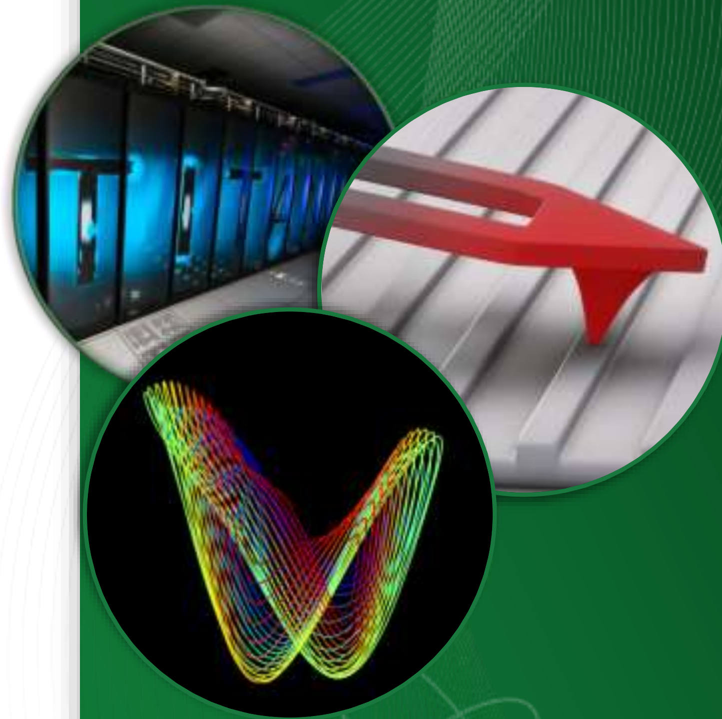
Imaging in the Information Dimension

- Suhas Somnath
- Chris R. Smith
- Stephen Jesse



Oak Ridge National Laboratory | Oak Ridge Leadership Computing Facility

Institute for Functional Imaging of Materials, Oak Ridge National Laboratory | Center for Nanophase Materials Sciences

ORNL is managed by UT-Battelle for the US Department of Energy

Multitude of Instruments

Micro Raman Microscope

Atomic Force Microscope (AFM)

AFM with Infrared spectroscopy (AFM-IR)

Scanning Tunneling Microscope (STM)

Scanning Transmission Electron Microscope (STEM)

AFM with Raman spectroscopy

What we wanted

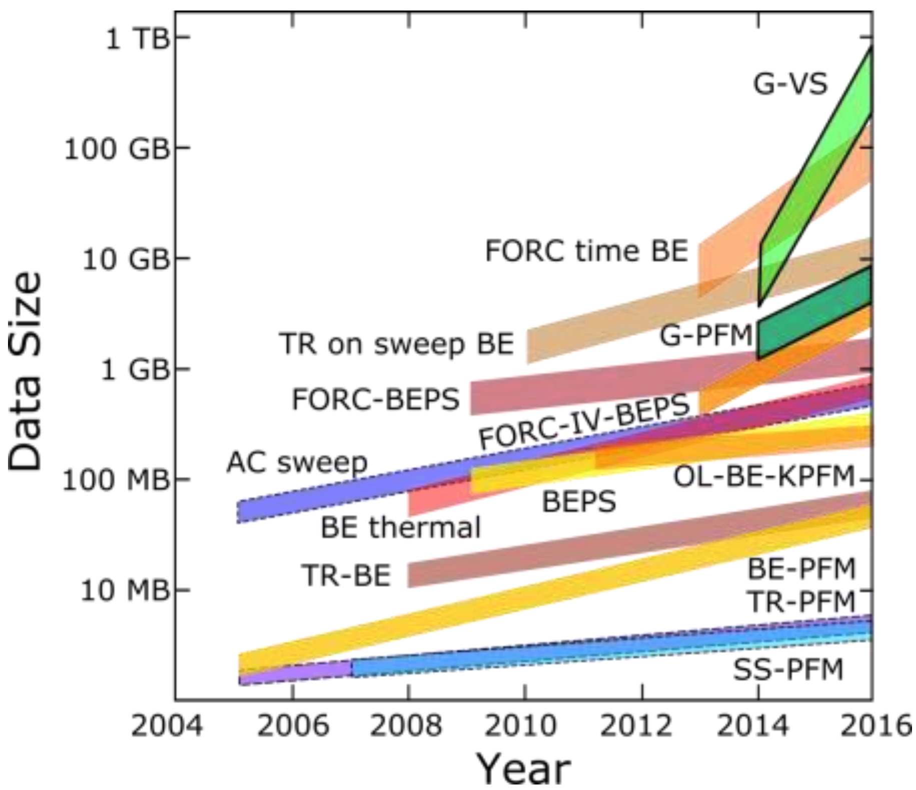
Instrument Tier

?

Interactive visualization, analysis, storage on supercomputers

Growing Data Sizes and Dimensionality

Evolution of Scanning Probe Microscopy Data



- Data sizes have grown from ~ 10 MB to ~ 1 TB in 10 years!
- Dimensionality ranges from 1D spectra to 7D hyperspectral datasets
- Cannot use laptops to analyze data

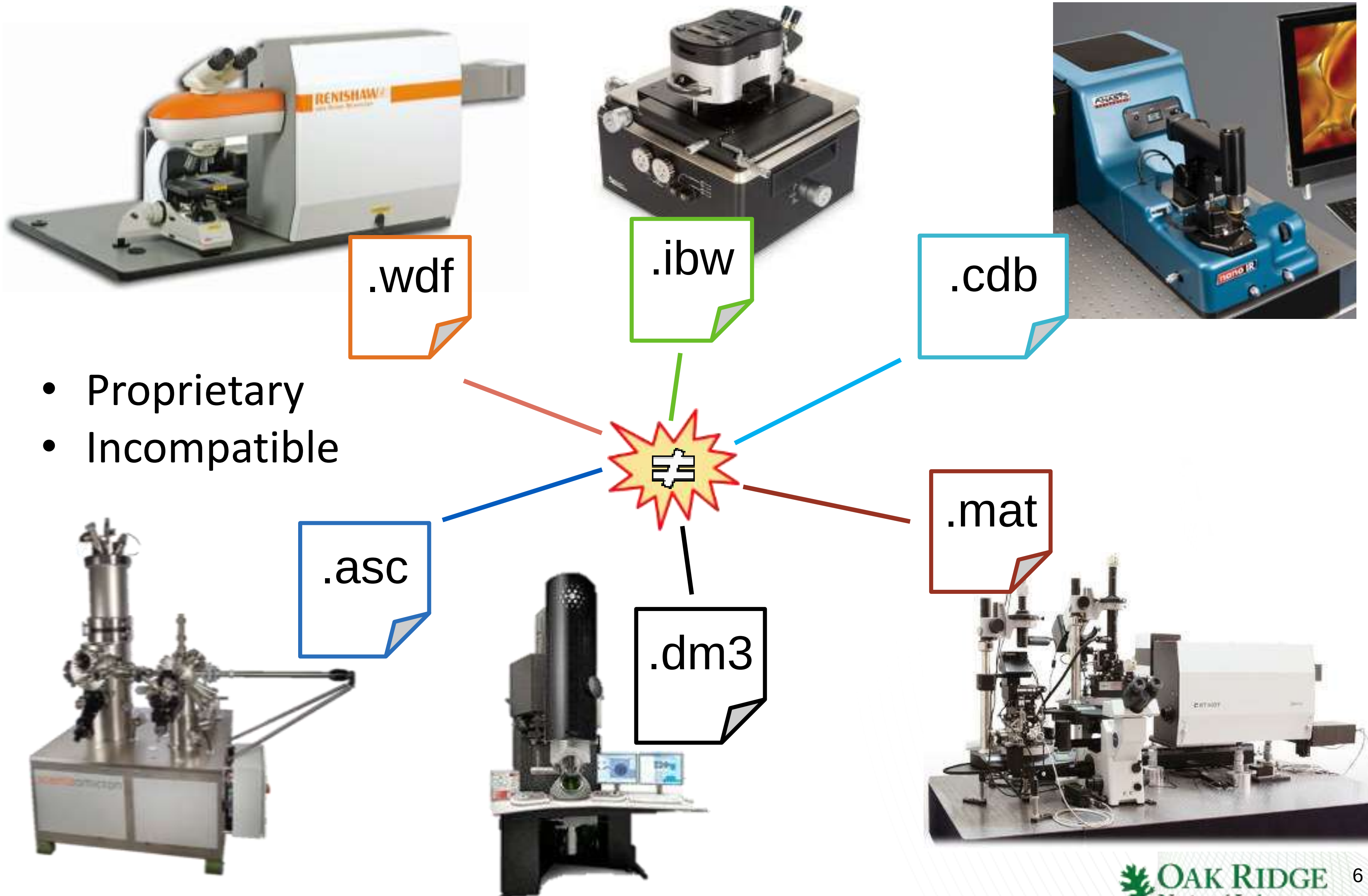
Kalinin et al., *ACS Nano*, 9068-9086, 2015

Instrumentation Software Inadequate for Analysis

- Software provided for controlling instruments typically only comes with basic data analysis capabilities
- Integrating user-developed functionality often impossible

Multitude of File Formats

- Proprietary
- Incompatible



Disjoint & Unorganized Communities

- Clustering
- Fit spectra …

- Filter Image
- Register Image …

- Fit Spectra
- SVD Filtering …

- FFT Filtering
- SVD Filtering …

- FFT Filtering
- Classify Images …

- Register Images
- Clustering

Cannot Share Code Efficiently



- HIGHLY instrument-specific code
- Different programming languages
- Often licensed / costly software like Matlab
- Most popular sharing method = email!
- No centralized repository



~~Problems~~ Opportunities in Imaging

1. Closed science
   a. No traceability for data analysis
   b. Results not (readily) reproducible

2. Multiple, incompatible, proprietary data formats

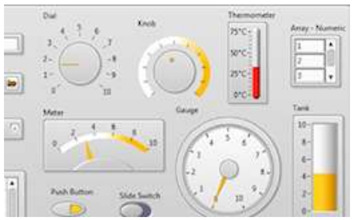
3. Disorganized and unorganized communities

4. No proper analysis software

5. Growing data volumes, variety, and dimensionality

The Solution


Instrument Tier



Automated, standardized, modularized data acquisition

Instrument-agnostic, self-describing, model in HPC-friendly file format

Centralized repository for data processing, analysis

Interactive visualization + analysis + storage on supercomputers

Expectation of Data Model

- Store data of different shapes, dimensionalities, precision and sizes.
- Accommodate data without N-dimensional form
  - Compressed sensing / sparse sampling
  - Not all combinations of spectroscopic variables
  - Incomplete experimental data

Universal Imaging and Spectroscopic Data (USID)

- Data stored as 2D matrix of (position x spectral values) regardless of dimensionality
- Ancillary datasets explain the data

Example data types:

- 2D images = (N_{pixels} x 1)
- Single spectra = (1 x Z_{steps})
- Spectroscopy on grid = (N_{pixels}x V_{steps})

Position Values

x location value	y location value	z location value
0.5	0.5	0.5
1	0.5	0.5
1.5	0.5	0.5
0.5	1	0.5
1	1	0.5
1.5	1	0.5
0.5	1.5	0.5
1	1.5	0.5
1.5	1.5	0.5
0.5	0.5	1
1	0.5	1
1.5	0.5	1
0.5	1	1
1	1	1
1.5	1	1
0.5	1.5	1
1	1.5	1
1.5	1.5	1

Position Indices

x location index	y location index	z location index
1	1	1
2	1	1
3	1	1
1	2	1
2	2	1
3	2	1
1	3	1
2	3	1
3	3	1
1	1	2
2	1	2
3	1	2
1	2	2
2	2	2
3	2	2
1	3	2
2	3	2
3	3	2

Measurement / Analysis parameters→ Attribute A … Attribute Z

Time / Spectral →

←Location

Main Dataset

Spectroscopic Indices

observable D index	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
observable C index	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
observable B index	1	1	1	1	2	2	2	2	3	3	3	3	4	4	4	4
observable A index	1	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4

observable D index	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
observable C index	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
observable B index	1	1	1	1	2	2	2	2	3	3	3	3	4	4	4	4
observable A index	1	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4

Spectroscopic Values

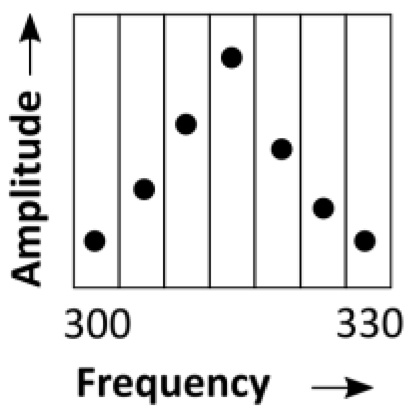
observable D value	0.125	0.125	0.125	0.125	0.125	0.125	0.125	0.125	0.125	0.125	0.125	0.125	0.125	0.125	0.125	0.125
observable C value	0.125	0.125	0.125	0.125	0.125	0.125	0.125	0.125	0.125	0.125	0.125	0.125	0.125	0.125	0.125	0.125
observable B value	0.125	0.125	0.125	0.125	0.25	0.25	0.25	0.25	0.375	0.375	0.375	0.375	0.5	0.5	0.5	0.5
observable A value	0.125	0.25	0.375	0.5	0.125	0.25	0.375	0.5	0.125	0.25	0.375	0.5	0.125	0.25	0.375	0.5

observable D value	0.125	0.125	0.125	0.125	0.125	0.125	0.125	0.125	0.125	0.125	0.125	0.125	0.125	0.125	0.125	0.125
observable C value	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25
observable B value	0.125	0.125	0.125	0.125	0.25	0.25	0.25	0.25	0.375	0.375	0.375	0.375	0.5	0.5	0.5	0.5
observable A value	0.125	0.25	0.375	0.5	0.125	0.25	0.375	0.5	0.125	0.25	0.375	0.5	0.125	0.25	0.375	0.5

USID – 1D spectra

Original N-dimensional form

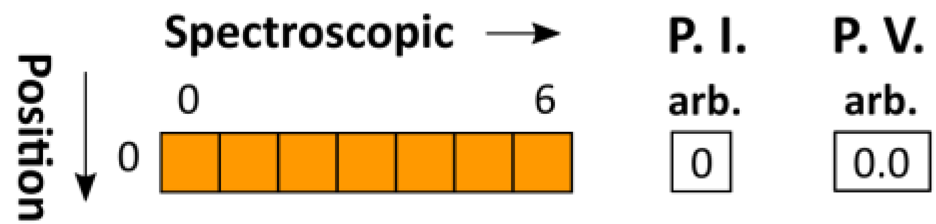
Spectra at X=3, Y=1



Shape: (7,)
Quantity: Amplitude
Units: V

USID 2-dimensional form

=

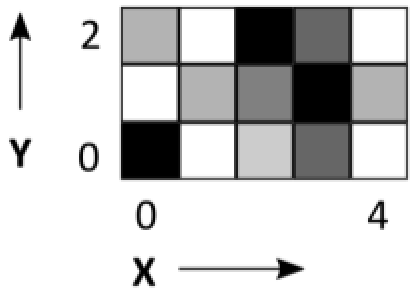


Shape: (1, 7)

S. I.	Frequency	0	1	2	3	4	5	6

S. V.	Frequency	300	305	310	315	320	325	330

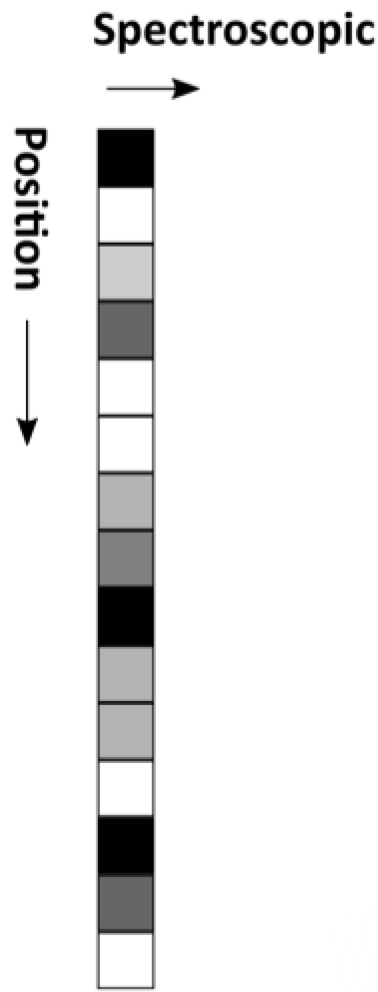
USID – 2D Image



Shape: (3, 5)

Original N-D form

=



P. I.

X	Y
0	0
1	0
2	0
3	0
4	0
0	1
1	1
2	1
3	1
4	1
0	2
1	2
2	2
3	2
4	2

P. V.

X	Y
-250	0
-125	0
0	0
125	0
250	0
-250	3.5
-125	3.5
0	3.5
125	3.5
250	3.5
-250	7
-125	7
0	7
125	7
250	7

USID 2D form

Quantity: Intensity
Units: arb. units

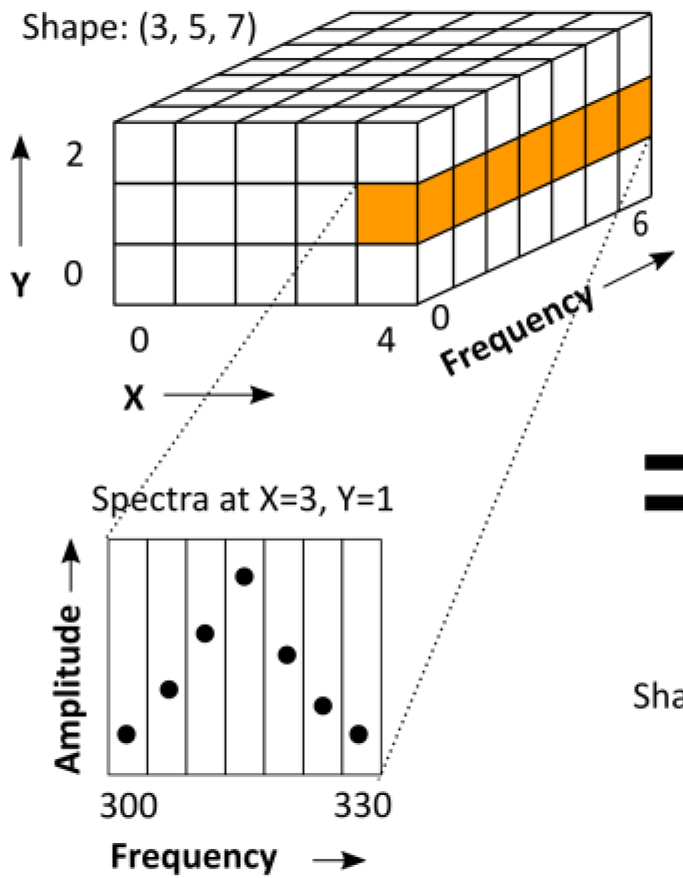
S. I. **arb.** 0

S. V. **arb.** 0.0

Shape: (15, 1)

USID – Spectra on Grid (3D)

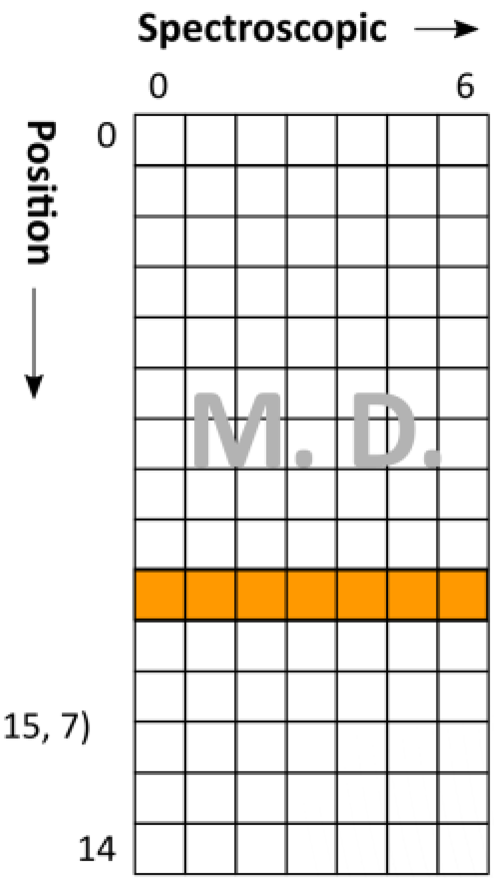
Original N-dimensional form



Quantity: Amplitude
Units: V

=

USID 2-dimensional Form



P. I.

X	Y
0	0
1	0
2	0
3	0
4	0
0	1
1	1
2	1
3	1
4	1
0	2
1	2
2	2
3	2
4	2

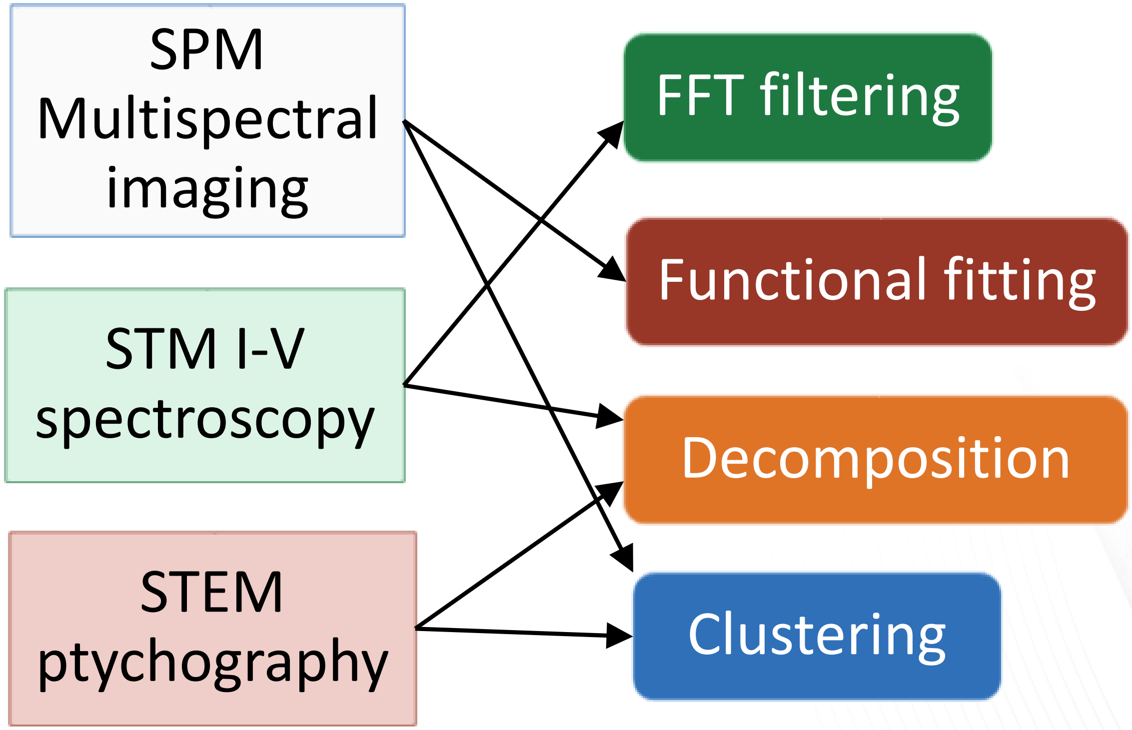
P. V.

X	Y
-250	0
-125	0
0	0
125	0
250	0
-250	3.5
-125	3.5
0	3.5
125	3.5
250	3.5
-250	7
-125	7
0	7
125	7
250	7

S. I. Frequency	0	1	2	3	4	5	6
S. V. Frequency	300	305	310	315	320	325	330

USID - Instrument Agnostic Code

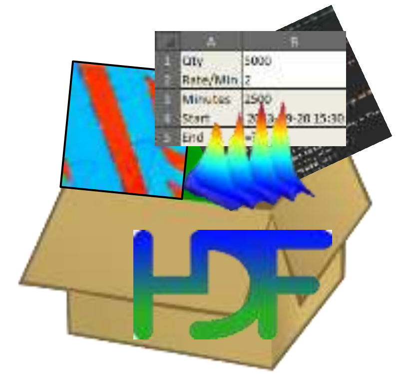
- Instrument-agnostic data allows instrument-agnostic code
- Single version of analysis and processing routine
- Brings multiple scientific communities together

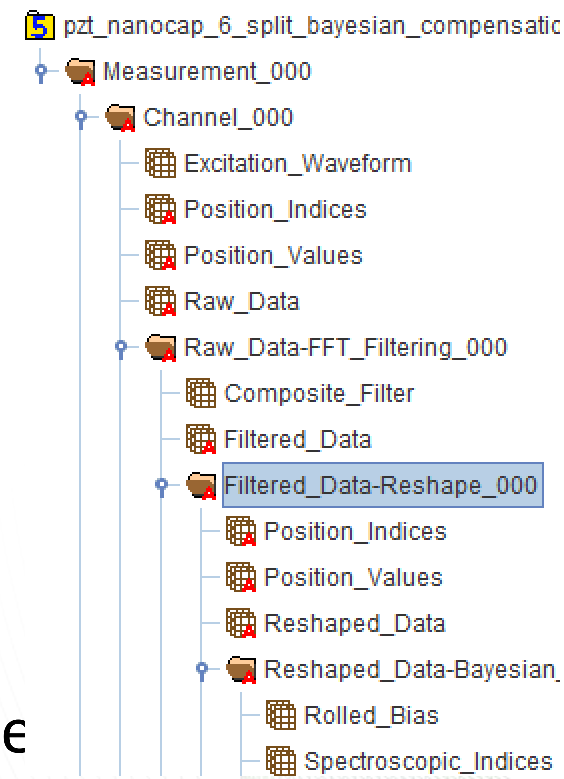


Suhas Somnath, somnaths@ornl.gov

Hierarchical Data Format (HDF5)

- A HDF5 file is a smart container
  - Capable of storing multidimensional datasets, Images, text, measurement parameters, etc.
  - Contents organized like traditional folders and files
    - **Groups** - Analogous to file folders
    - **Dataset** – 1 to N dimensional data
      - Integer, floating point, complex numbers etc
    - **Attributes** – {Key : value} pairs useful for describing data and experimental parameters, etc.
- Easily accessible – C, C++, python, Java….
- Tree structure + nomenclature +attributes are **records of workflow** applied to dataset
- Parallel read / write, HPC & cloud compatible



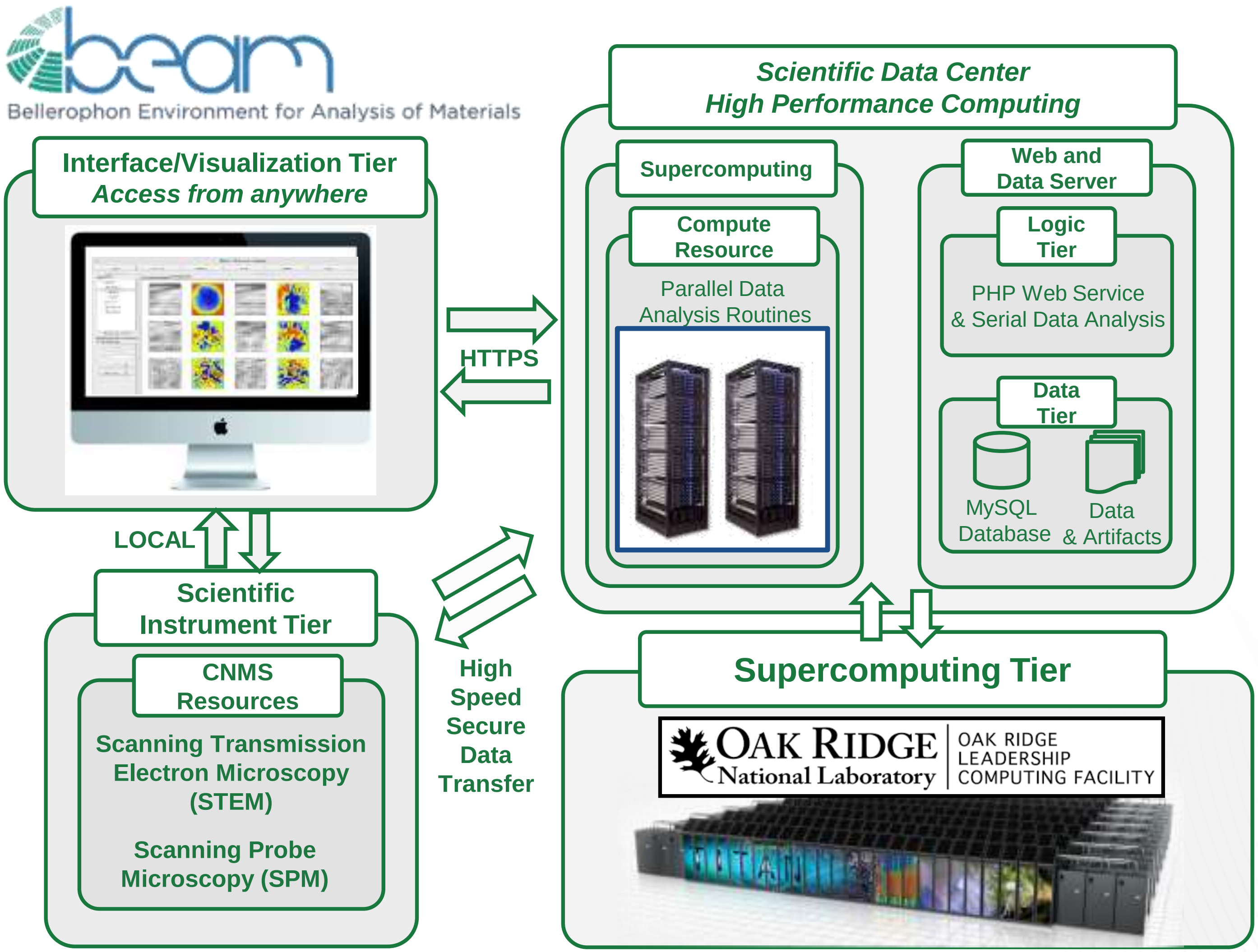


Expectation from Software

- Easy to learn and understand
- Strong support-base
- Established community standard
- Straightforward to implement and maintain
- Optimized libraries for scientific and numeric algorithms
- Access to existing imaging related packages
- Free
- Scalable to multiple CPU cores + distributed computing

(Purely) Programmer-Driven Solution

Software connecting scientific instruments to supercomputers



- **Successes**:
  - Easy to use – Point-click
  - Fast – on super-computers
- **Shortcomings**:
  - Very long development cycle
  - Very expensive
  - Brittle (points of failure)
  - Scientists had no control!!

Lingerfelt et al., *Procedia Computer Science* **80**, 2276-2280 (2016).

Python for Scientific Research

Very easy to learn + code

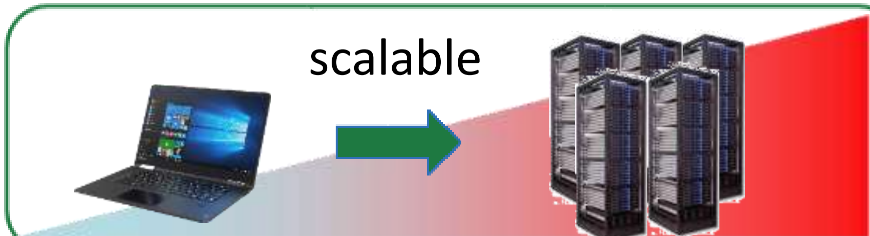
Numerous, **powerful** libraries for science

scikit learn

NumPy

SciPy

scalable



Strong user community

stackoverflow

open source™

- Facilitates innovation
- More robust code
- Improved adoption of new methods / standards
- Accelerates scientific progress

Cross-platform

MacOS

Established standard for:

- Microscopy
- Microbiology
- Deep learning
- Data science
- Neutron science
- More!

All for a princely sum of …. **$0!**

Software Packages

- Written in Python
- Open source & free
- Written by scientists
- Data centric
- Instrument-independent data model in HDF5
- Instrument-independent analysis algorithms
  - Reusable across scientific domains

pyUSID

pycroscopy

Software Organization

pycroscopy

I/O
- Data translators (proprietary formats to HDF5)

Visualization
- Plotting utilities
- Jupyter widgets

Simulation
- AFM Force-distance …

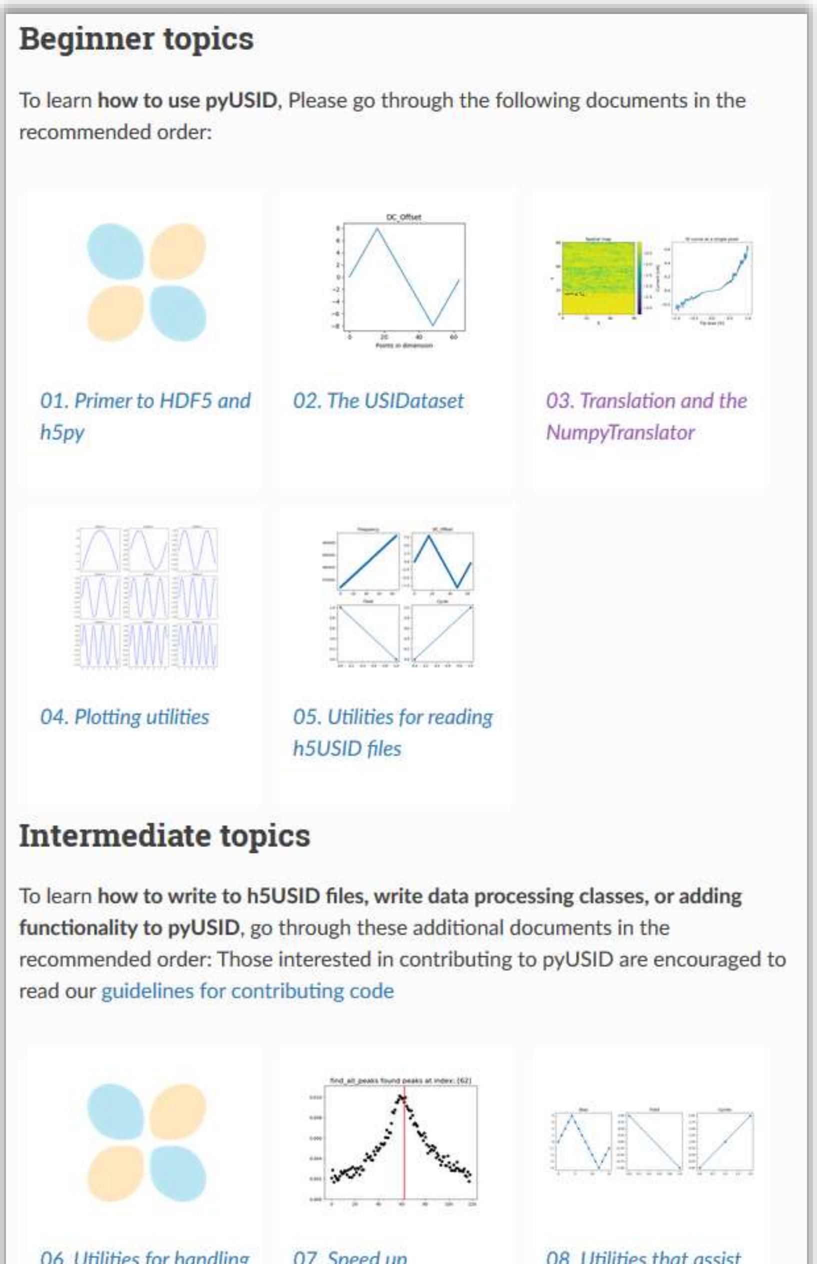
Analysis
- Physical model specific
- Fitting to model, etc.
- Physics based regression

Processing
- Physical model agnostic
- Image filtering, registration,
- Multivariate analysis

pyUSID
- HDF5 file i/o operations
- Base data processing,
- visualization…

Software Organization

PyUSID & Pycroscopy - Well documented



Beginner topics

To learn **how to use pyUSID**, Please go through the following documents in the recommended order:

01. Primer to HDF5 and h5py

02. The USIDataset

03. Translation and the NumpyTranslator

04. Plotting utilities

05. Utilities for reading h5USID files

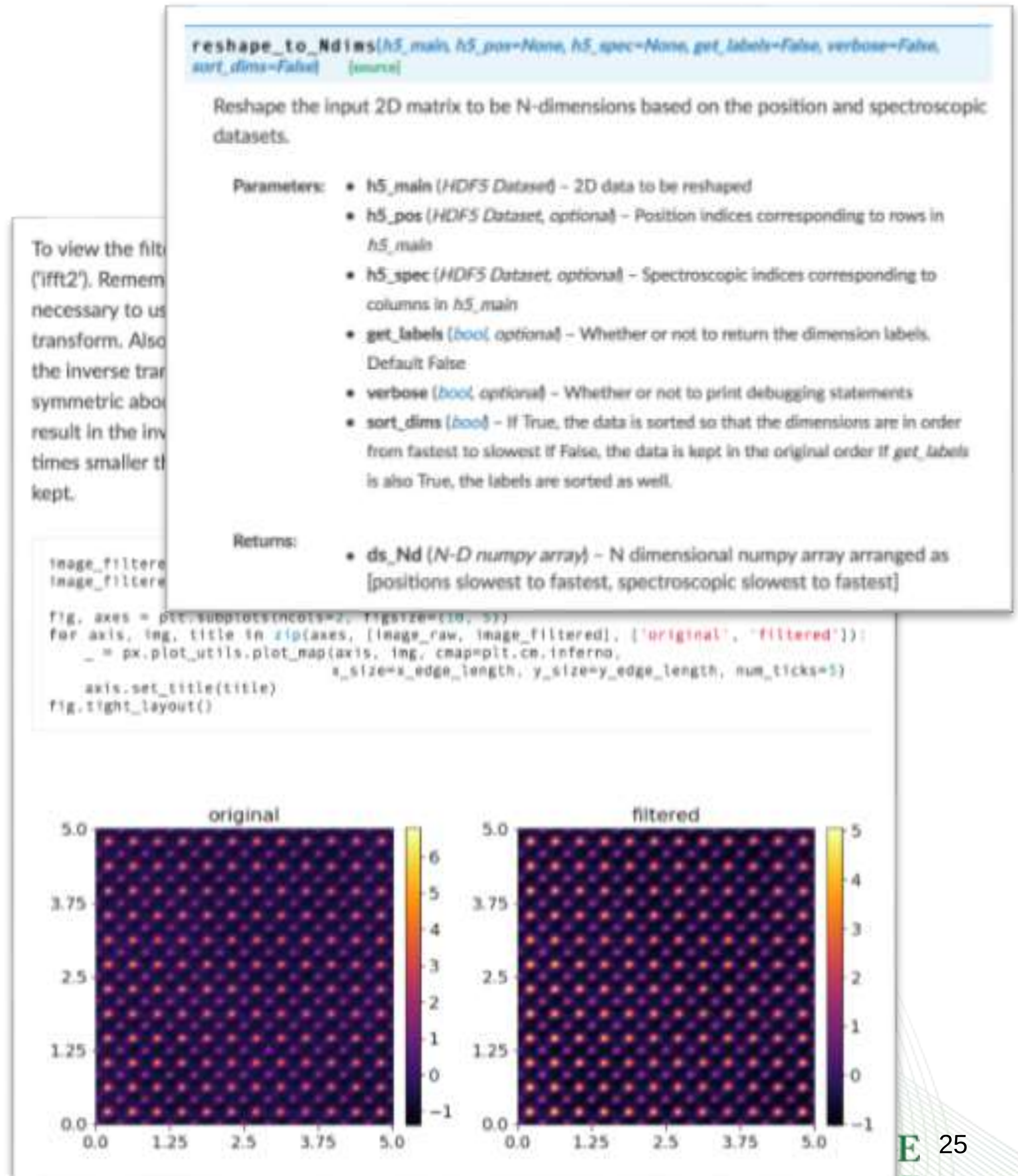
Intermediate topics

To learn **how to write to h5USID files, write data processing classes, or adding functionality to pyUSID**, go through these additional documents in the recommended order: Those interested in contributing to pyUSID are encouraged to read our guidelines for contributing code

06. Utilities for handling

07. Speed up

08. Utilities that assist



reshape_to_Ndims(*h5_main, h5_pos=None, h5_spec=None, get_labels=False, verbose=False, sort_dims=False*) [source]

Reshape the input 2D matrix to be N-dimensions based on the position and spectroscopic datasets.

Parameters:
- **h5_main** (*HDF5 Dataset*) – 2D data to be reshaped
- **h5_pos** (*HDF5 Dataset, optional*) – Position indices corresponding to rows in *h5_main*
- **h5_spec** (*HDF5 Dataset, optional*) – Spectroscopic indices corresponding to columns in *h5_main*
- **get_labels** (*bool, optional*) – Whether or not to return the dimension labels. Default False
- **verbose** (*bool, optional*) – Whether or not to print debugging statements
- **sort_dims** (*bool*) – If True, the data is sorted so that the dimensions are in order from fastest to slowest If False, the data is kept in the original order If *get_labels* is also True, the labels are sorted as well.

Returns:
- **ds_Nd** (*N-D numpy array*) – N dimensional numpy array arranged as [positions slowest to fastest, spectroscopic slowest to fastest]

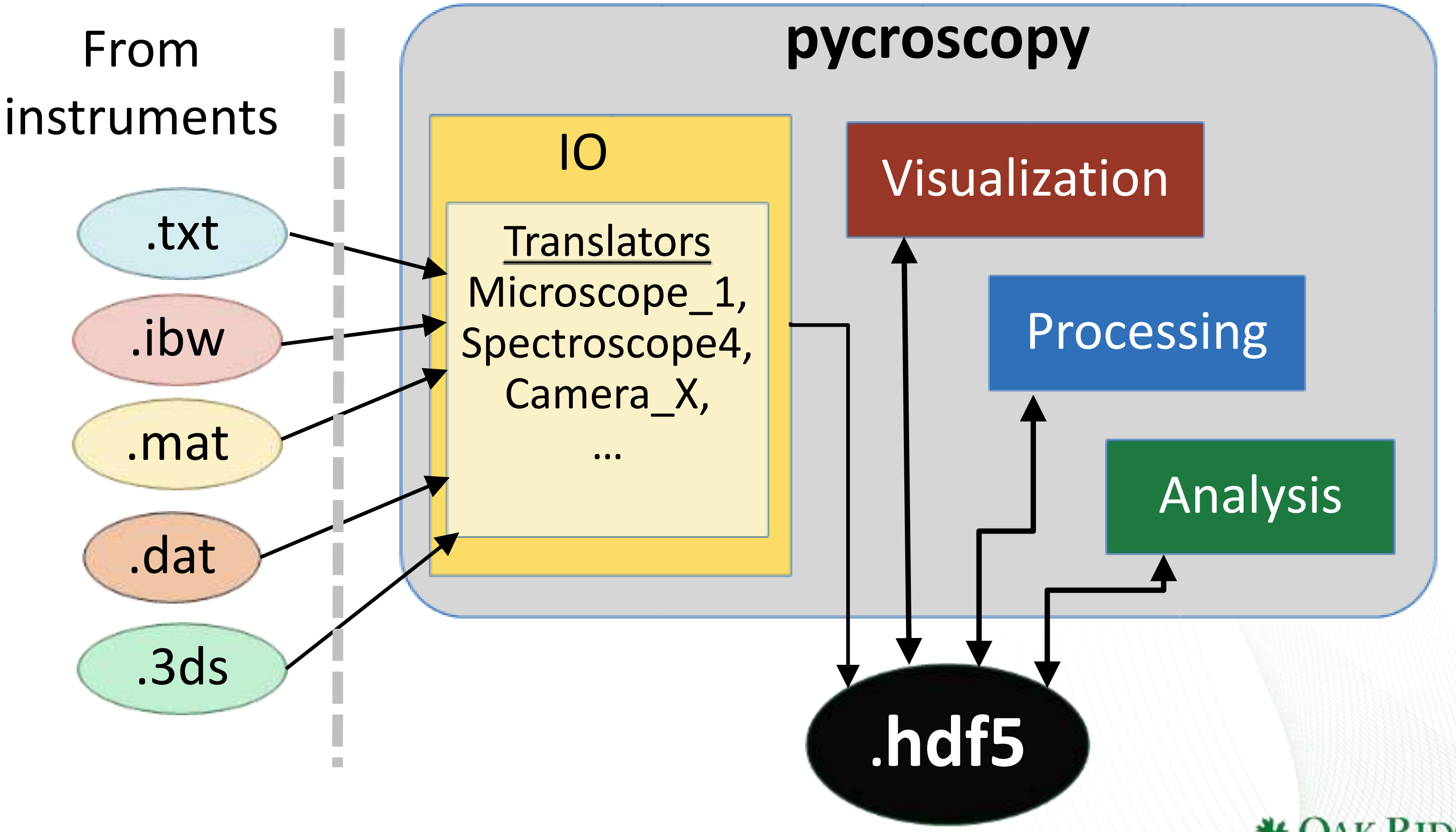
To view the filt
('ifft2'). Remem
necessary to us
transform. Also
the inverse tra
symmetric abo
result in the inv
times smaller t
kept.

```
image_filtere
image_filtere

fig, axes = plt.subplots(ncols=2, figsize=(10, 5))
for axis, img, title in zip(axes, [image_raw, image_filtered], ['original', 'filtered']):
    _ = px.plot_utils.plot_map(axis, img, cmap=plt.cm.inferno,
                               x_size=x_edge_length, y_size=y_edge_length, num_ticks=5)
    axis.set_title(title)
fig.tight_layout()
```

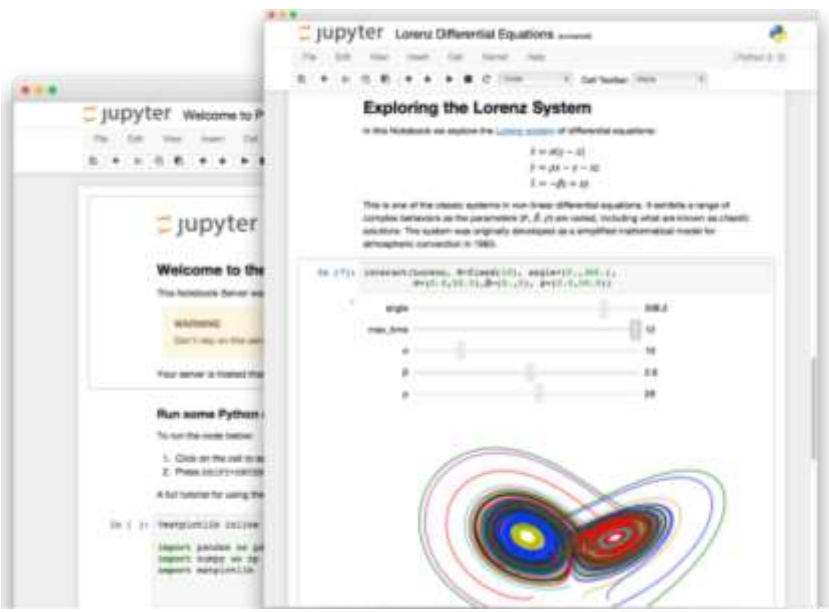
Entering the Pycroscopy Ecosystem

- hdf5 file is the hub for all operations
- Analysis, processing, visualization available after translation to .hdf5



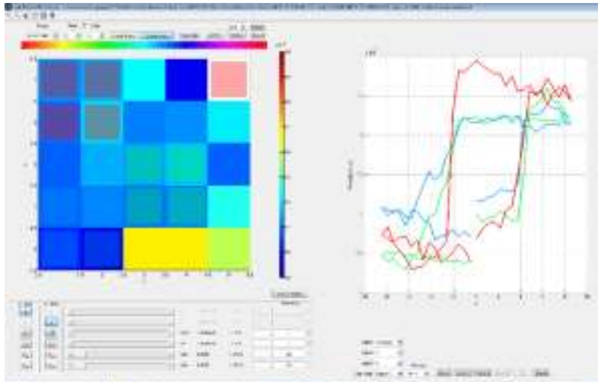
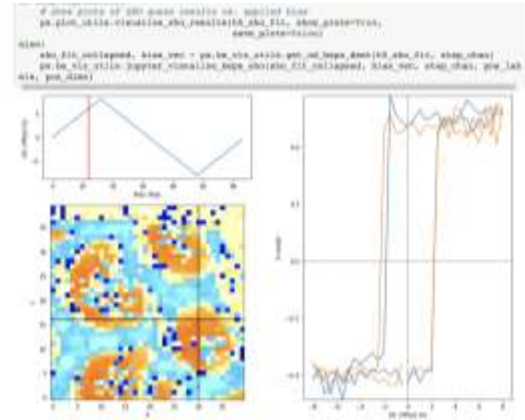
Jupyter Notebooks

Jupyter Notebook



- Interactive documents
- Exploratory programming
- Code
- Text
- Images
- Interactive – slice through data, pan, move, rotate …

Pycroscopy - Supporting User Research

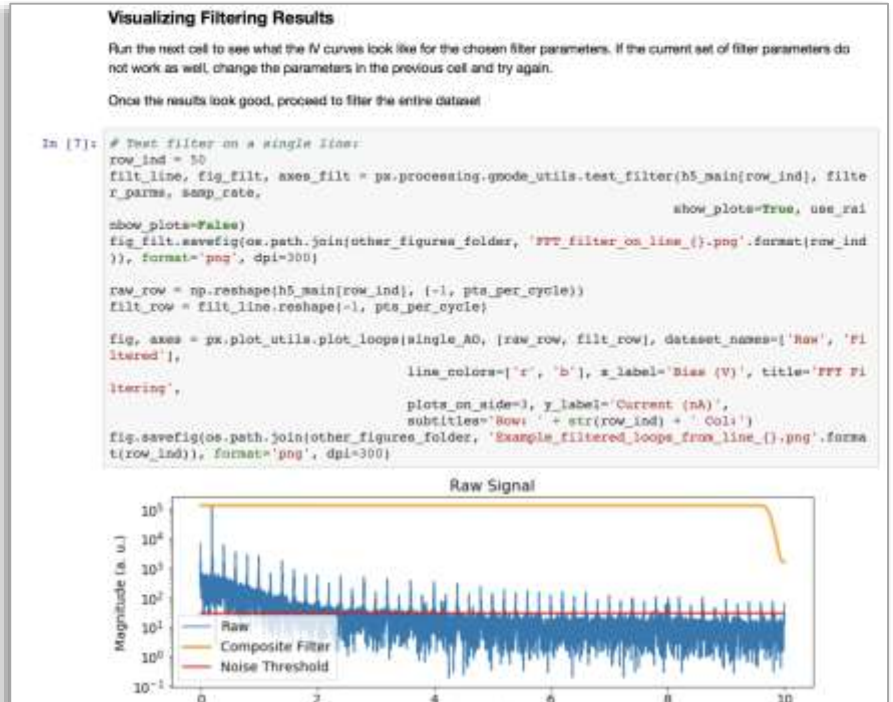
Before 2016	Since 2016
 + 	
Scripts + complicated, Matlab GUI	Set of simple Jupyter notebooks
Witten by dedicated software engineer	Written by material scientists
Not customizable	Completely customizable.
2-3 hours of training before use	Notebooks include instructions. NO training required!
Deployed only on two offline workstations due to licensing restrictions = queue	Each user gets VMs with jupyter notebook server
Will remain on off-line desktops	In the process of switching to computations on clusters

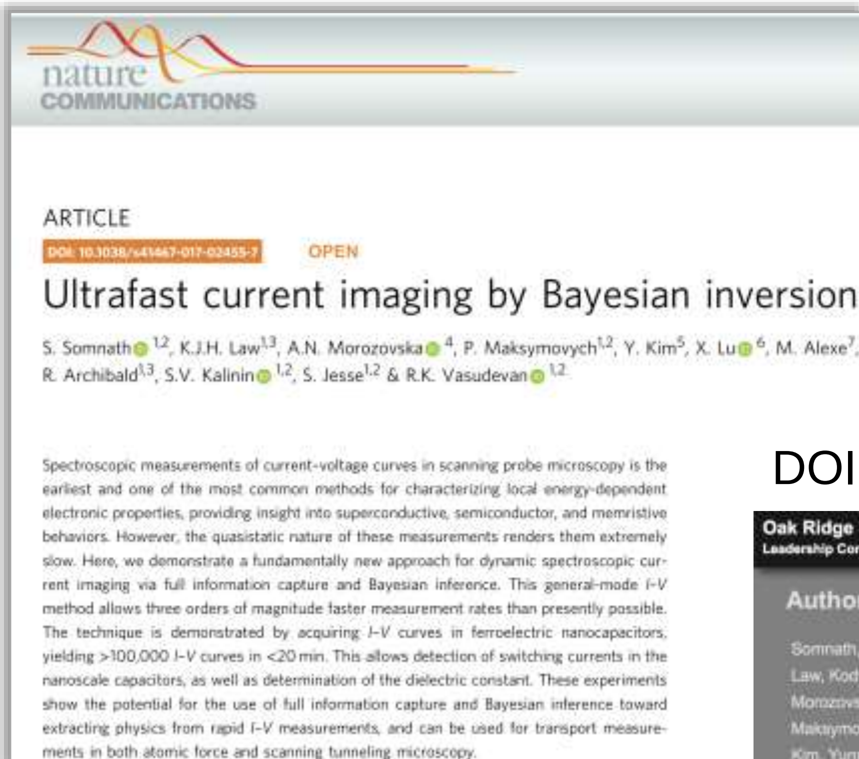
Truly Achieving Open Science, Reproducibility

Aim – ALL scientific journal papers accompanied with:

- Jupyter notebook that shows all analysis (raw data → figures).
- Data with DOI number

Jupyter notebook associated with paper





nature COMMUNICATIONS

ARTICLE

DOI: 10.1038/s41467-017-02455-7 OPEN

Ultrafast current imaging by Bayesian inversion

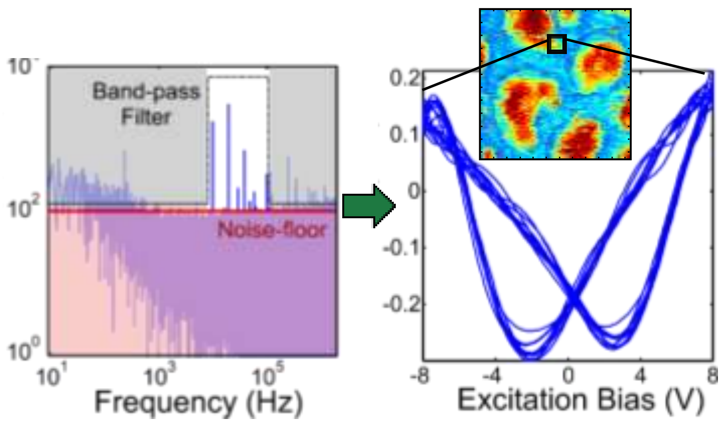
S. Somnath[1,2], K.J.H. Law[1,3], A.N. Morozovska[4], P. Maksymovych[1,2], Y. Kim[5], X. Lu[6], M. Alexe[7], R. Archibald[1,3], S.V. Kalinin[1,2], S. Jesse[1,2] & R.K. Vasudevan[1,2]

Spectroscopic measurements of current-voltage curves in scanning probe microscopy is the earliest and one of the most common methods for characterizing local energy-dependent electronic properties, providing insight into superconductive, semiconductor, and memristive behaviors. However, the quasistatic nature of these measurements renders them extremely slow. Here, we demonstrate a fundamentally new approach for dynamic spectroscopic current imaging via full information capture and Bayesian inference. This general-mode I-V method allows three orders of magnitude faster measurement rates than presently possible. The technique is demonstrated by acquiring I-V curves in ferroelectric nanocapacitors, yielding >100,000 I-V curves in <20 min. This allows detection of switching currents in the nanoscale capacitors, as well as determination of the dielectric constant. These experiments show the potential for the use of full information capture and Bayesian inference toward extracting physics from rapid I-V measurements, and can be used for transport measurements in both atomic force and scanning tunneling microscopy.

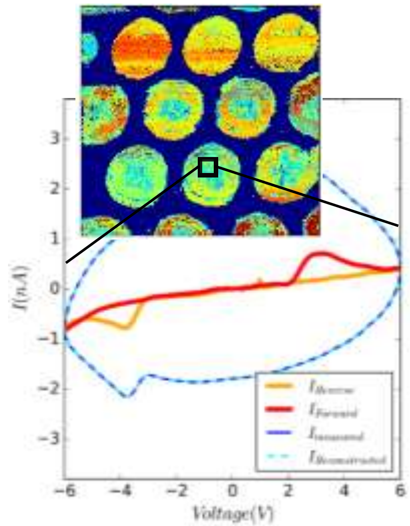
DOI associated with data (raw → paper figures)

Pycroscopy - Scientific Advancements

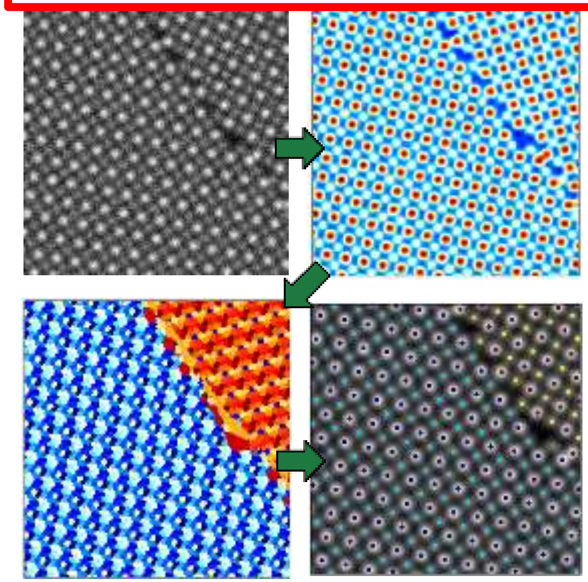
3,500x faster imaging via adaptive signal filtering, linear unmixing of signals



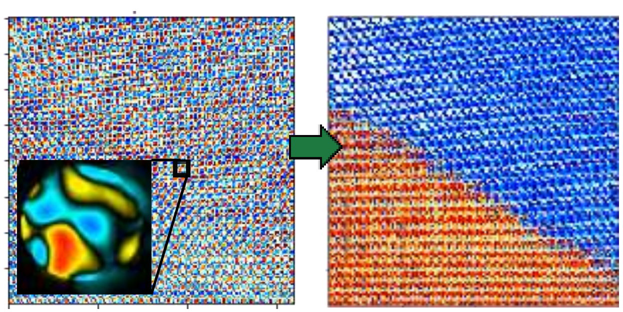
200x faster spectroscopy via Bayesian inference



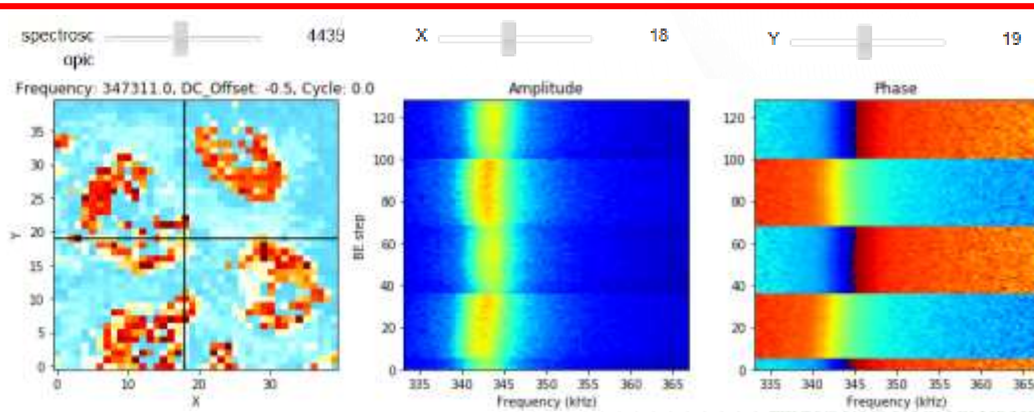
Separating uncorrelated data from correlated data to clean images



Identifying invisible patterns using multivariate analysis



Simplified navigation multidimensional data - users



Software Progression

Scaling up Computing:

2016
Single core

2017
Multi-core
Single CPU

2018
Multi-core
Multi CPU

2019
JupyterHub
On HPC

Emphasis always on ease-of-development instead of raw performance

New Scientific Domains:

Atomic Force Microscopy

+ Scanning Transmission Electron Microscopy

+ Mass Spectrometry
+ Bio-Chemistry

2016

2017

2018

2019

Thank you

Questions?

Suhas Somnath, somnaths@ornl.gov