OAK RIDGE National Laboratory

December 16th, 2024

Ecosystems for Microscopy

Microscopy Hackathon

Rama Vasudevan[1]

[1]Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge TN

U.S. DEPARTMENT OF ENERGY

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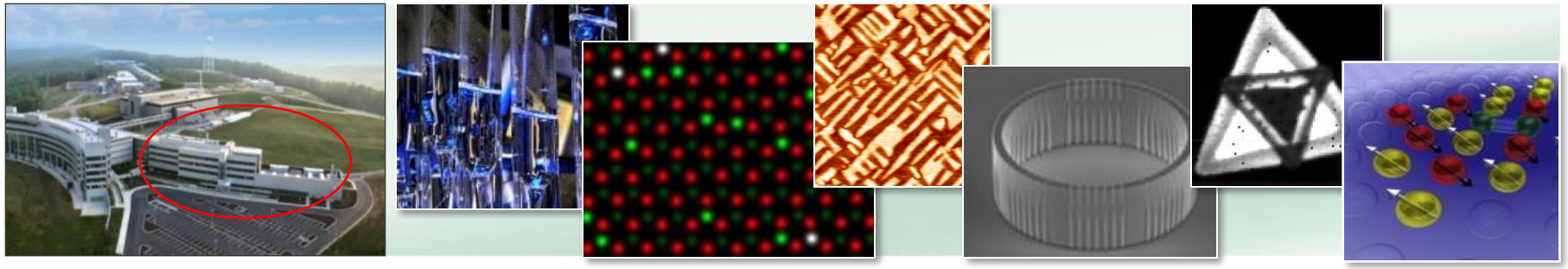
CNMS is a national user facility with a mission to advance nanoscience

- About CNMS:
  - **Unlike many user facilities, you don't need to have samples to apply for time**
  - **Two calls per year for continuous access; anytime for short-term projects**
  - **Simple 2-page proposal**
  - **Free access to laboratories, equipment and expertise if you agree to publish**
  - **Proposal deadlines: early May and mid-October**
  - **Joint proposals with neutron sources (SNS, HFIR)**

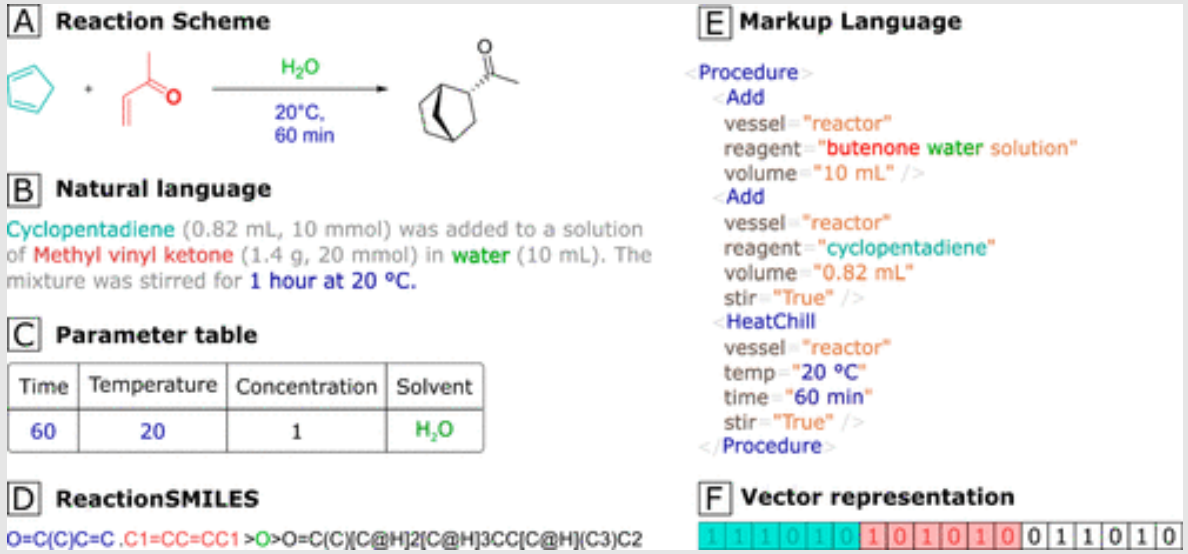
- Research areas:
  - **Synthesis –** 2D, precision synthesis, selective deuteration
  - **Nanofabrication –** direct-write, microfluidics, cleanroom
  - **Advanced Microscopy –** AFM, STM, aberration-corrected TEM/STEM, atom-probe tomography
  - **Functional Characterization –** laser spectroscopy, transport, magnetism, electromechanics
  - **Theory and Modelling –** including gateway to leadership-class high performance computing



CNMS is a Nanoscale Science Research Center supported by the U.S. Department of Energy, Office of Science, Scientific User Facilities Division

Abstractions make the (automated) world go round

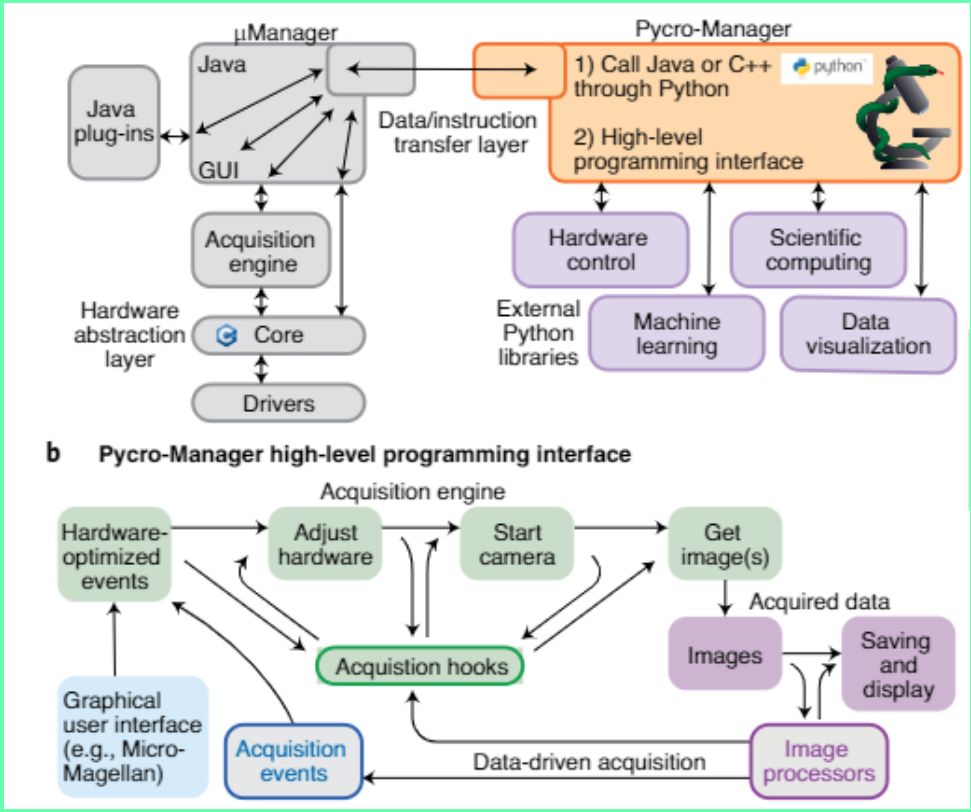
"Chemputation" – Digital chemistry



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)

Systems for automated microscopy

Software Infrastructure

AEcroscopy

Welcome to AEcroscopy

Get Started

Get Started

Experiment

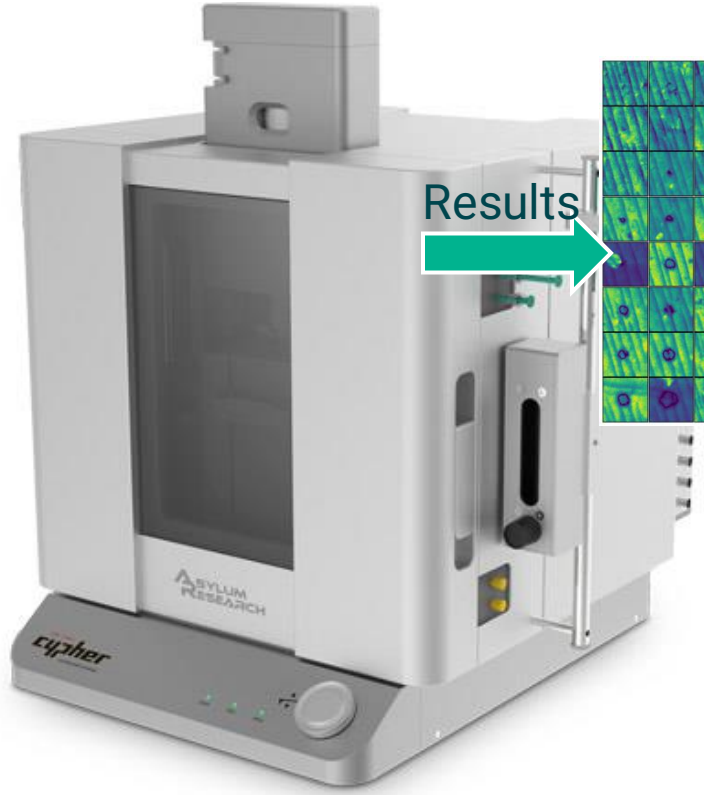
Experiments

Step 4. Do a BEPFM at the whole experiment area

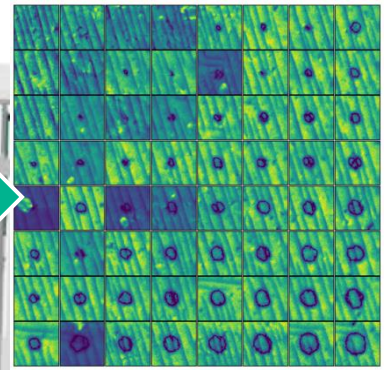
```
dset_pfm, dset_chns, dset_cs = newexp.raster_scan(raster_parms_dict = {"scan_pixel": 32, "s
                                                                       "scan_y_start": -1.0,
                                                                       "scan_y_stop": 1.0},
                                                  file_name = "pfm_whole", ploton = False)

f, (ax1, ax2, ax3, ax4, ax5, ax6) = plt.subplots(1, 6, figsize = (30, 5), dpi = 100)
ax1.imshow(dset_pfm[:,:,0])
ax2.imshow(dset_pfm[:,:,1])
ax3.imshow(dset_pfm[:,:,2])
ax4.imshow(dset_pfm[:,:,3])
ax5.imshow(dset_chns[0,:,:])
ax6.imshow(dset_chns[1,:,:])
plt.show()
```

Deploy

Y. Liu et al. Small Methods 2301740 (2024)



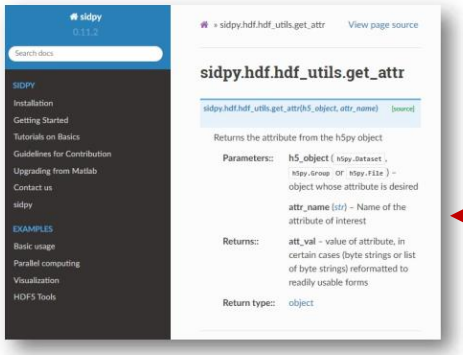
Results



sidpy.Dataset

pycroscopy

An ecosystem for microscopy data ingestion, analytics and visualization



pycroscopy
A general-purpose package for microscopy imaging and spectroscopy data analytics, including registration, image cleaning, unmixing, etc.

scifireaders	pyusid	pynsid	sidpy	bglib	atomai	stemtools	pytemlib
For ingesting a variety of microscopy files for output to sidpy dataset objects	Python package for reading and visualizing our universal spectral imaging dataset format	Python package for reading and visualizing our N-dimensional spectral imaging dataset format	Python utilities for storing, visualizing and fitting Spectroscopic Imaging Data	Utilities to analyze, fit and visualize Band - Excitation and G - mode imaging data primarily for CNMS SPM Users	Deep learning toolkit for analysis of atomically resolved imaging and spectroscopy datasets	Python based codes for analysis of 4D - STEM and aberration - corrected vanilla STEM datasets	Python tools for simulation, registration, analysis and visualization of TEM datasets

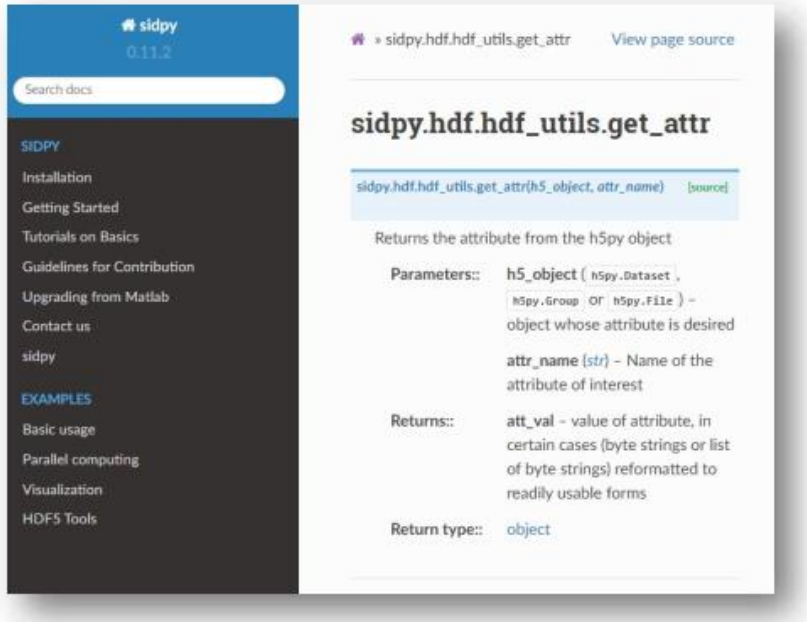
Vasudevan et al. Advanced Theory and Simulations **6**, 2300247 (2023)

- Standardized data model
- In-built processing and viz utilities

Pycroscopy

pycroscopy

An ecosystem for microscopy data ingestion, analytics and visualization



pycroscopy

A general-purpose package for microscopy imaging and spectroscopy data analytics, including registration, image cleaning, unmixing, etc.

scifireaders

For ingesting a variety of microscopy files for output to sidpy dataset objects

pyusid

Python package for reading and visualizing our universal spectral imaging dataset format

pynsid

Python package for reading and visualizing our N-dimensional spectral imaging dataset format

sidpy

Python utilities for storing, visualizing and fitting Spectroscopic Imaging Data

bglib

Utilities to analyze, fit and visualize Band-Excitation and G-mode imaging data primarily for CNMS SPM Users

atomai

Deep learning toolkit for analysis of atomically resolved imaging and spectroscopy datasets

stemtools

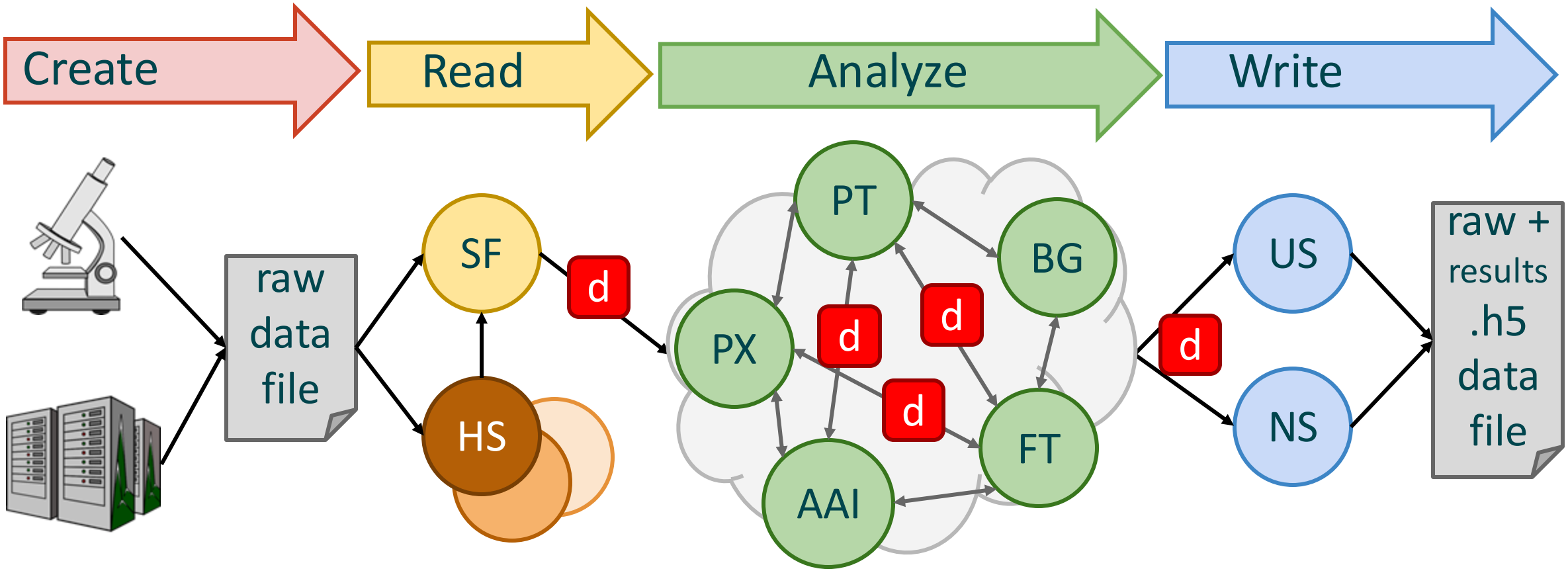
Python based codes for analysis of 4D-STEM and aberration-corrected vanilla STEM datasets

pytemlib

Python tools for simulation, registration, analysis and visualization of TEM datasets

Github.com/pycroscopy

Pycroscopy philosophy

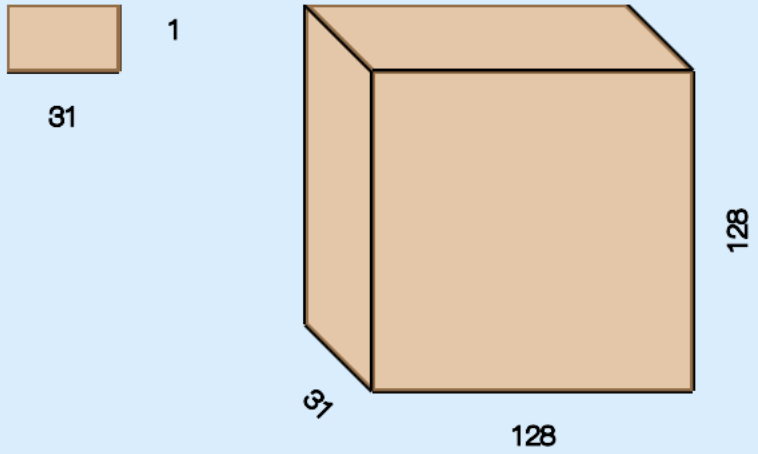


Data from measurements or simulations are read into **`sidpy.Dataset`** (d) objects directly by **`SciFiReaders`** (SF). Data are processed using multiple science packages in the Pycroscopy ecosystem that interoperate via **`Dataset`** objects. **`Dataset`** objects are written to HDF5 files via **`pyUSID`** (US) or **`pyNSID`** (NS).

NSID Model (implemented as sidpy.Dataset)

Dataset Object built on top of dask arrays

	Array	Chunk
Bytes	120.12 MiB	120.12 MiB
Shape	(31, 31, 128, 128)	(31, 31, 128, 128)
Count	1 Tasks	1 Chunks
Type	float64	numpy.ndarray

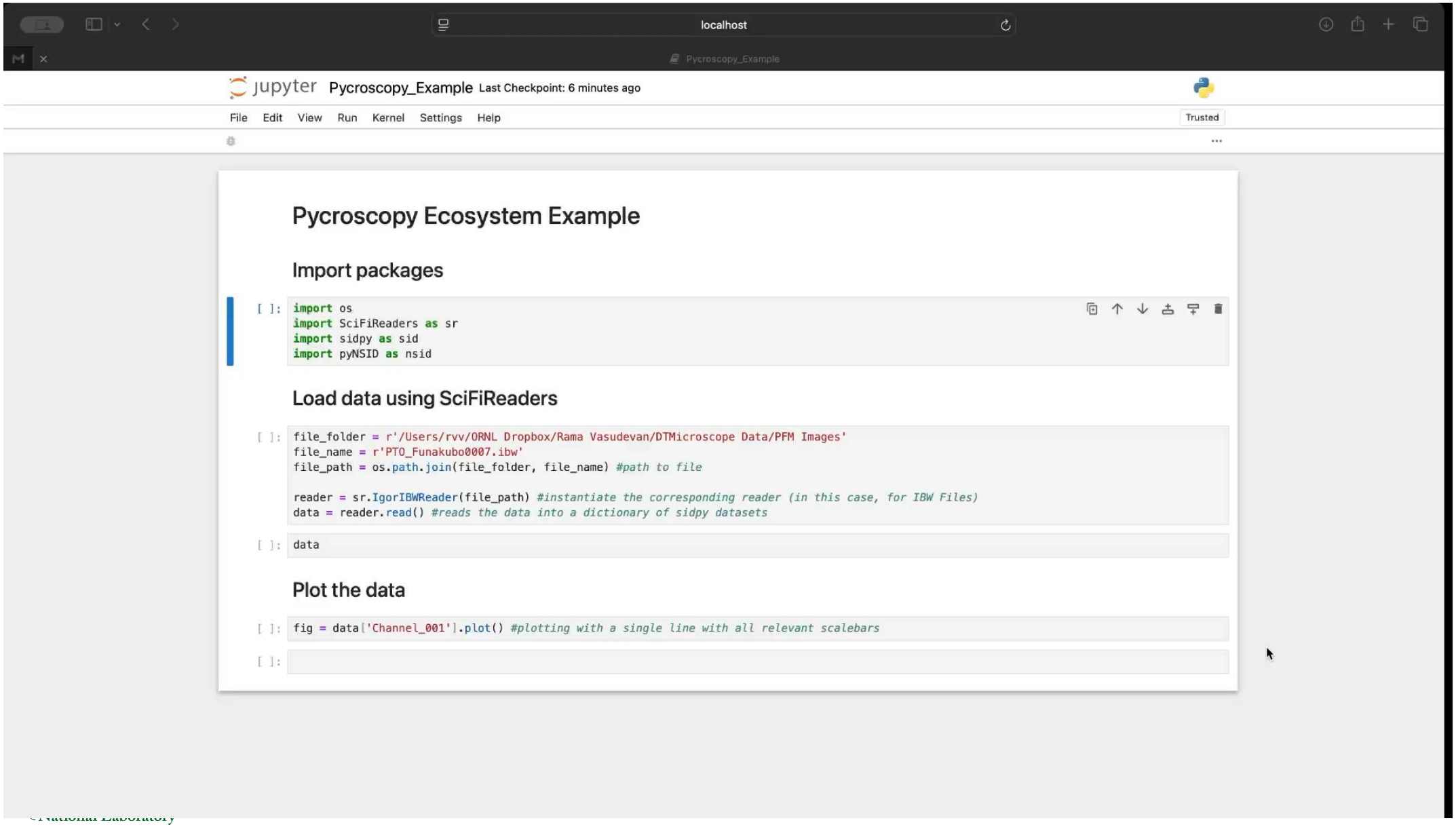


Benefits of the model:

- Easy to understand
- sidpy takes care of plotting (dataset.plot())
- Can easily perform parallel computations
- Easy to push to file including metadata
- Useful for data pipelining

- Maintain N-dimensional form
- All of the advantages of dask (large sizes, parallel compute)
- Additional data given for each dimension of dataset, such as name, quantity, units
- Metadata stored in dictionary
- Can be readily pushed to hdf5 files

Example: Load data into a sidpy dataset and plot it

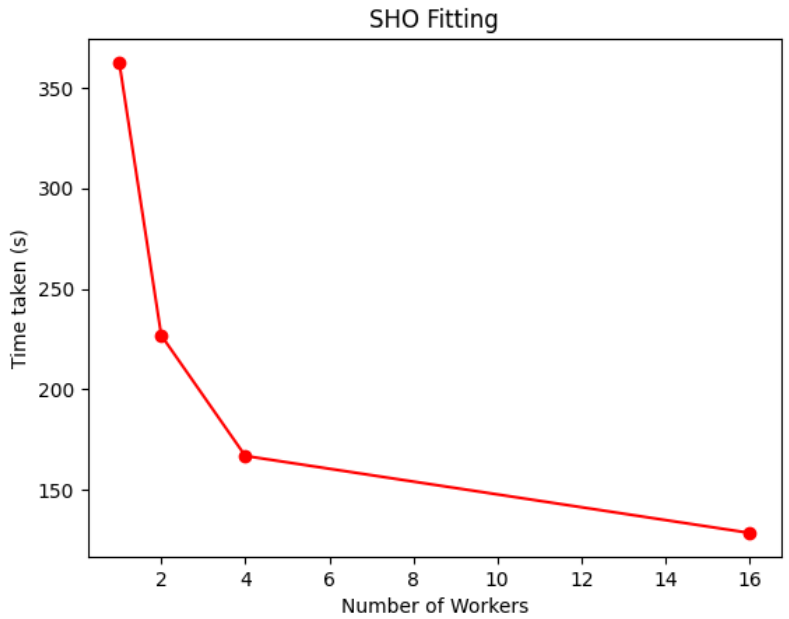


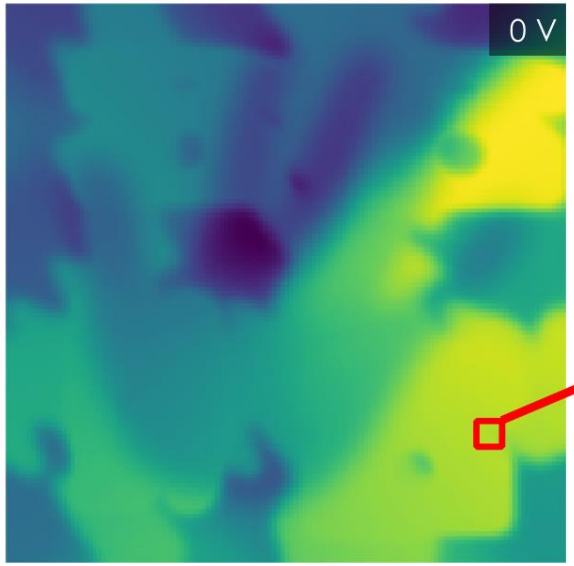
Dask backend means we can enable rapid parallel fitting

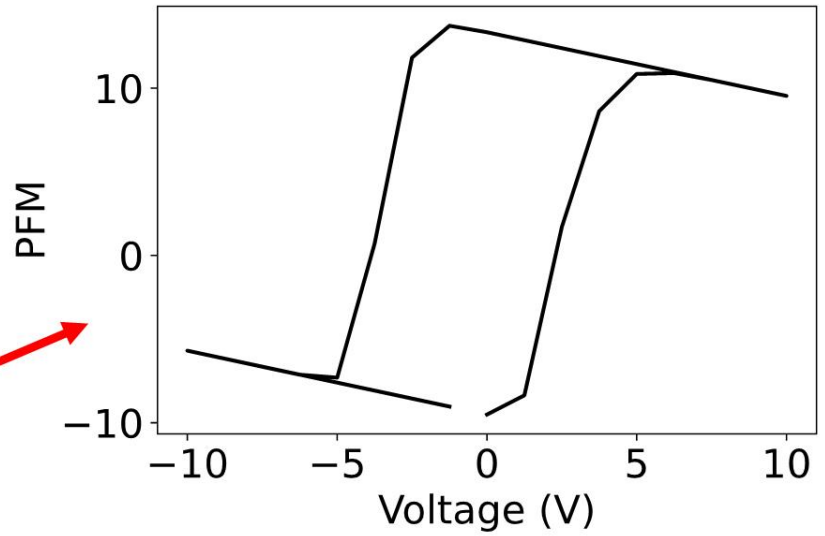
```
pserver = ProcessServer(server_loc = 'remote')
```

```
Please start the server at the remote location if it is
not already running.
```

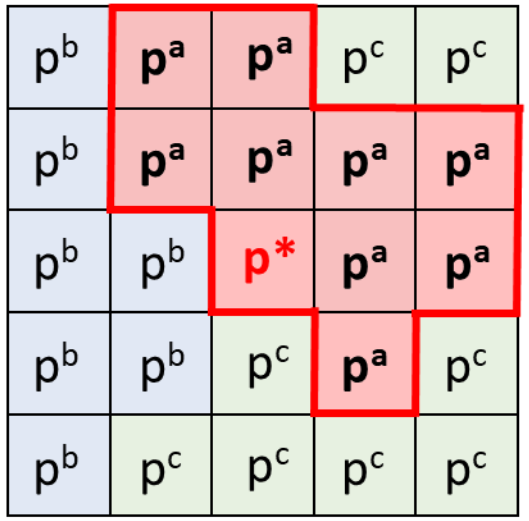
```
times = []
for num_workers in [1,2,4,16]:
    t0 = time.time()
    process_args = {'num_workers':num_workers,
                    'ind_dims':[0,1],
                    'return_cov':False,
                    'return_fit':False}
    processed_data = pserver.run_process(beline_sidpy,
                                         'SHO Fit',
                                         **process_args )
```

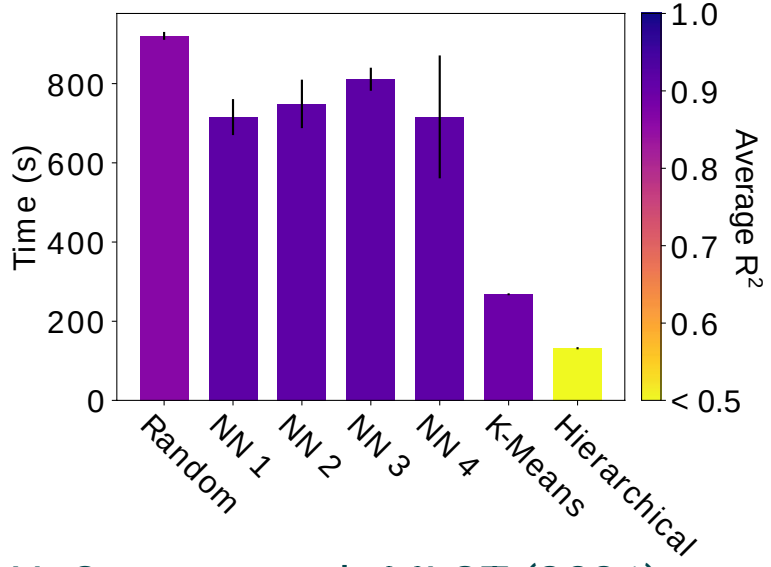






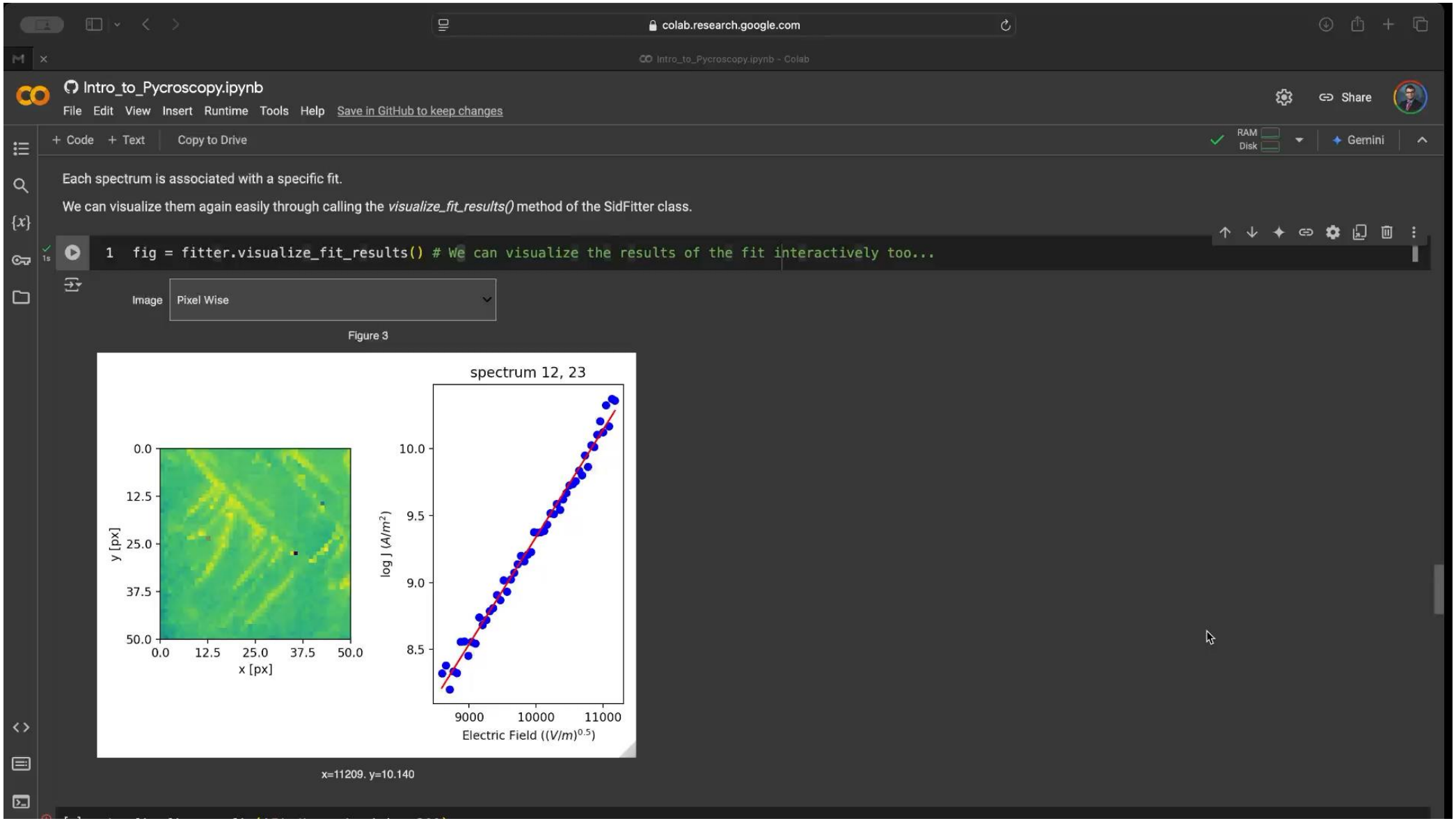
K-Means





N. Creange et al., MLST (2021)

Example: Save and reload data from hdf5 files



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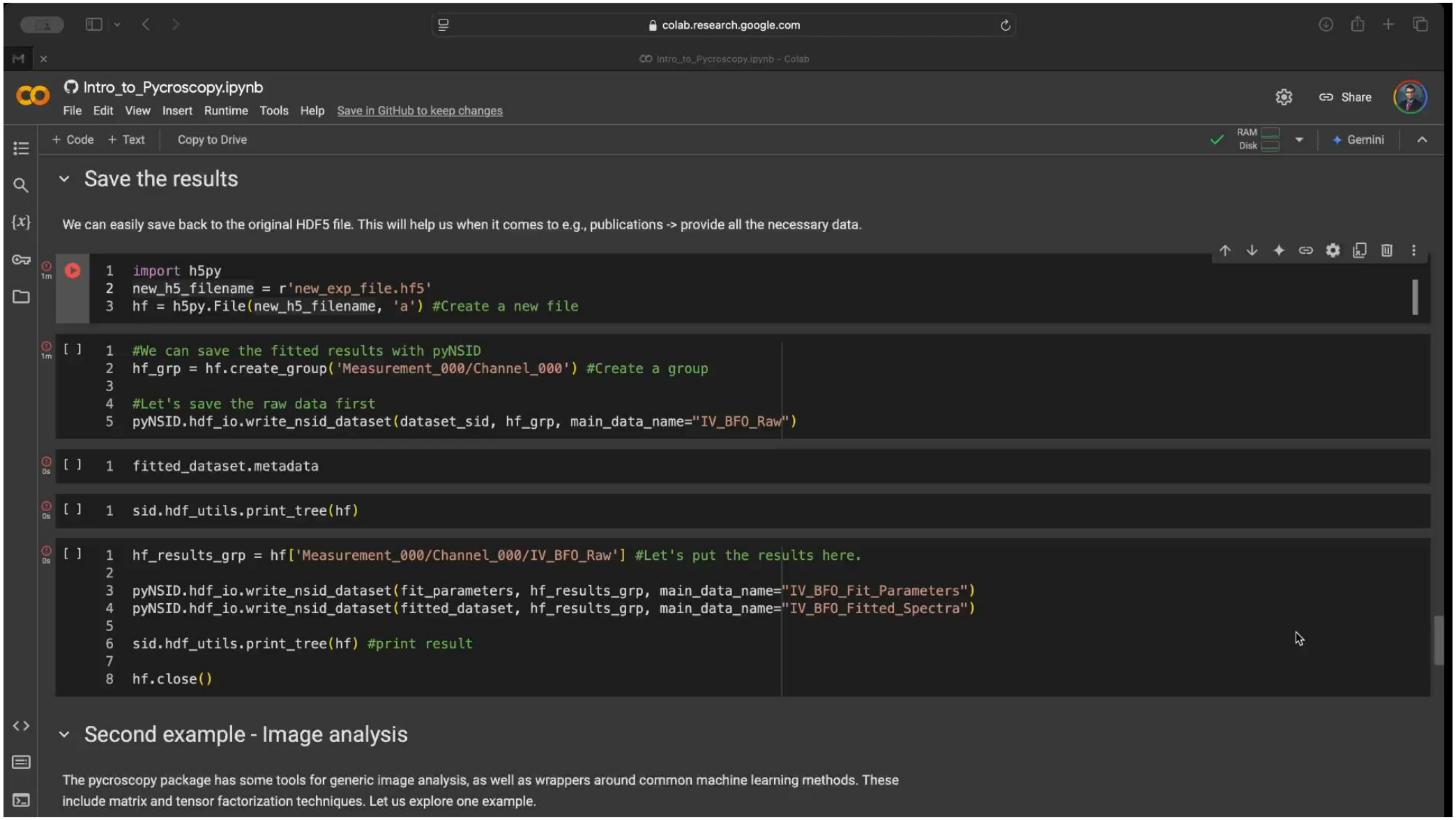
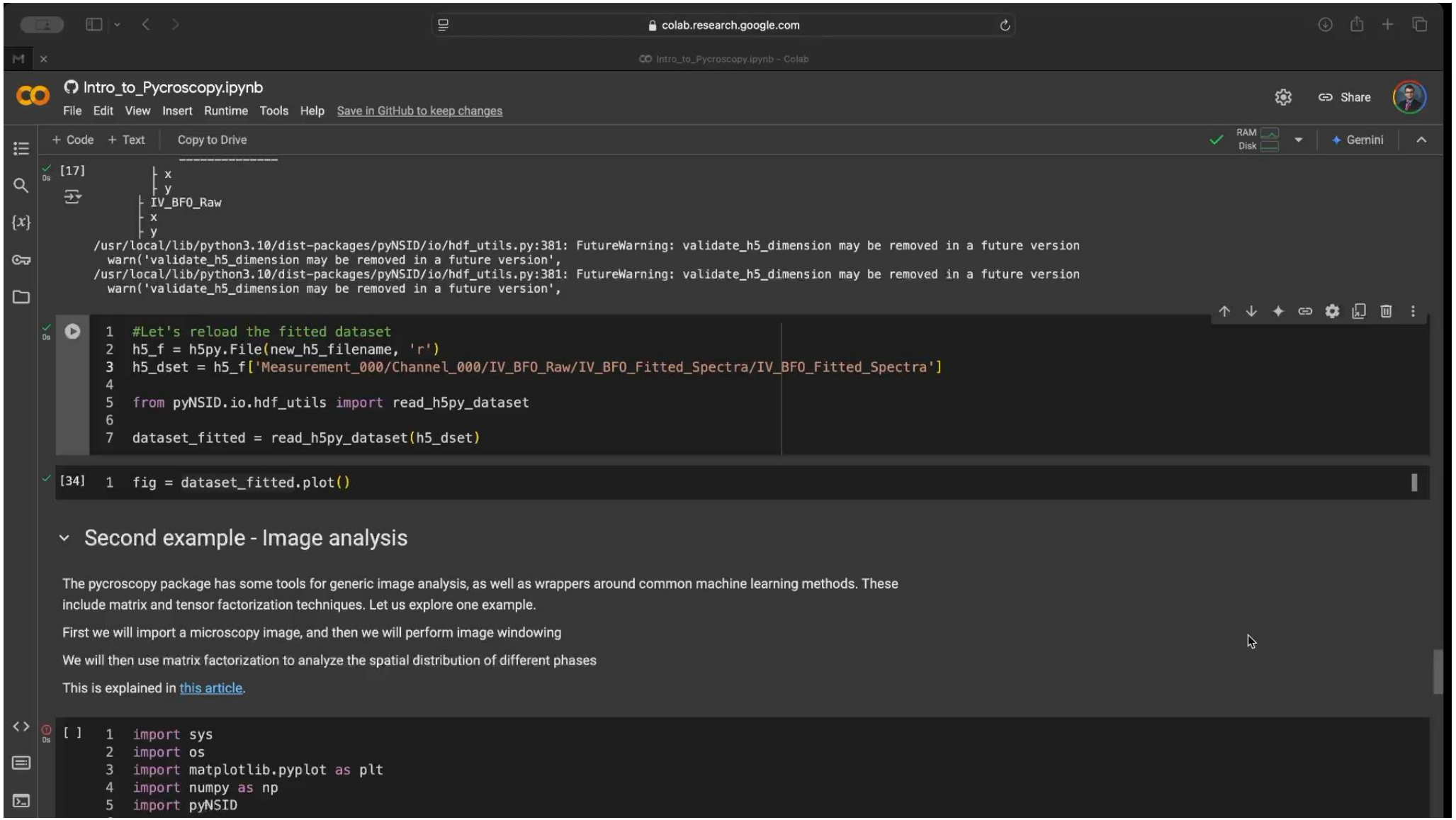
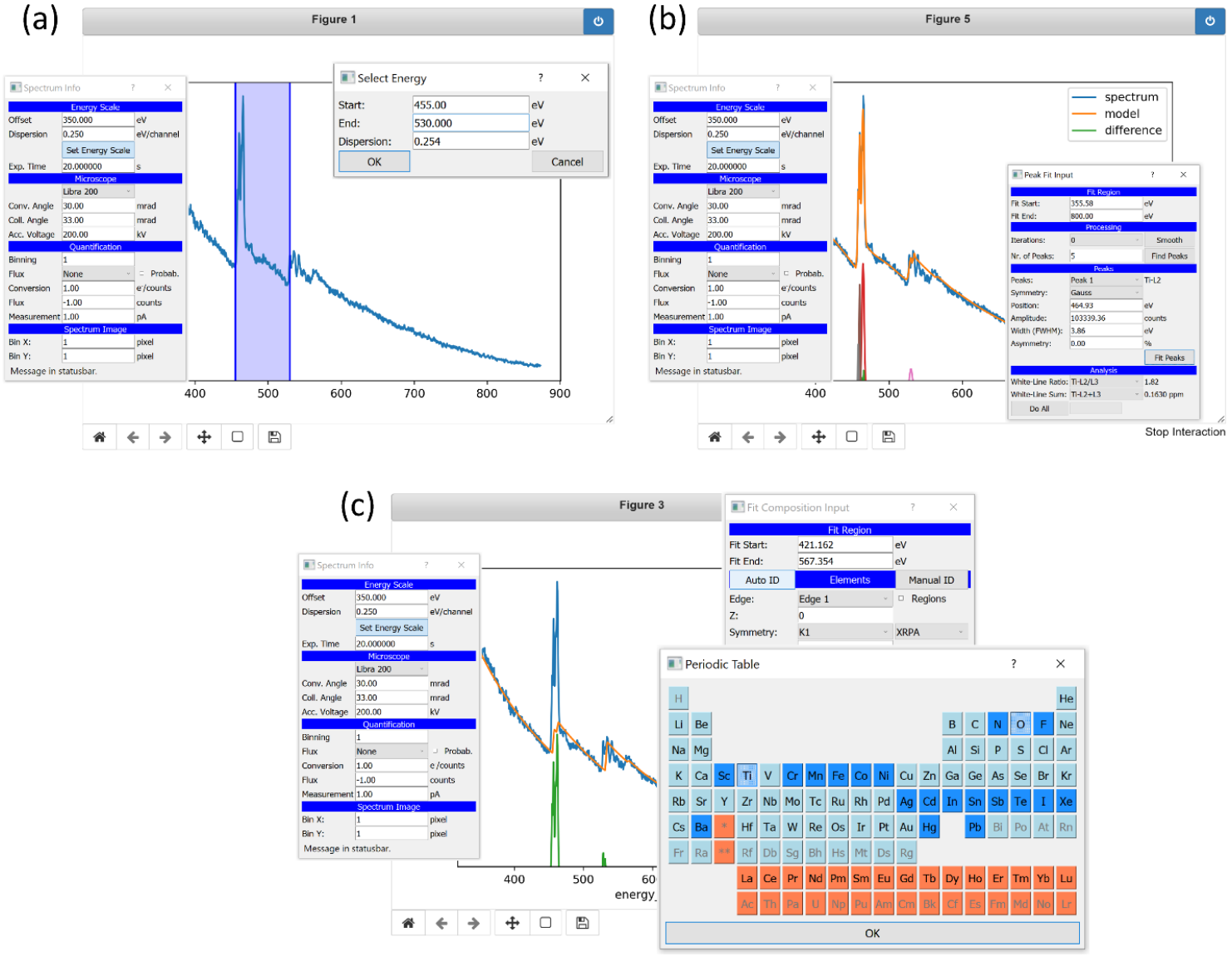


Example: Save and reload data from hdf5 files



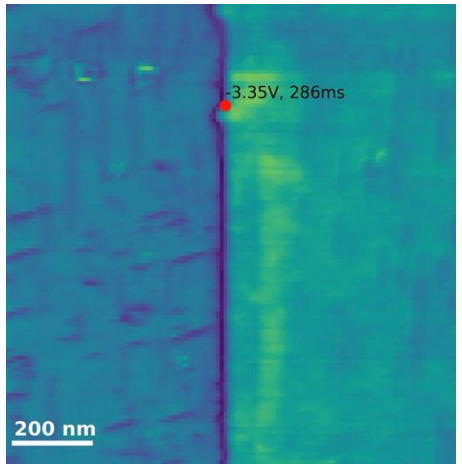
Domain-specific analysis available within the ecosystem



Domain-specific analysis, e.g. can analyze electron microscopy data in pyTEMlib, or atomic force microscopy data in BGLib, etc.

Automated workflows enable materials manipulation

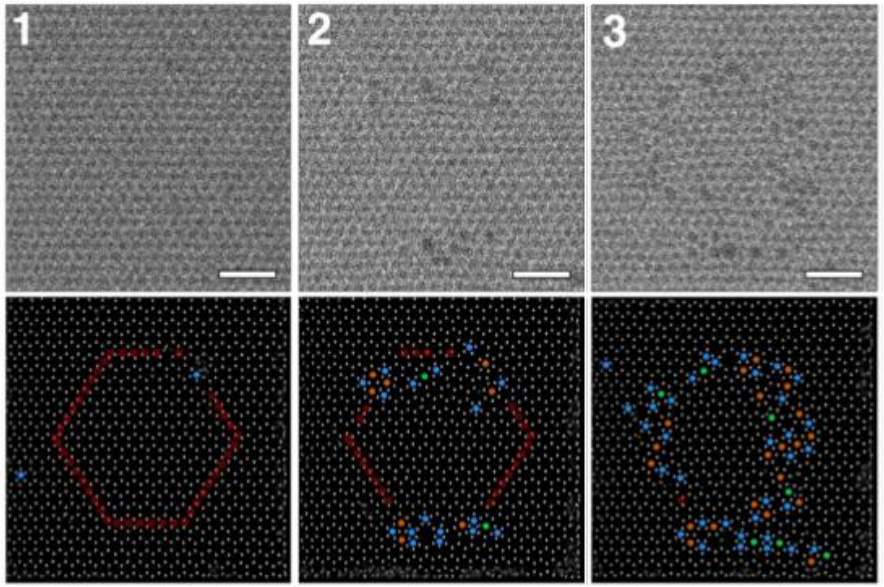
SPM: Autonomous Wall Manipulation



B. Smith et al. RSC Dig. Disc. (2024)

- Automated transition acquisition: write and perturb domain walls with voltages from the SPM tip
- Train physics-guided neural networks for prediction and digital twin, for arbitrary wall configurations and pulse parameters
- Use digital twin to train AI Agents for autonomous wall manipulation

STEM: Workflows for Defect Writing



K. Roccapriore et al. ACS Nano 16, 17116 (2022)

- Graphene imaging – steer beam in desired path, image again, find defects with computer vision, avoid defective areas, repeat
- Fully automated 'avoidance patterning' workflow to create defective regions on demand

DTMicroscope on Github

Rather than need a real microscope for development, we have created several ‘digital twin’ microscopes that you can utilize

This will ensure minimal changes are required when porting the methods developed herein, onto the full microscope for real-time autonomous steering

Github.com/pycroscopy/DTMicroscope

main · 10 Branches · 0 Tags · Go to file · Code

ramav87 Merge pull request #30 from pycroscopy/updated_data · 975fb1b · 3 days ago · 152 Commits

DTMicroscope	test updates	last month
assets	update: STEM datasets_links.md	last month
data	add: CoAg data	3 weeks ago
notebooks	additional notebooks	3 days ago
.DS_Store	additional notebooks	3 days ago
.gitignore	Merge branch 'utk' of https://github.com/pycroscopy/DT...	last month
LICENSE	added files	4 months ago
README.md	Initial commit	4 months ago
__init__.py	added files	4 months ago
setup.py	structural changes	last month

README · MIT license

DTMicroscope

Digital Twin Microscope

Some Hackathon notes

- Use the Slack channels for communication. If you have a question, feel free to unmute or directly message us in Slack (preferred) or Zoom
- If you don’t know what to do or are stuck, we have several helpers available. We will direct you to a breakout room for further discussion
- The key point is to join a group tackling a problem, and work on that problem over the course of the hackathon. If you need ideas you can again feel free to ask us – there are several computer scientists and machine learning experts on hand
- The point is to have fun and learn something cool – we are building the future of microscopy with the merging of automation, software ecosystems, and machine learning capabilities.


Questions?
Enjoy the hackathon!