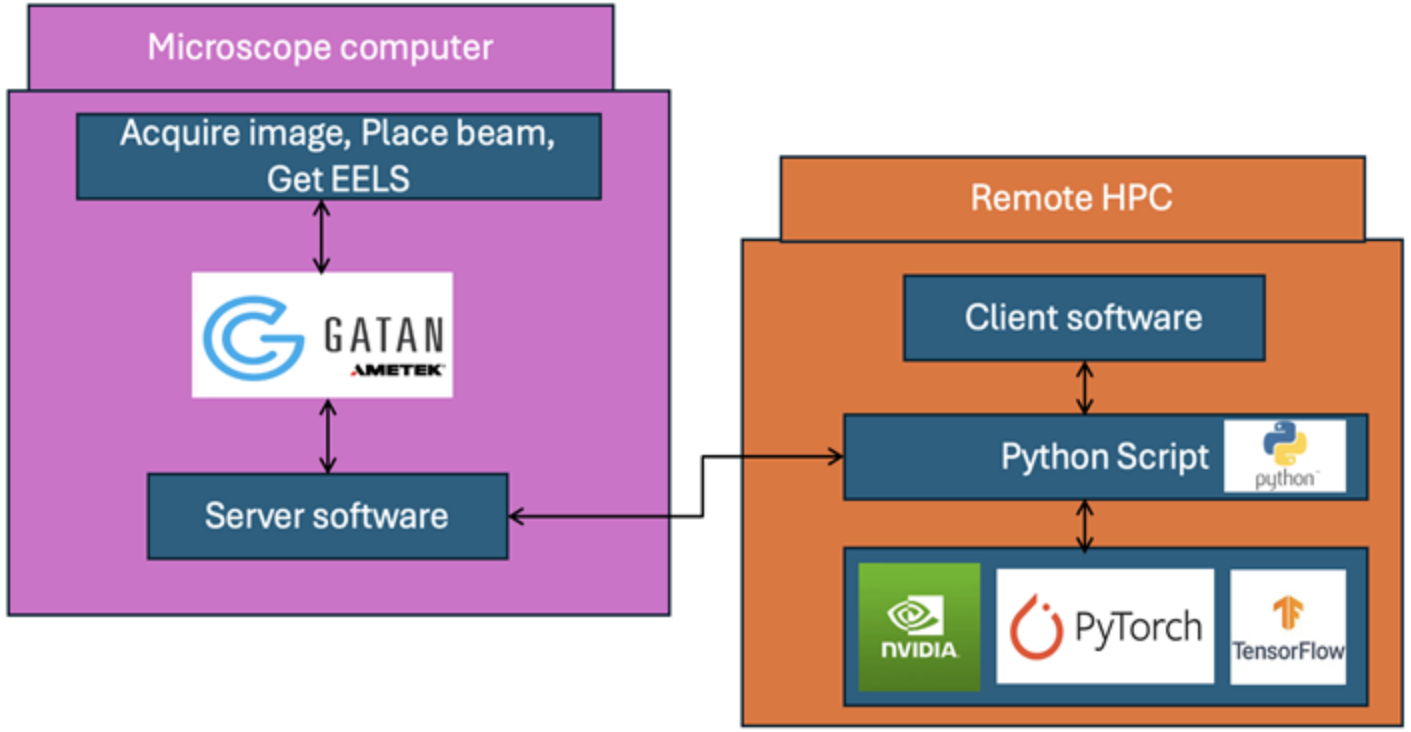
```
DigitalMicrograph
->Survey image:
    ->DM.GetActiveCamera()
    ->cam.PrepareForAcquire()
    ->DS_StartAcquisition()

->Beam control:
    ->DM.DS_GetScanControl()
    ->DM.DS_MoveBeamTo()
        ->Offset from img metadata
    ->DM.DS_GetBeamDSPosition()

->Acquire EELS:
    ->cam.CreateImageForAcquire()

->For debugging:
    ->DM.GetFrontImage()
```

ADD more!

Pyro - Python Remote Objects - 5.15
-> Offset correction
-> Data serialization

Brief overview of connection



Features:

- In Memory data handling
- Multiple acquisition if data is processing
- Interfaces directly with any STEM having Digital Micrograph installed

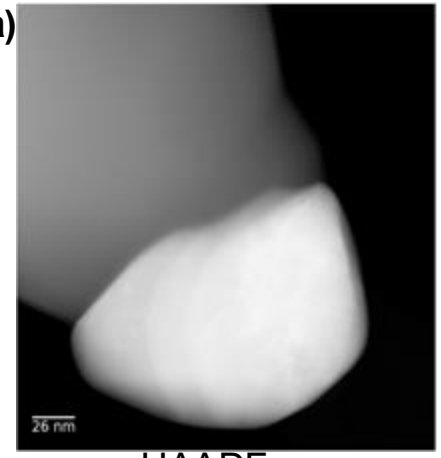
Recommend to take a look at our manuscript for timing details

Source: Realizing smart scanning transmission electron microscopy using high performance computing
Utkarsh Pratiush, Austin Houston, Sergei V. Kalinin, Gerd Duscher, Rev. Sci. Instrum. 95, 103701 (2024). DOI: 10.1063/5.0225401

Workflow 1: Canny filter based smart EELS

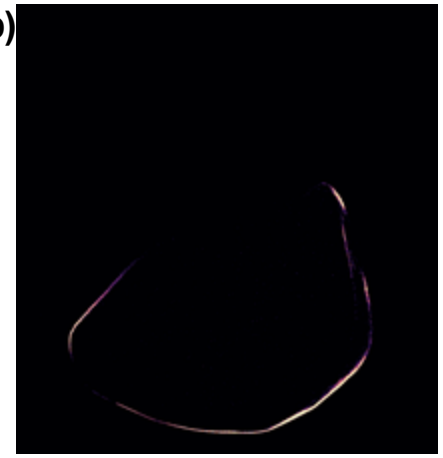
The GaAs-Au nanowire sample.

a)



HAADF

b)



Edge detected

Interesting physics in interface

Grid-based Spectrum Image:
- 128*128 image

4.5 seconds to acquire the survey image

Total time for spectrum image: 80 minutes

considerable beam exposure

Sparsely-sampled Spectrum image:

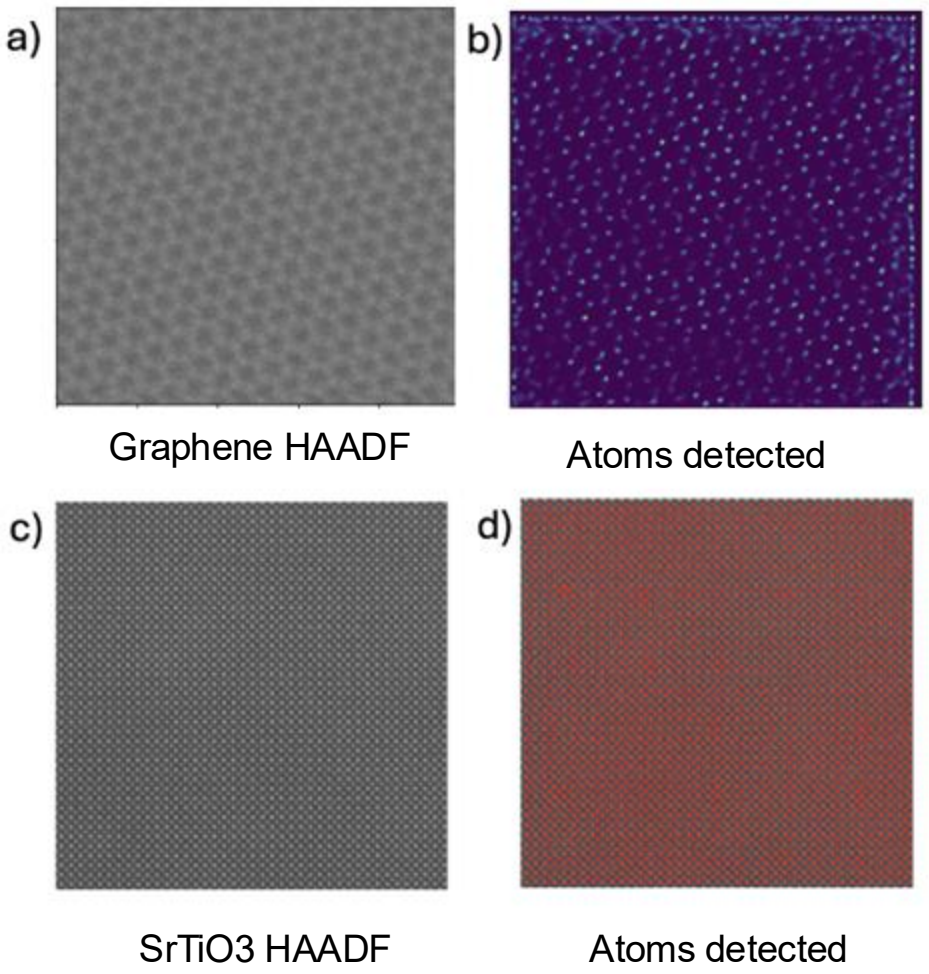
137 pixels were identified to be interesting
- 1% of total pixels

Total time: 2 minutes

400X faster and less beam damage

Source: Realizing smart scanning transmission electron microscopy using high performance computing Utkarsh Pratiush, Austin Houston, Sergei V. Kalinin, Gerd Duscher, Rev. Sci. Instrum. 95, 103701 (2024). DOI: 10.1063/5.0225401

Workflow 2: Ensembled DCNN for atom finding



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Article | Open access | Published: 02 July 2021

Ensemble learning-iterative training machine learning for uncertainty quantification and automated experiment in atom-resolved microscopy

Ayana Ghosh, Bobby G. Sumpter, Ondrej Dyck, Sergei V. Kalinin & Maxim Ziatdinov

npj Computational Materials **7**, Article number: 100 (2021) | Cite this article

4517 Accesses | **28** Citations | **4** Altmetric | Metrics

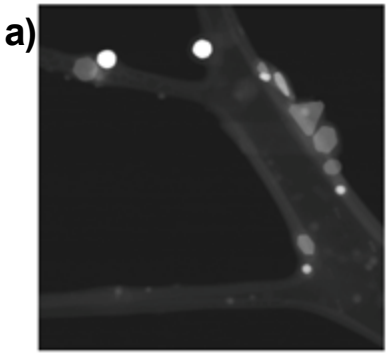
Real time Segmentation of atoms:

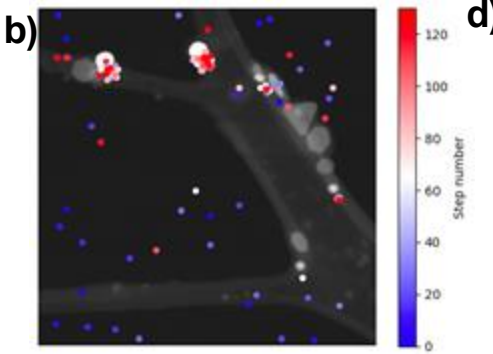
Number of UNETS: 8
GPU memory required: 20 GB

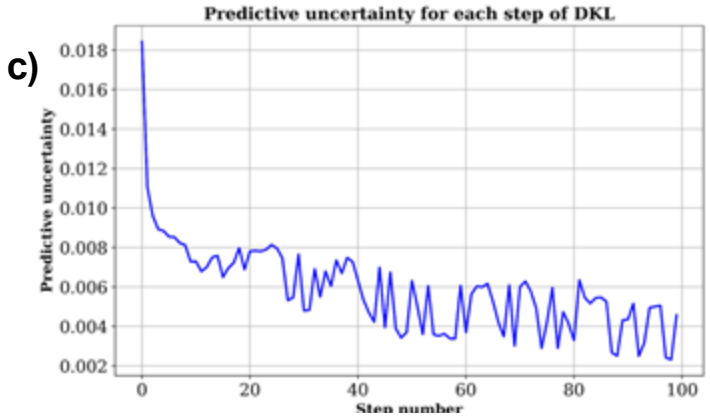
We were able to run this due to gpu's accessible remotely!

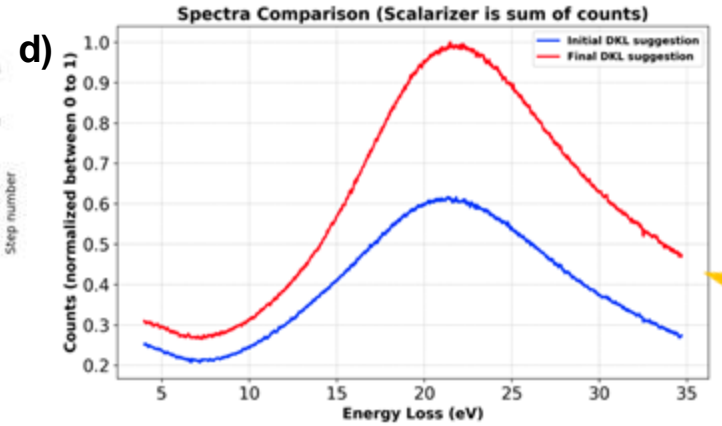
Source: Realizing smart scanning transmission electron microscopy using high performance computing
Utkarsh Pratiush, Austin Houston, Sergei V. Kalinin, Gerd Duscher, Rev. Sci. Instrum. 95, 103701 (2024). DOI: 10.1063/5.0225401

Workflow 3: Deep kernel learning – Example collect eels in those pixels where the sum of counts is maximum.









nature > npj computational materials > perspectives > article

Perspective | Open access | Published: 20 December 2023

Machine learning for automated experimentation in scanning transmission electron microscopy

Sergei V. Kalinin, Debangshu Mukherjee, Kevin Roccapriore, Benjamin J. Blaiszik, Ayana Ghosh, Maxim A. Ziatdinov, Anees Al-Najjar, Christina Doty, Sarah Akers, Nageswara S. Rao, Joshua C. Agar & Steven R. Spurgeon

npj Computational Materials **9**, Article number: 227 (2023) | Cite this article

5813 Accesses | **6** Citations | **2** Altmetric | Metrics

Q. Can you see the problem?

As experiment progresses the algorithm learns to measure in regions with high values of scalarizer

Source: Implementing dynamic high-performance computing supported workflows on Scanning Transmission Electron Microscope arXiv:2406.11018

Friday – 2pm to 2:50pm,
New opportunities enabled by remote ML controlled acquisition

Hands on!

https://github.com/pycroscopy/pyAutoMic/

- Setup remote acquisition for EELS
  - Client side
    - Clone the repository
    - Install the dependencies
    - Connect to the network
    - Running the workflow
  - Server side:
    - If needed install the offline package
      - https://www.gatan.com/products/tem-analysis/gatan-microscopy-suite-software
    - DM scripting mode
    - Accessing the dm environment and installing
    - Importing the server script – run on a **port**