Edge Computing and Microscopy: Autonomous and Automated Experiments Leveraging Advances in Computing, Control Systems and Algorithms

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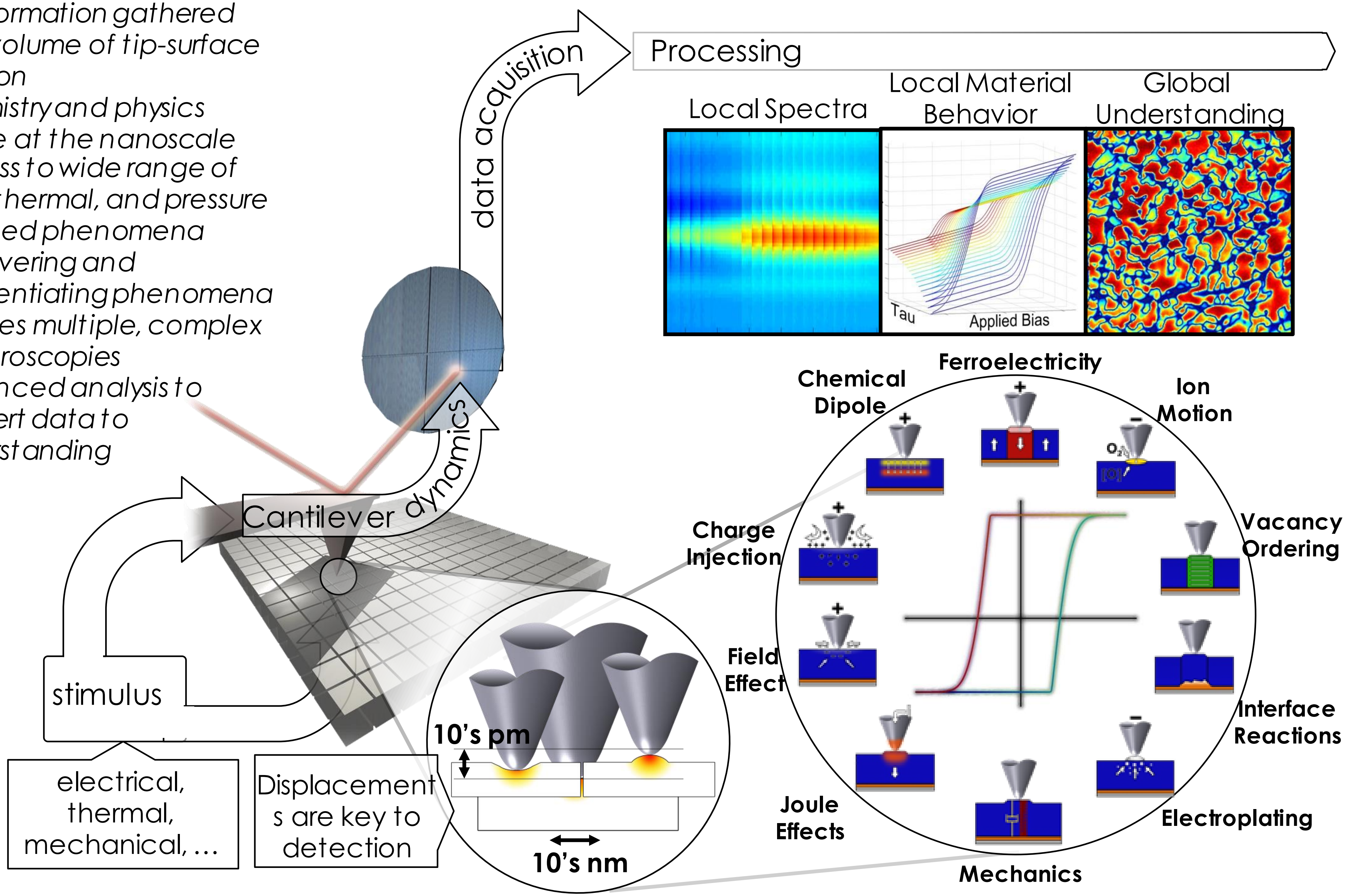
Information flow in SPM

- *All information gathered from volume of tip-surface junction*
- *Chemistry and physics merge at the nanoscale*
- *Access to wide range of bias, thermal, and pressure induced phenomena*
- *Discovering and differentiating phenomena requires multiple, complex spectroscopies*
- *Advanced analysis to convert data to understanding*



Slide by S. Jesse

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REVIEW

Automated and Autonomous Experiments in Electron and Scanning Probe Microscopy

Sergei V. Kalinin,* Maxim Ziatdinov, Jacob Hinkle, Stephen Jesse, Ayana Ghosh, Kyle P. Kelley, Andrew R. Lupini, Bobby G. Sumpter, and Rama K. Vasudevan

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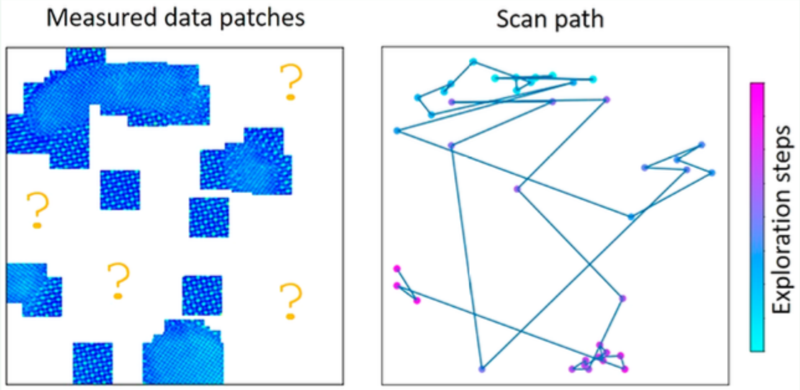
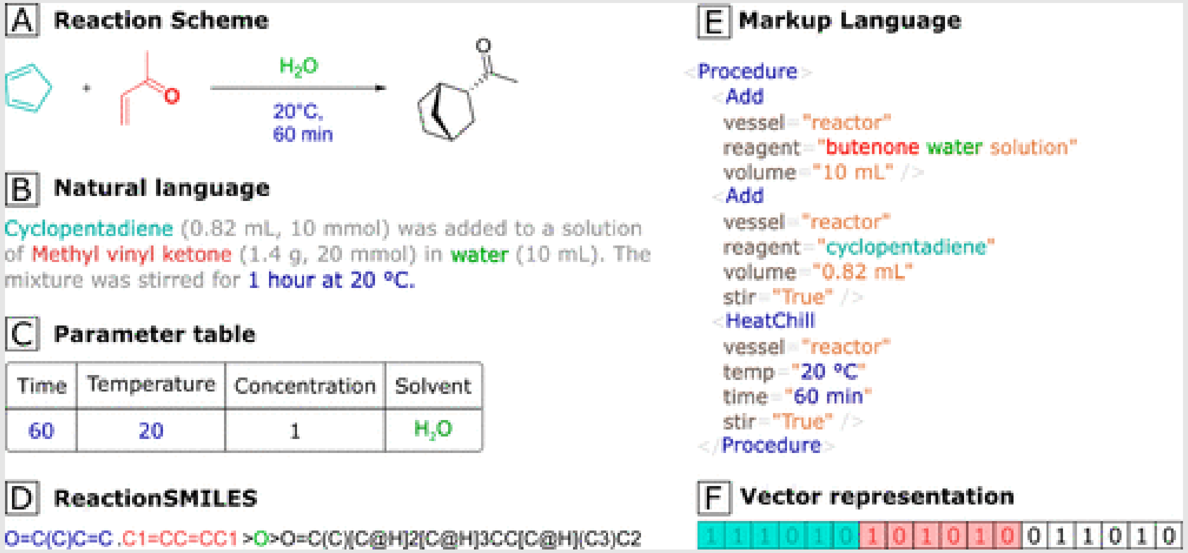
ABSTRACT: Machine learning and artificial intelligence (ML/AI) are rapidly becoming an indispensable part of physics research, with domain applications ranging from theory and materials prediction to high-throughput data analysis. In parallel, the recent successes in applying ML/AI methods for autonomous systems from robotics to self-driving cars to organic and inorganic synthesis are generating enthusiasm for the potential of these techniques to enable automated and autonomous experiments (AE) in imaging. Here, we aim to analyze the major pathways toward AE in imaging methods with sequential image formation mechanisms, focusing on scanning probe microscopy



Abstractions make the (automated) world go round

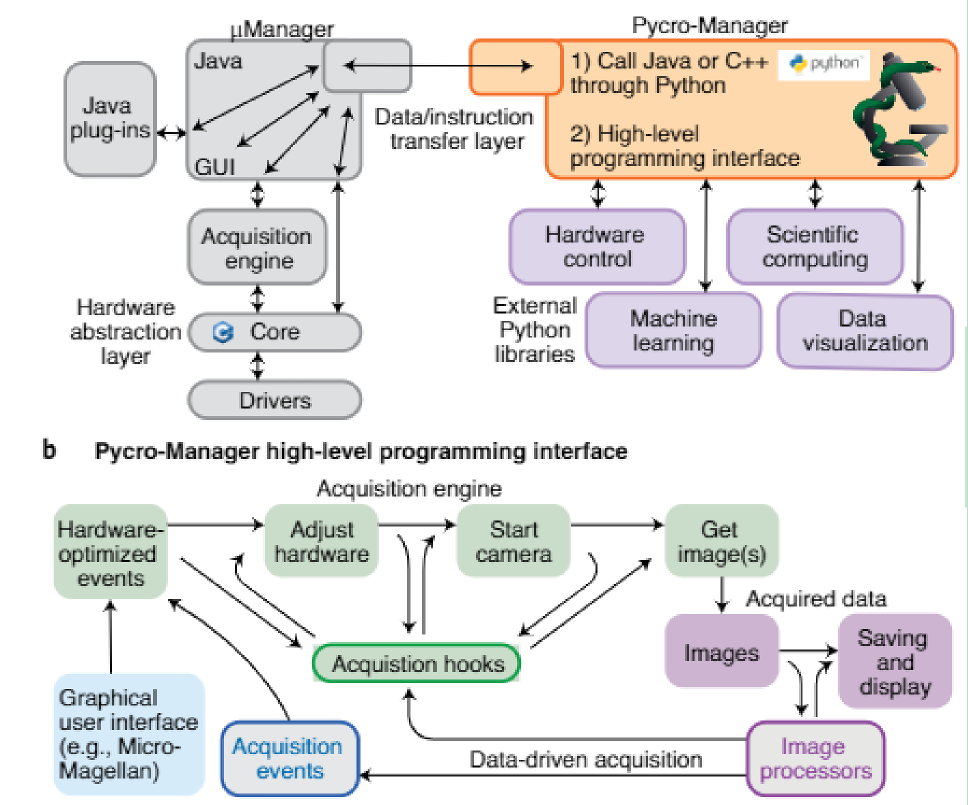
"Chemputation" – Digital chemistry



Hammer, Leonov, Bell and Cronin, JACS 1, 1572 (2021)

A complete programming language for chemistry that can run on open hardware

PycroManager



Pinkard, et al. Nat. Methods. 18, 226 (2021)

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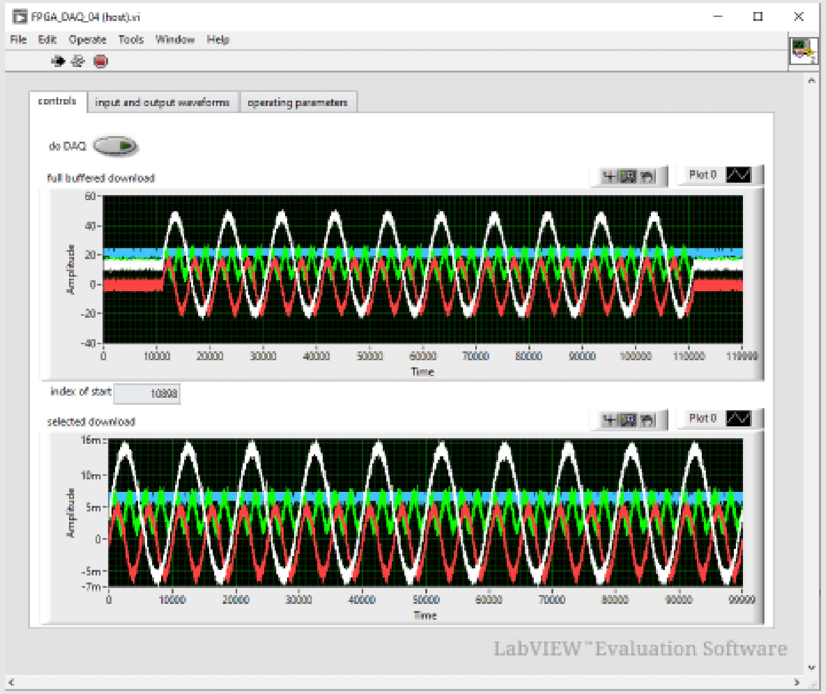
Hardware abstraction - FPGA

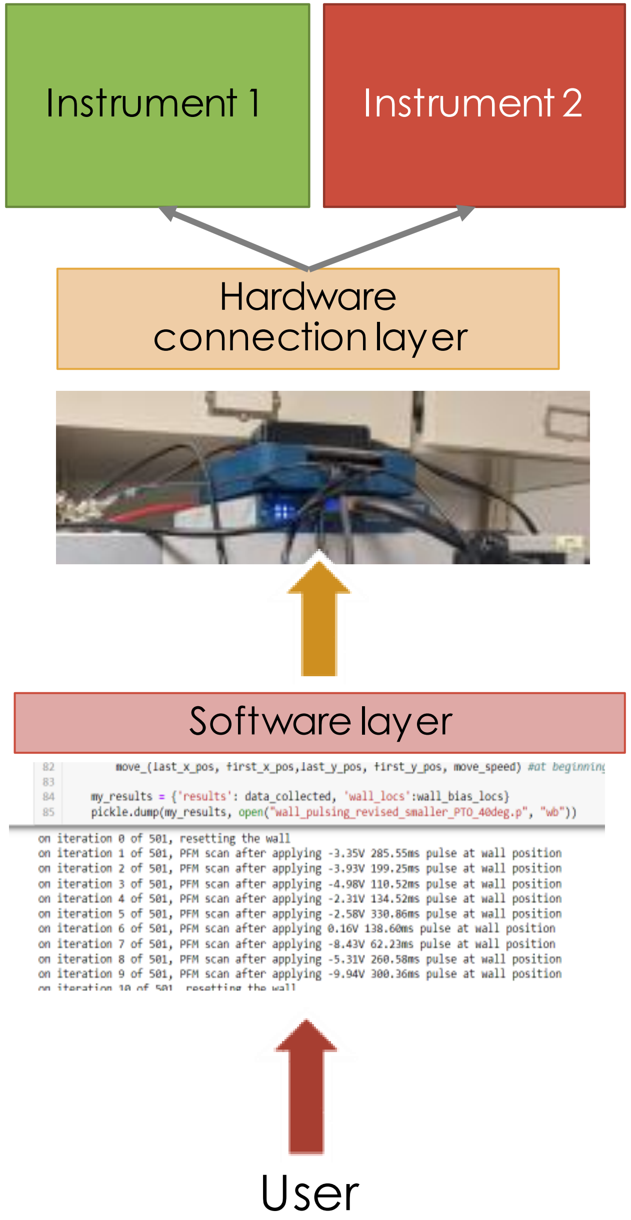


Software abstraction - python

```python
# Pole half the sample
# Locate the position of the wall
# Randomly select a location on the wall, and randomly select a bias pulse magnitude and pulse width
# Move tip to that location and apply a bias pulse, move the tip back to the start
# Then scan to observe effects

wall_bias_locs = []

for k in range(num_iters):
    if k%reset_freq==0:
        print('on iteration {} of {}, resetting the wall'.format(k, num_iters))
        data_output, d, x , y = raster_scan(volt,pix,num_lines, IO_rate,trig,offsetvx,offsetvy, tip_volt=reset_bias,
                                apply_half=True, left_bias=False)

        last_x_pos = x[-1]
        last_y_pos = y[-1]
        first_x_pos = x[0]
        first_y_pos = y[0]

        move_(last_x_pos, first_x_pos,last_y_pos, first_y_pos, move_speed) #at beginning of scan, move to starting p

        data_output, d, x , y = raster_scan(volt,pix,num_lines, IO_rate,trig,offsetvx,offsetvy, tip_volt=-reset_bias
                                apply_half=True, left_bias=True)
        move_(last_x_pos, first_x_pos,last_y_pos, first_y_pos, move_speed) #at beginning of scan, move to starting p

        #Do a standard scan, without any bias.
        data_output, d, x , y = raster_scan(volt,pix,num_lines, IO_rate,trig,offsetvx,offsetvy, tip_volt=0.0,
                                      apply_half=False)
        data_collected.append(data_output)

    else:
        #find the mean wall position
        amp_img = data_output[2].reshape(-1, pix*2)[:,:pix]
        phase_img = data_output[2].reshape(-1, pix*2)[:,:pix]
        bias_amp, bias_pw, wall_x_pos, wall_y_pos, xpos_v, ypos_v = get_next_action(amp_img, phase_img, pix=pix)
```

Call low-level functions to control tip position, scanning (e.g., raster, spiral, move etc.), specify voltage waveforms, collect data all in Jupyter notebook

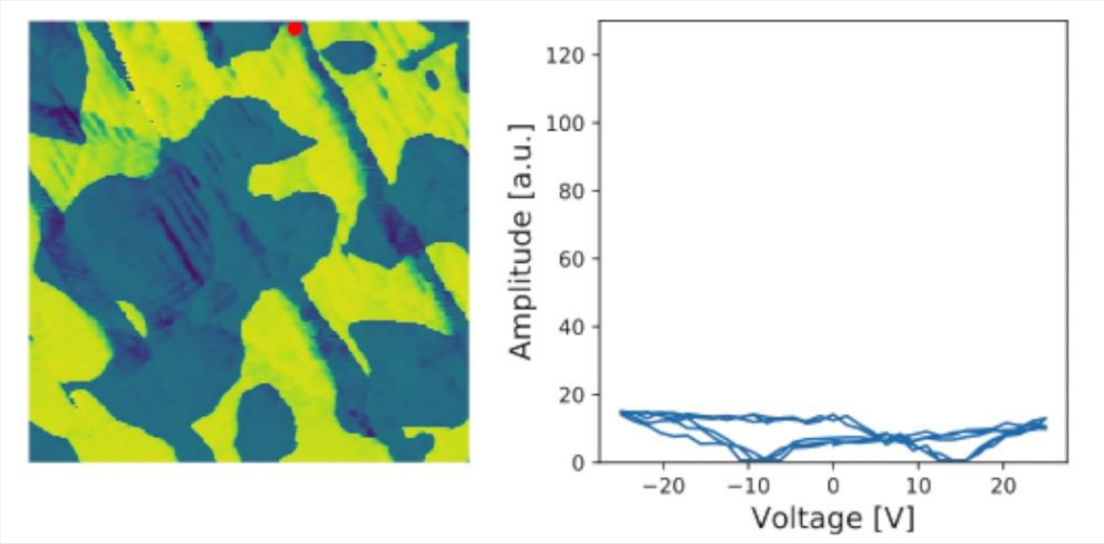
Enables design of complicated automated and autonomous experiments, hardware independent



Progress: Real-time automated experiments in SPM

In-line inference

Image-based feature finding

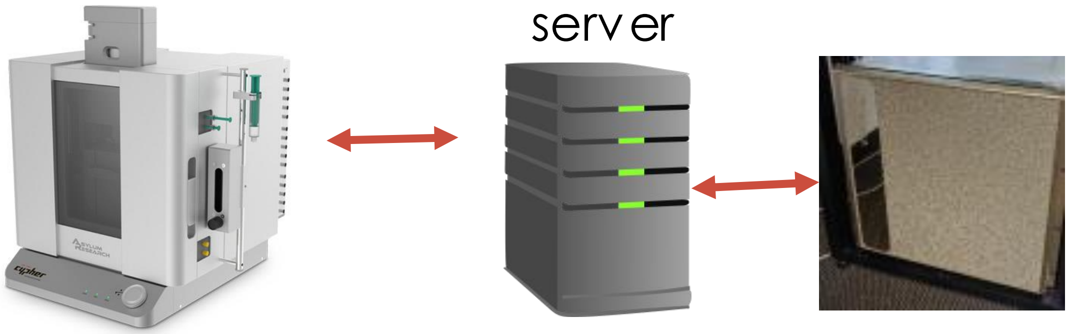


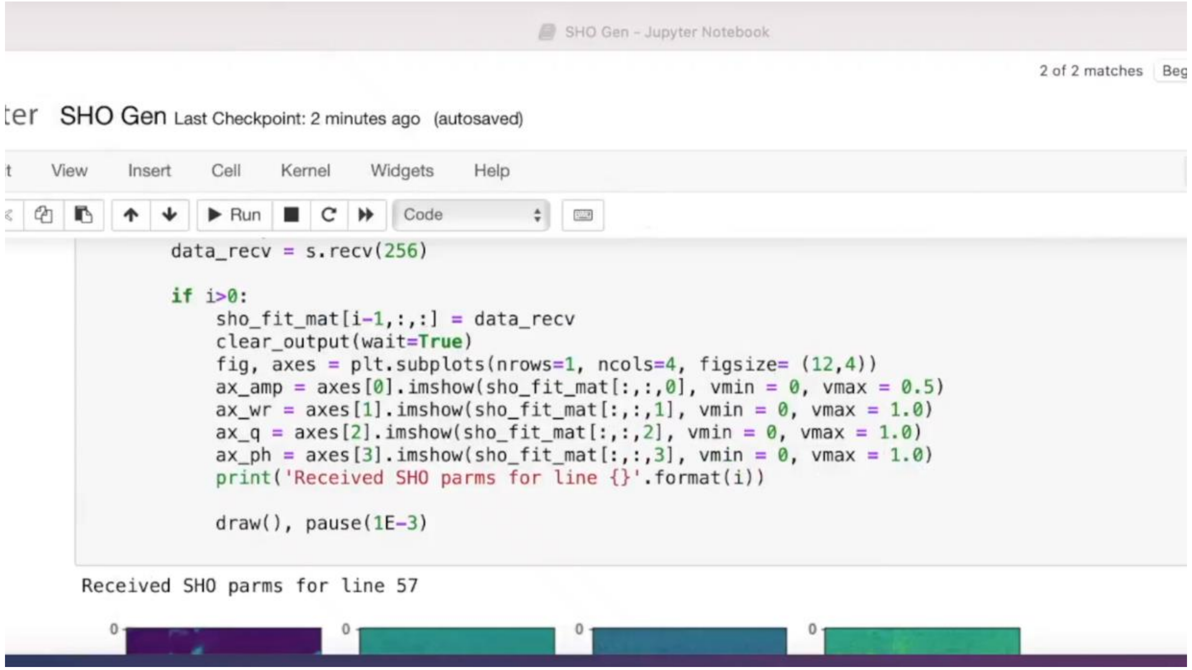
Streaming functional fitting during scanning on the microscope

Instrument

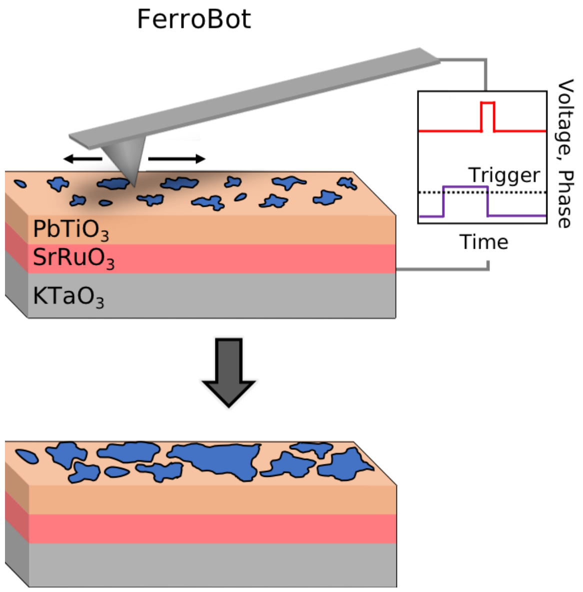
'Gateway' server

GPU Server

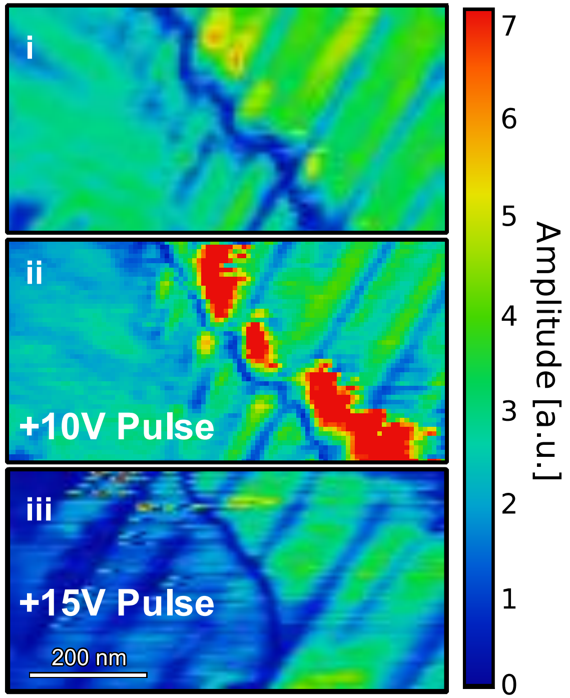




“Smart” Microscopy Experiments



Kelley et al. ACS Nano **14**, 10569 (2020).



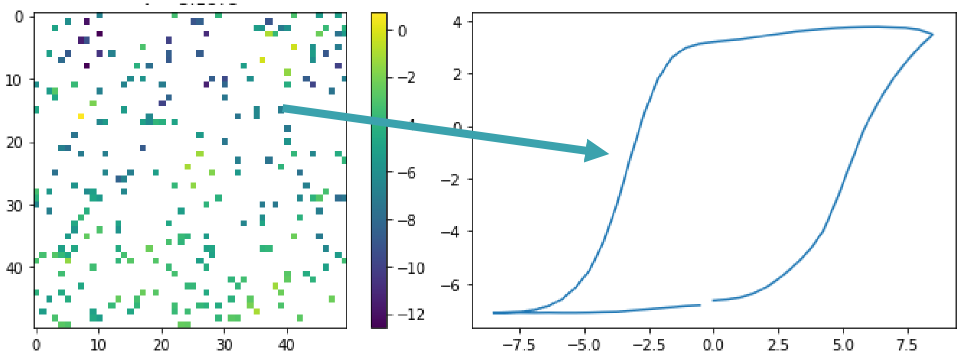
Techniques
- Adaptive sampling
- Structure-triggered events
- Streaming analysis with model comparisons “on the fly”

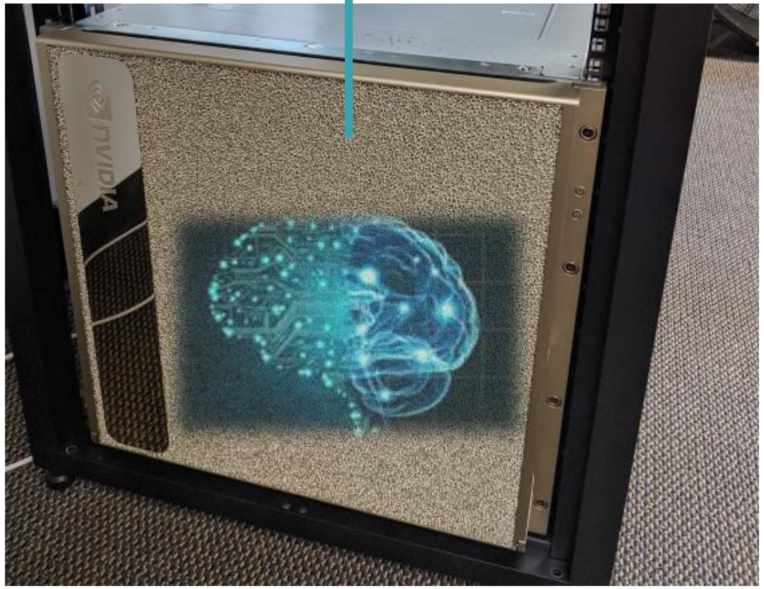
Yields:
- Enables more efficient and more complex measurements
- Engineering new metastable states
- Better hypothesis testing for physics discovery

Real-time automated SPM

Provide list of new measurement conditions

Measure a batch of hysteresis loops

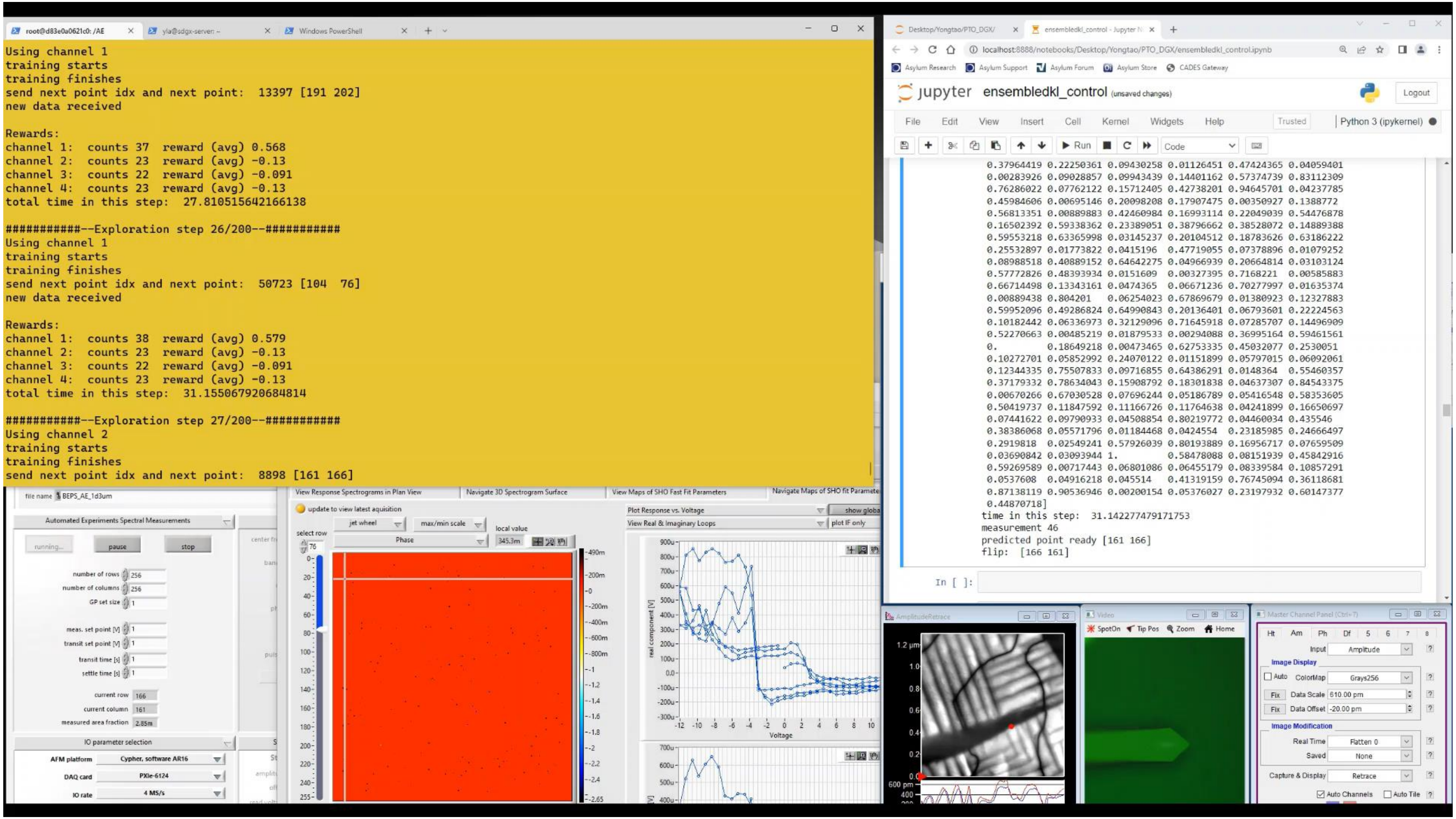




Upload to dgx for Bayesian Optimization

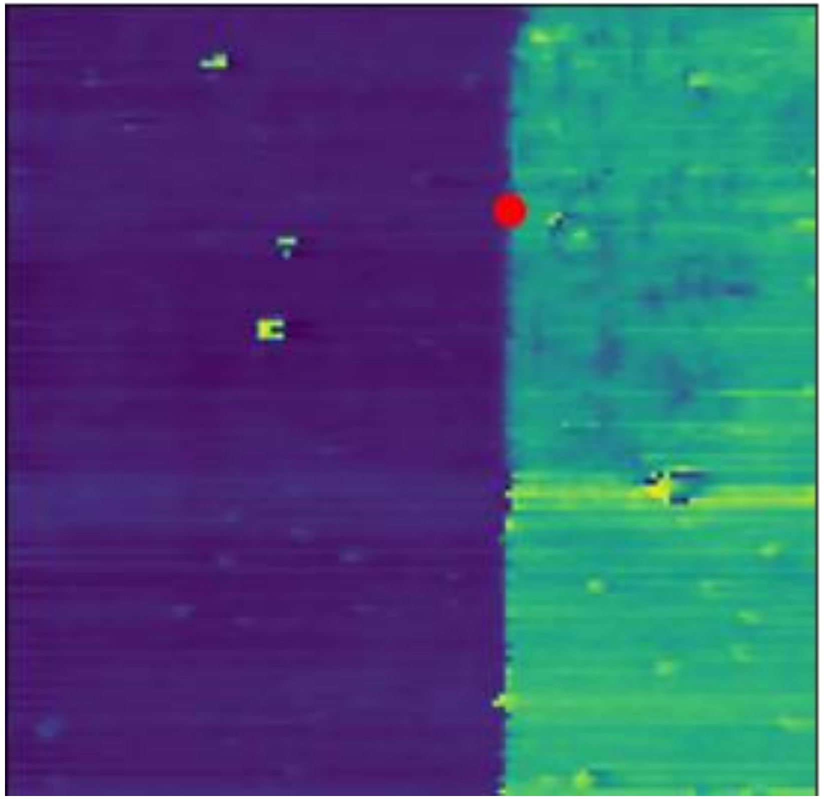
Data preprocessing

- For long spectroscopies, measuring every pixel across a grid is not feasible. Bayesian optimization enables sampling only those points that will maximize a property of choice, enabling new experiments that would otherwise not be possible


Using channel 1
training starts
training finishes
send next point idx and next point: 13397 [191 202]
new data received
Rewards:
channel 1: counts 37 reward (avg) 0.568
channel 2: counts 23 reward (avg) -0.13
channel 3: counts 22 reward (avg) -0.091
channel 4: counts 23 reward (avg) -0.13
total time in this step: 27.810515642166138
###########--Exploration step 26/200--###########
Using channel 1
training starts
training finishes
send next point idx and next point: 50723 [104 76]
new data received
Rewards:
channel 1: counts 38 reward (avg) 0.579
channel 2: counts 23 reward (avg) -0.13
channel 3: counts 22 reward (avg) -0.091
channel 4: counts 23 reward (avg) -0.13
total time in this step: 31.155067920684814
###########--Exploration step 27/200--###########
Using channel 2
training starts
training finishes
send next point idx and next point: 8898 [161 166]
jupyter ensembledkl_control (unsaved changes)
File Edit View Insert Cell Kernel Widgets Help
Trusted
Python 3 (ipykernel)
Logout
0.37964419 0.22250361 0.09430258 0.01126451 0.47424365 0.04059401
0.00283926 0.09028857 0.09943439 0.14401162 0.57374739 0.83112309
0.76286022 0.07762122 0.15712405 0.42738201 0.94645701 0.04237785
0.45984606 0.00695146 0.20098208 0.17907475 0.00350927 0.1388772
0.56813351 0.00889883 0.42460984 0.16993114 0.22049039 0.54476878
0.16502392 0.59338362 0.23389051 0.38796662 0.38528072 0.14889388
0.59553218 0.63365998 0.03145237 0.20104512 0.18783626 0.63186222
0.25532897 0.01773822 0.0415196 0.47719055 0.07378896 0.01079252
0.08988518 0.40889152 0.64642275 0.04966939 0.20664814 0.03103124
0.57772826 0.48393934 0.0151609 0.00327395 0.7168221 0.00585883
0.66714498 0.13343161 0.0474365 0.06671236 0.70277997 0.01635374
0.00889438 0.804201 0.06254023 0.67869679 0.01380923 0.12327883
0.59952096 0.49286824 0.64990843 0.20136401 0.06793601 0.22224563
0.10182442 0.06336973 0.32129096 0.71645918 0.07285707 0.14496909
0.52270663 0.00485219 0.01879533 0.00294088 0.36995164 0.59461561
0. 0.18649218 0.00473465 0.62753335 0.45032077 0.2530051
0.10272701 0.05852992 0.24070122 0.01151899 0.05797015 0.06092061
0.12344335 0.75507833 0.09716855 0.64386291 0.0148364 0.55460357
0.37179332 0.78634043 0.15908792 0.18301838 0.04637307 0.84543375
0.00670266 0.67030528 0.07696244 0.05186789 0.05416548 0.58353605
0.50419737 0.11847592 0.11166726 0.11764638 0.04241899 0.16650697
0.07441622 0.09790933 0.04508854 0.80219772 0.04460034 0.435546
0.38386068 0.05571796 0.01184468 0.0424554 0.23185985 0.24666497
0.2919818 0.02549241 0.57926039 0.80193889 0.16956717 0.07659509
0.03690842 0.03093944 1. 0.58478088 0.08151939 0.45842916
0.59269589 0.00717443 0.06801086 0.06455179 0.08339584 0.10857291
0.0537608 0.04916218 0.045514 0.41319159 0.76745094 0.36118681
0.87138119 0.90536946 0.00200154 0.05376027 0.23197932 0.60147377
0.44870718]
time in this step: 31.142277479171753
measurement 46
predicted point ready [161 166]
flip: [166 161]
In [ ]:
Automated Experiments Spectral Measurements
pause
stop
number of rows 256
number of columns 256
current row 166
current column 161
IO parameter selection
AFM platform Cypher, software AR16
DAQ card PXIe-6124
IO rate 4 MS/s
View Response Spectrograms in Plan View
Navigate 3D Spectrogram Surface
View Maps of SHO Fast Fit Parameters
Plot Response vs. Voltage
View Real & Imaginary Loops
Voltage
Master Channel Panel
Image Display
Image Modification

Autonomous workflows

Materials design problem in microscopy: how we can modify materials intelligently



Workflow

Write automation script

Collect data on state transitions with policy

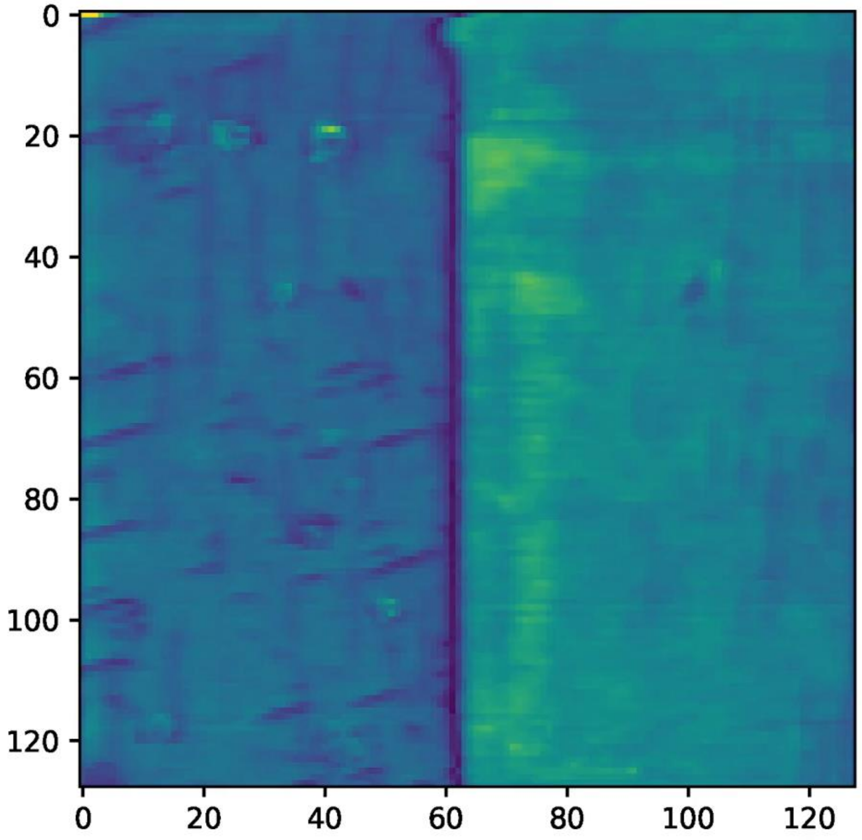
Domain knowledge, Simulations

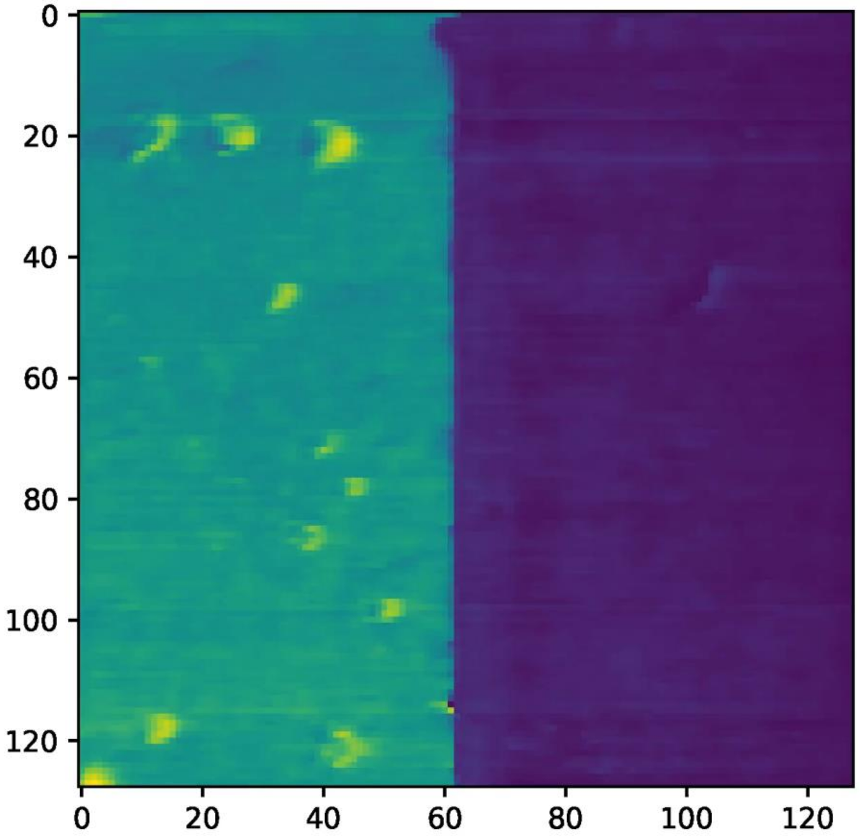
From data, train a surrogate model

Train autonomous agent, obtain policy

Update Policy

Random Policy-> data collection





Workflow elaboration (future idea – not current)

Workflow

Write automation script

Collect data on state transitions with policy

Surrogate model training

Massively parallel simulations

Train autonomous agent, obtain policy

Computational Needs: Streaming, Near Edge and HPC

Instrument

~64 MB/s

"Streaming" Edge

FPGA*

Jetson Nano

~ MB-GB/run

GPU "Far" Edge

DGX-2
16 GPUs

~ 10+GB/job

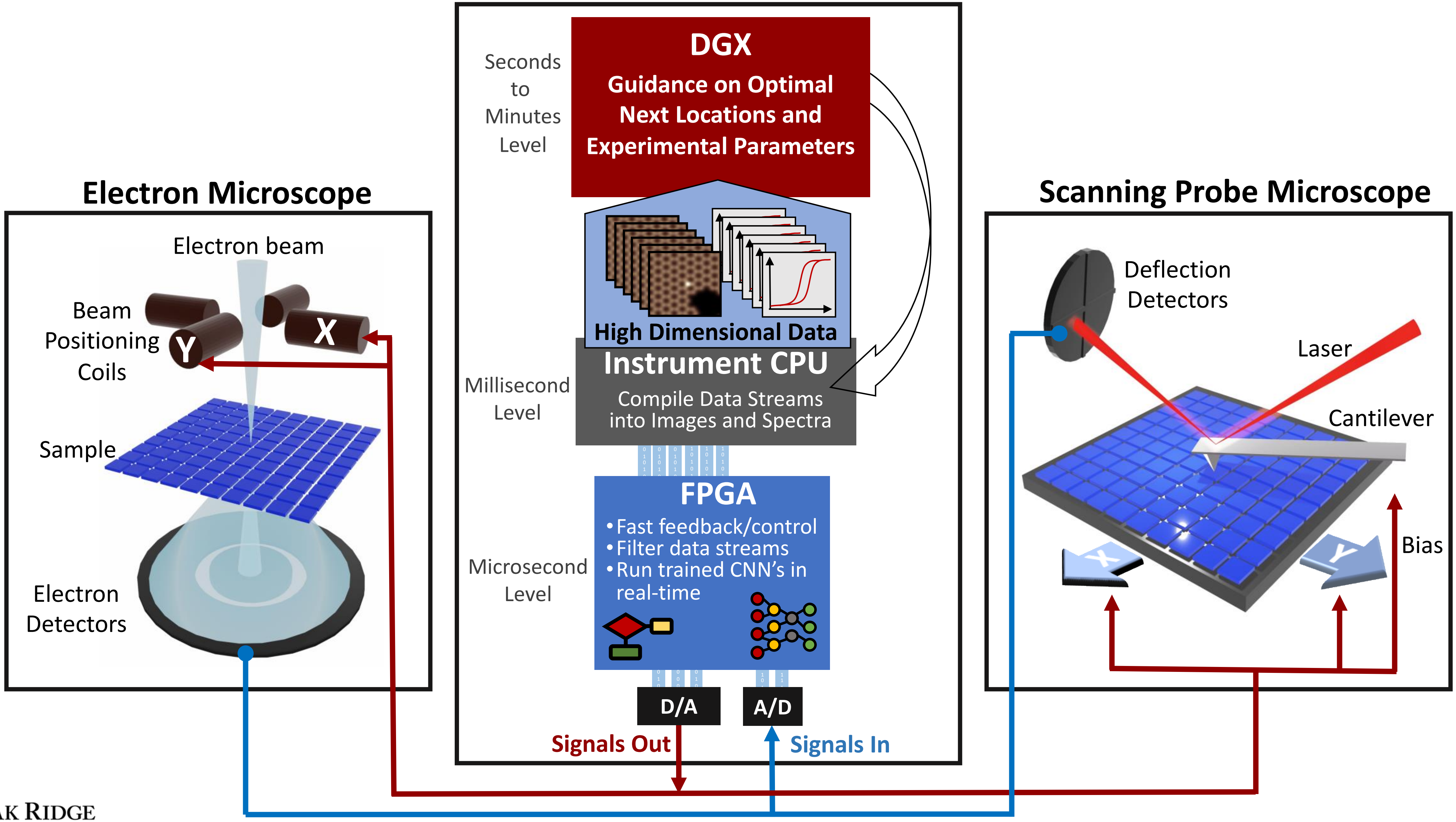
Leadership Class

Summit
~27000 GPUs

Simulations and Model Refinements

Feedback for control

Edge Computing at the Instrument Level



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