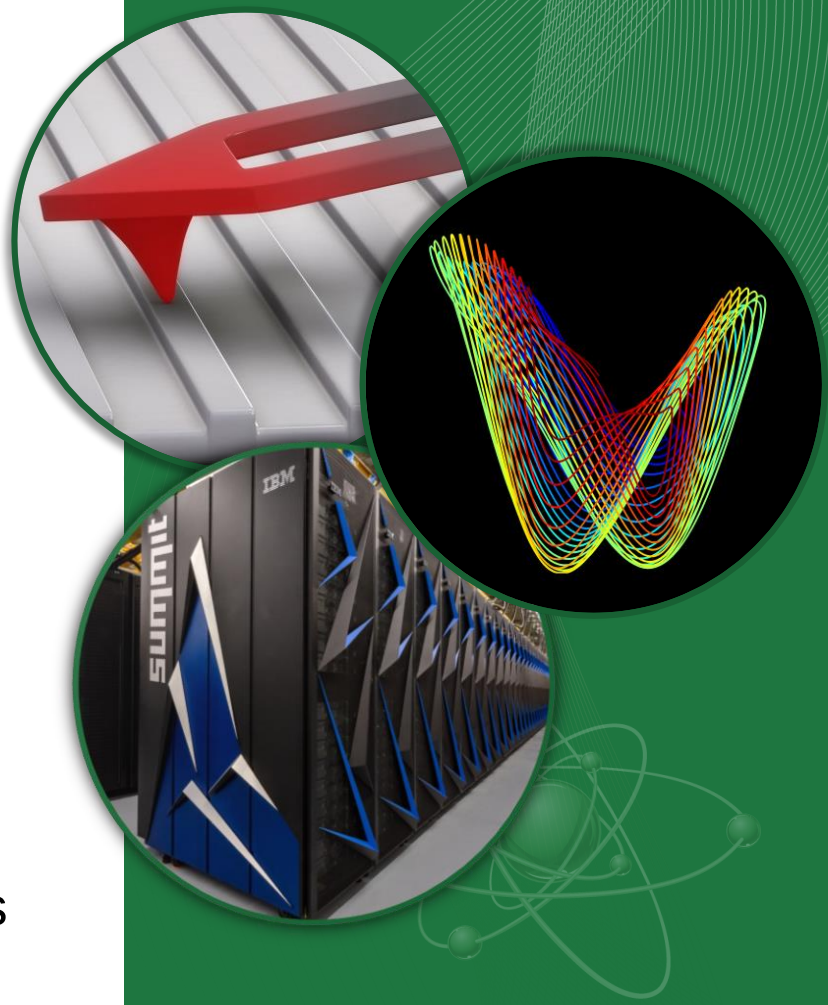
Scaling Data-Driven Scientific Discovery in the Big-Data Era –

A Data Lifecycle View

12/06/2018

Suhas Somnath

Advanced Data and Workflows Group
National Center for Computational Sciences



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ORNL is managed by UT-Battelle
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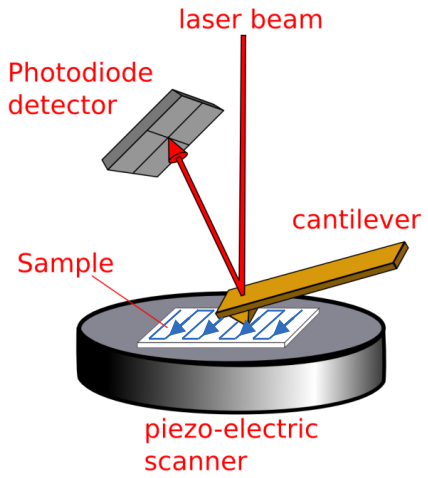
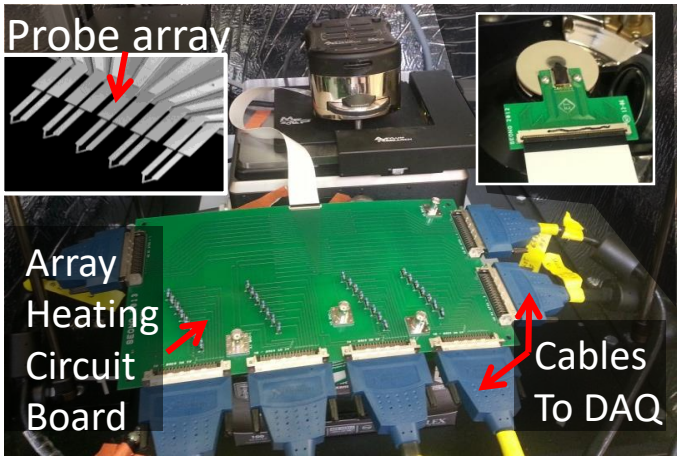
About me…

- PhD in Mechanical Engineering – University of Illinois @ Urbana-Champaign
- Postdoctoral Researcher at CNMS (2014 - 2017)
- Computer / Data Scientist at CCSD (2017 – Present)

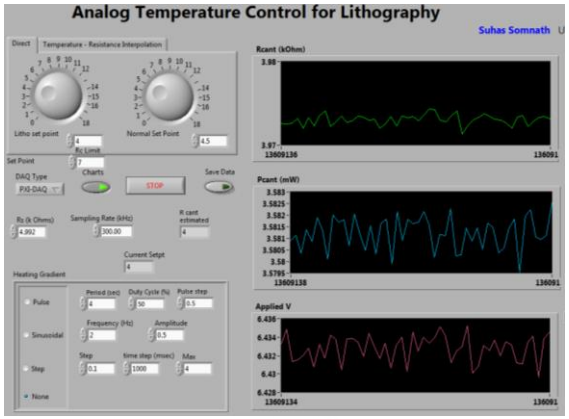
Atomic Force Microscopy



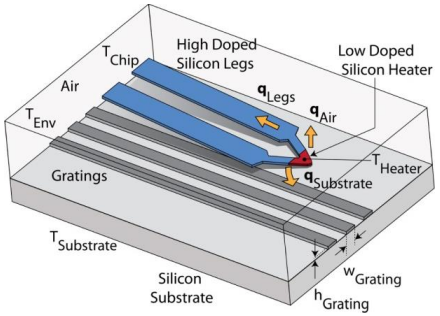
Instrument Development



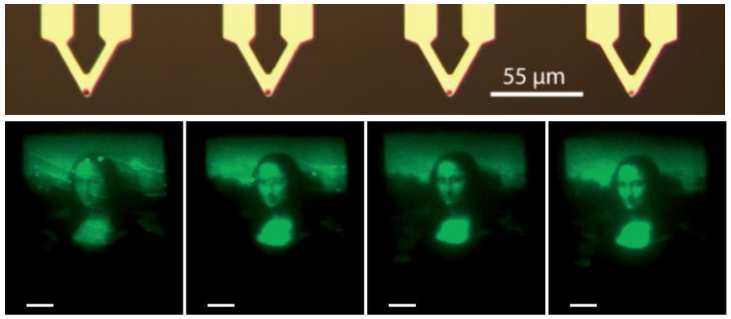
Instrumentation Software



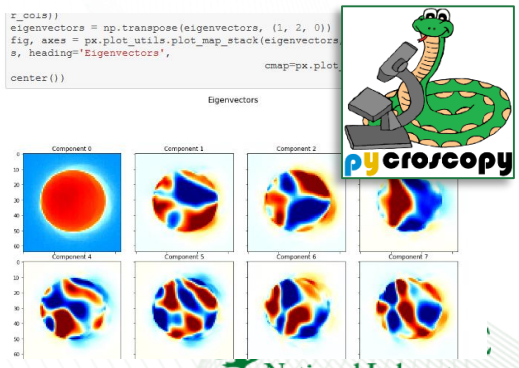
Simulation / Modeling



New measurement & manufacturing techniques

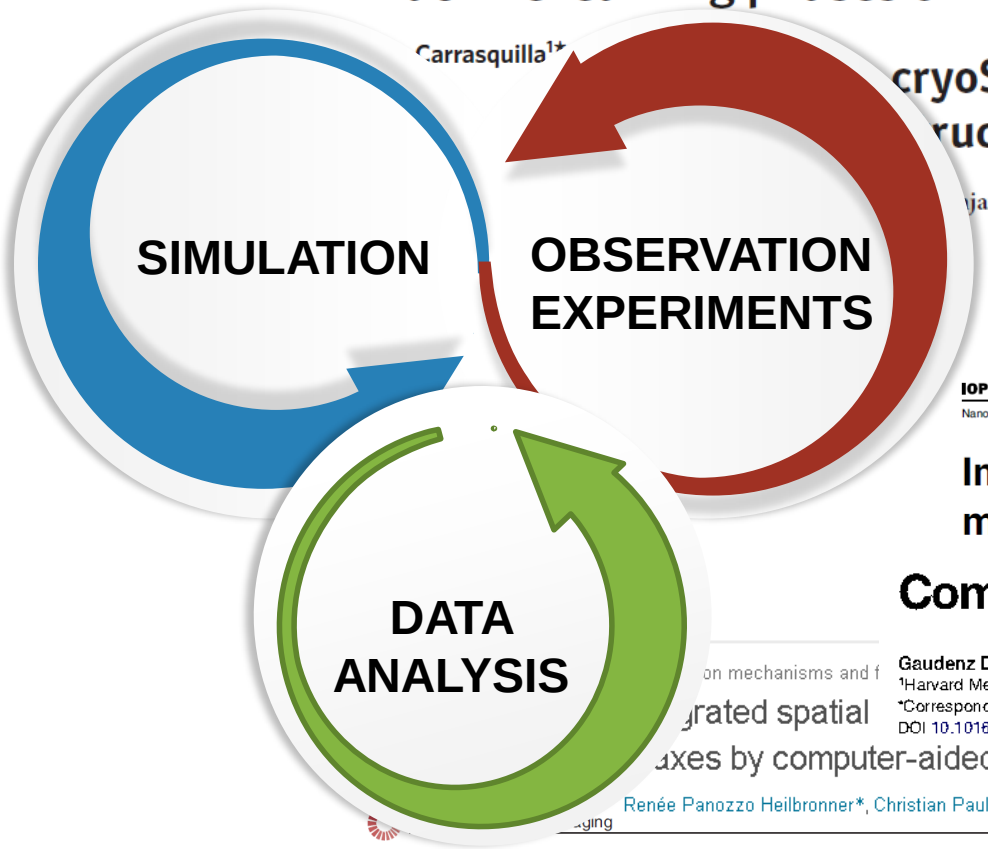


Data Analysis Software



National Laboratory

Paradigms of Scientific Discovery



nature physics

PUBLISHED

Deep Neural Networks Segment Neuronal Membranes in Electron Microscopy Images

Machine learning phases of matter

Carrasquilla[1]*

cryoSPARC: algorithms for rapid unsupervised cructure determination

jani[1], John L Rubinstein[2–4], David J Fleet[5] & Marcus A Brubaker[6]

Review

Review: Automatic Particle Detection in Electron Microscopy

IOP Publishing

Nanotechnology 27 (2016) 3740

William V. Nicholson[a], Robert M. Glaeser[a, b, c]

Imaging nanoscale lattice variations by machine learning of x-ray diffraction

Computer Vision in Cell Biology

Gaudenz Danuser[1,*]

[1]Harvard Medical School, 240 Longwood Avenue, Boston, MA 02140, USA

*Correspondence: gaudenz_danuser@hms.harvard.edu

DOI 10.1016/j.cell.2011.11.001

Bioinformatics, 32, 2016, i52–i59

doi: 10.1093/bioinformatics/btw252

ISMB 2016

on mechanisms and f

grated spatial

axes by computer-aided mic

Renée Panozzo Heilbronner*, Christian Pauli

Classifying and segmenting microscopy images with deep multiple instance learning

Oren Z. Kraus,[1, 2,*] Jimmy Lei Ba[1] and Brendan J. Frey[1,2]

[1]Department of Electrical and Computer Engineering, University of Toronto, Toronto, M5S 2E4, Canada and [2]The Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, M5S 3E1, Canada

Machine learning in cell biology – teaching com to recognize phenotypes

Christoph Sommer and Daniel W. Gerlich*

Institute of Molecular Biotechnology of the Austrian Academy of Sciences (IMBA), 1030 Vienna, Austria

*Author for correspondence (daniel.gerlich@imba.oeaw.ac.at)

Journal of Cell Science 126, 5529–5539

© 2013. Published by The Company of Biologists Ltd

doi: 10.1242/jcs.123604

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Facilitating Data Driven Science

Only possible with

LARGE VOLUMES

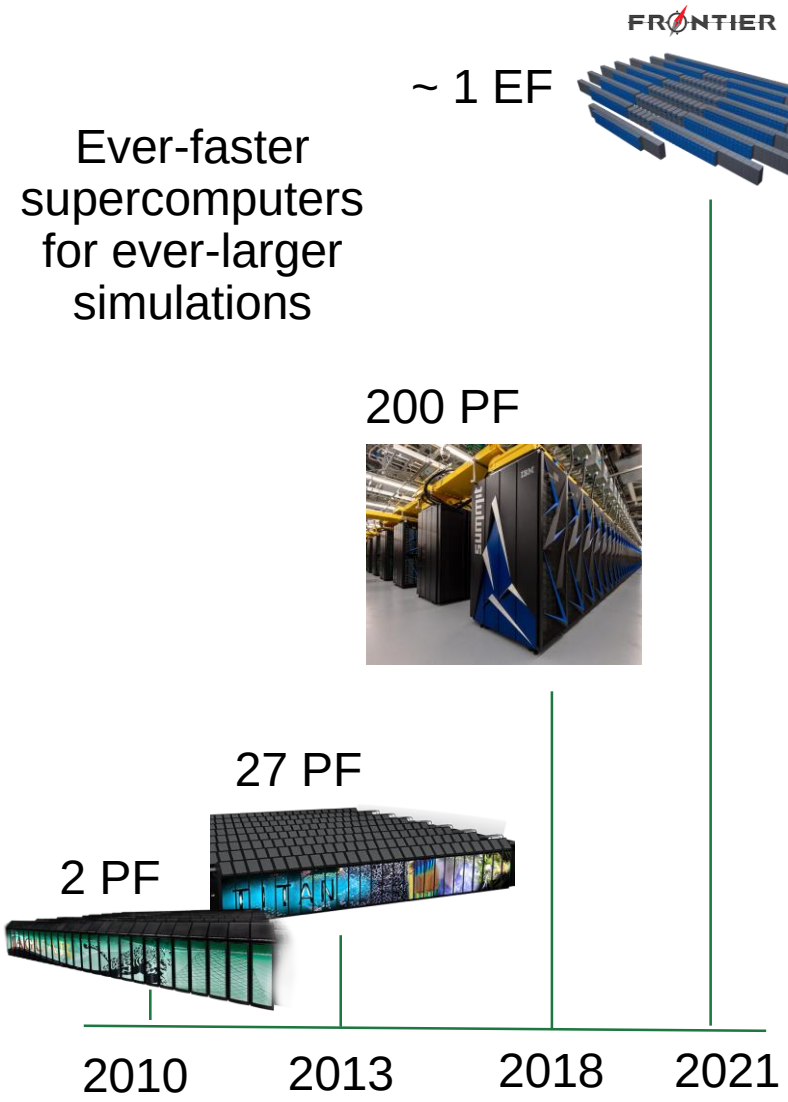
of

WELL CURATED

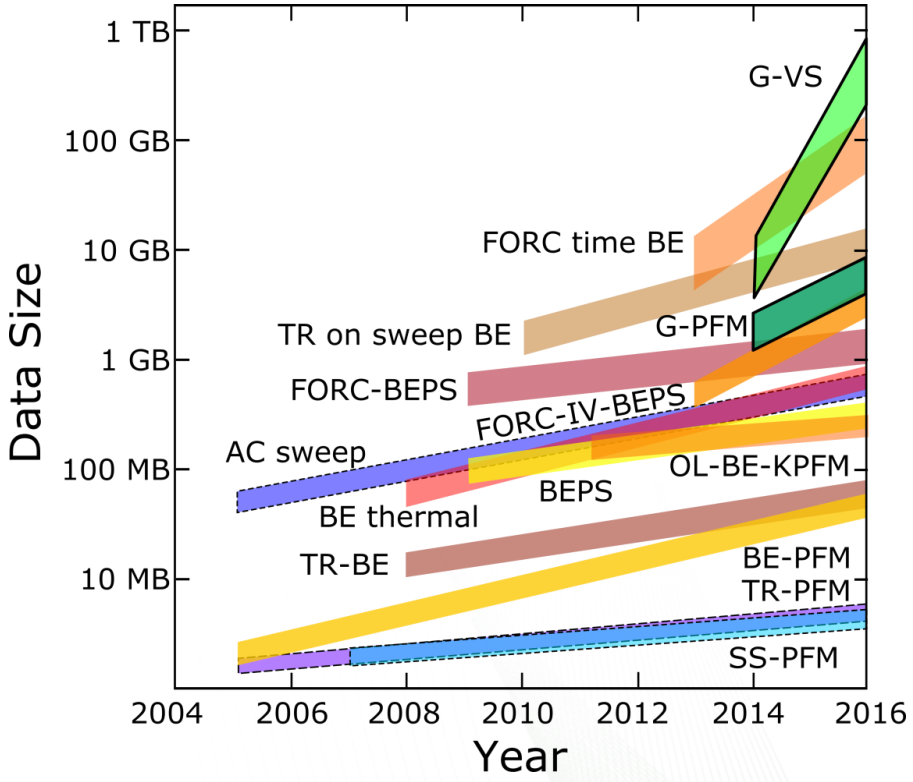
data

Explosion in Data Volumes

Ever-faster supercomputers for ever-larger simulations

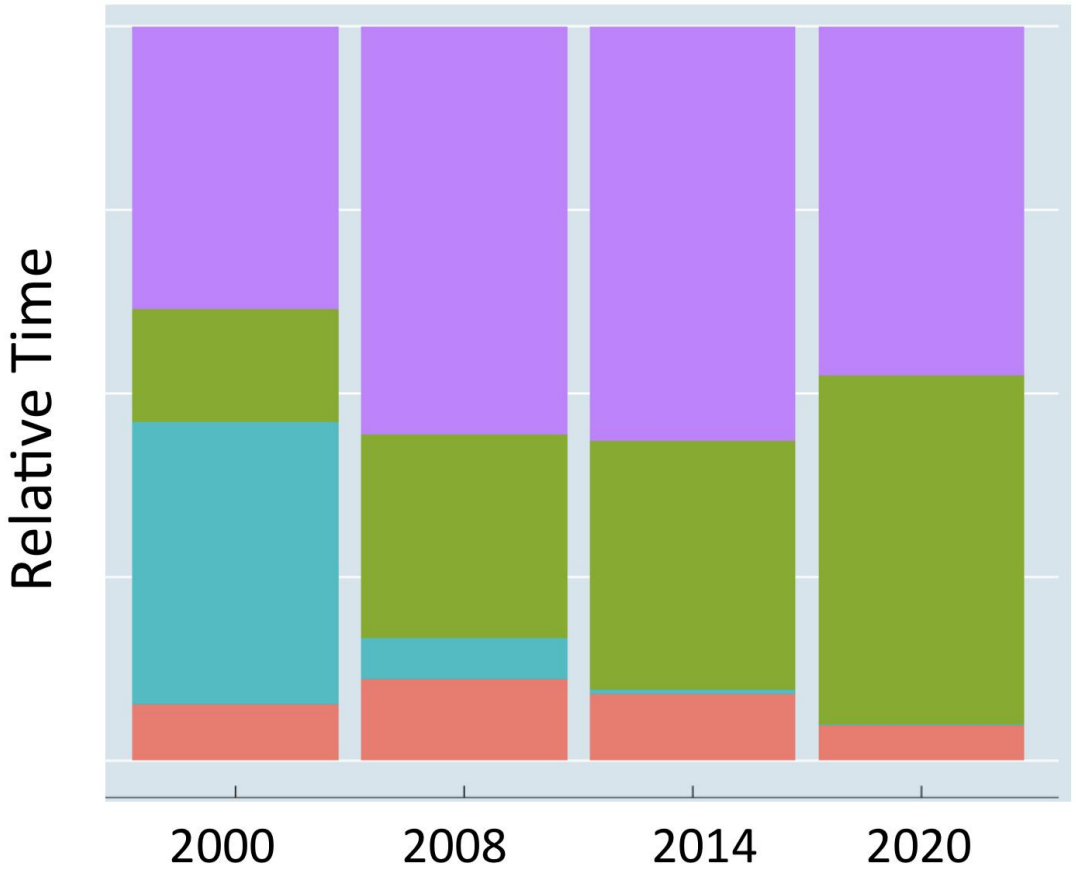


Evolution of Scanning Probe Microscopy Data



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

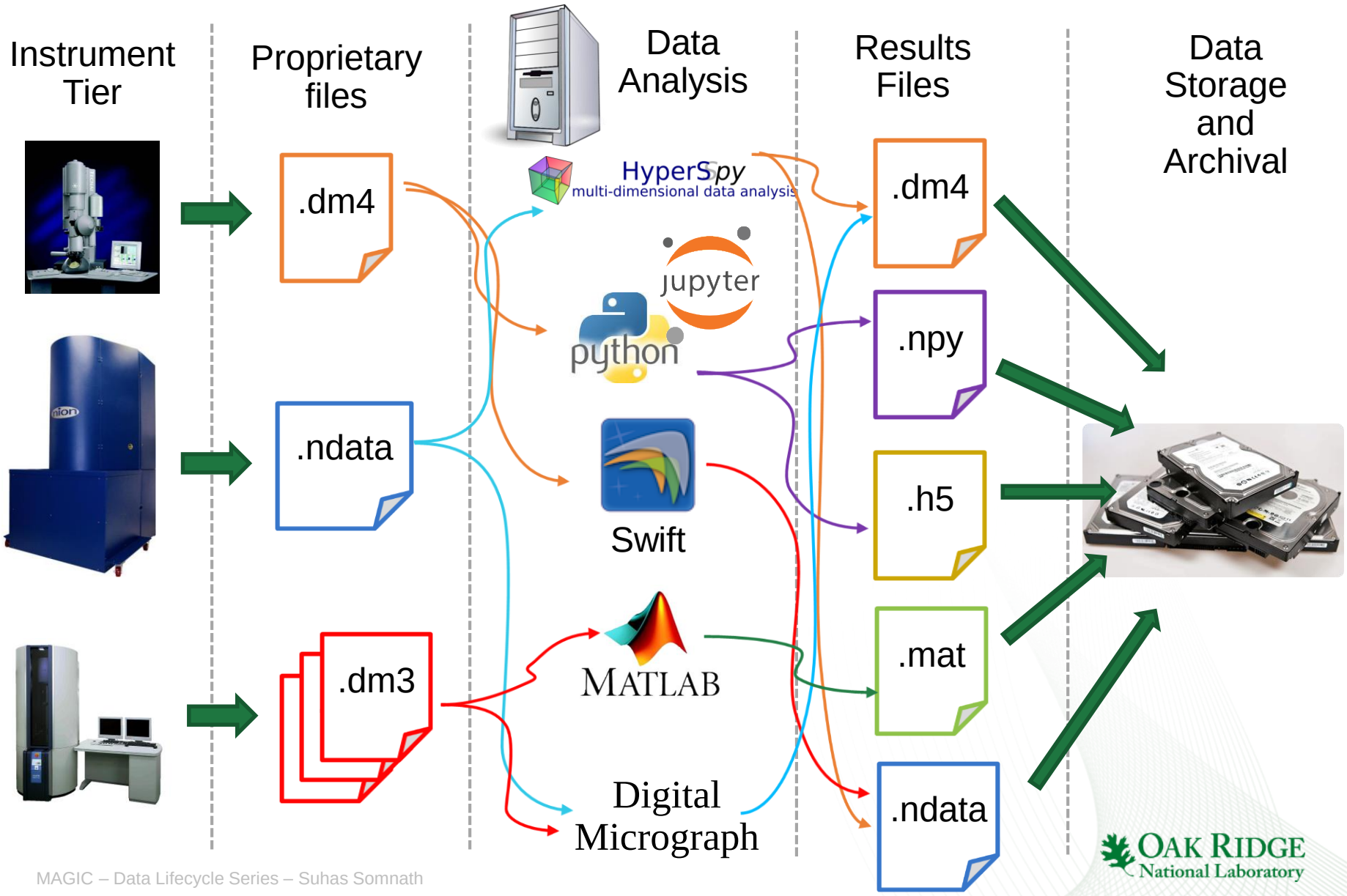
Data Management & Processing are Dominant



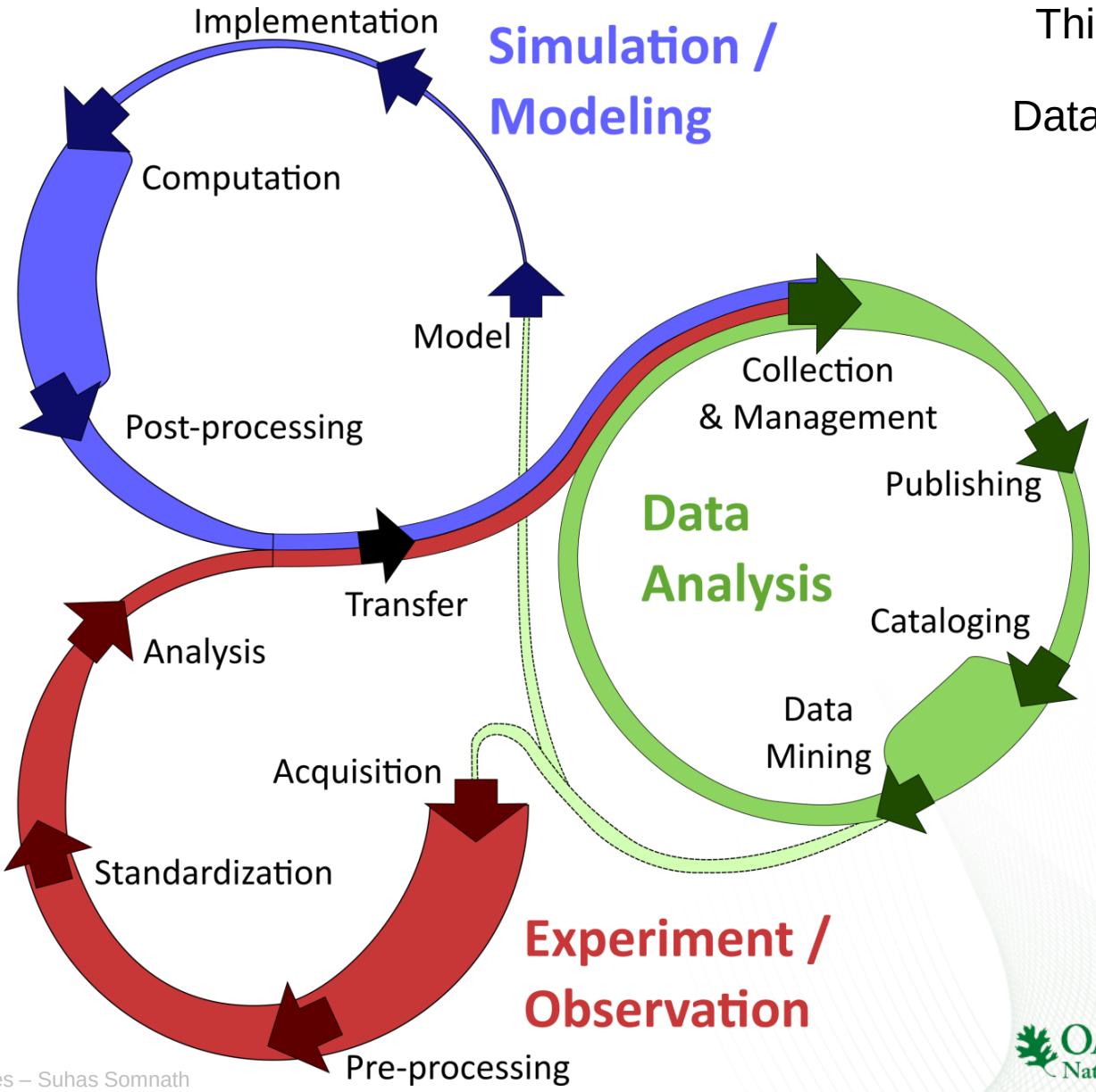
* at light sources

Figure from Kevin Mader
https://rawgit.com/4Quant/SRI2015/master/SRIPres.html#/

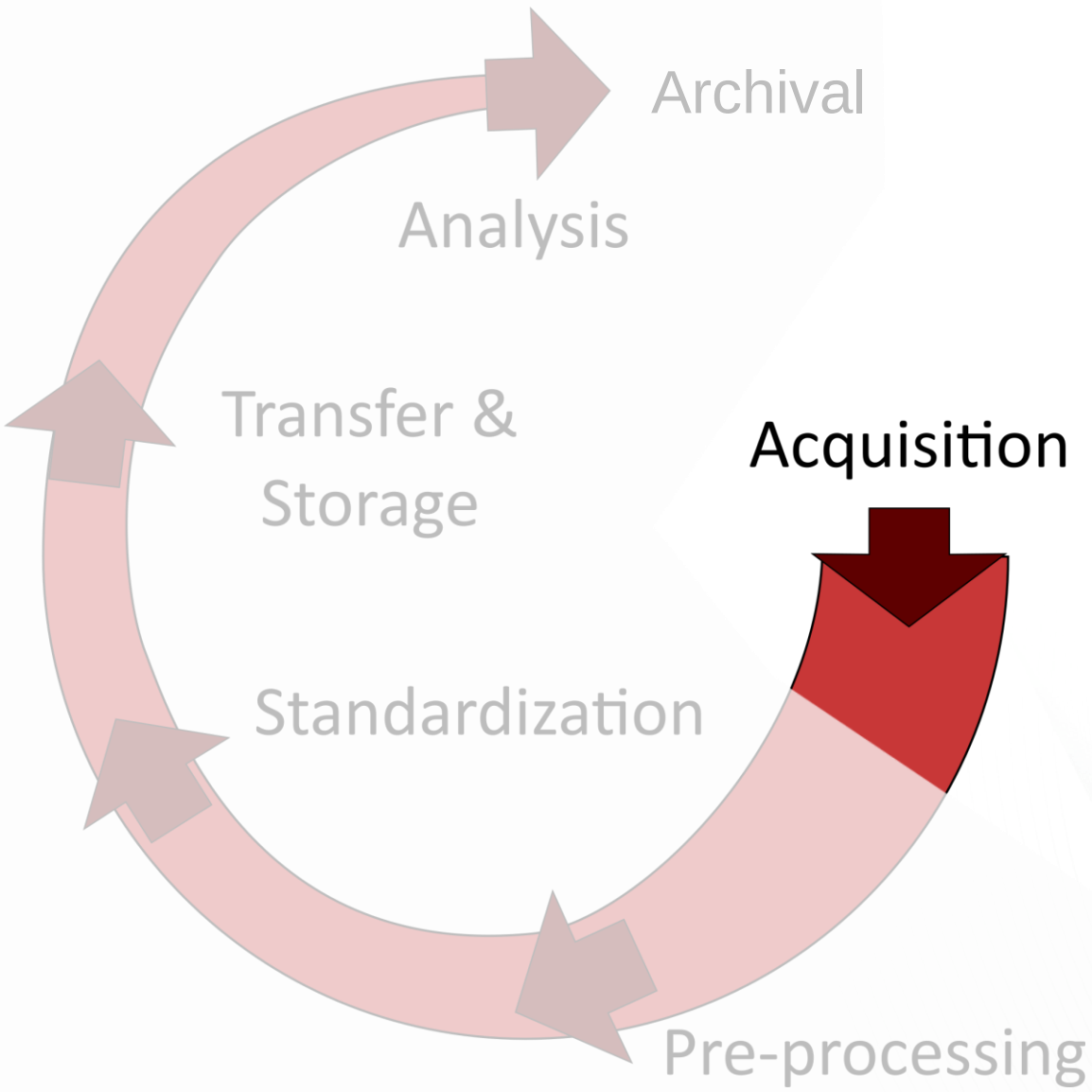
Current Data Life-Cycle in Experimental Facilities



Data Lifecycle



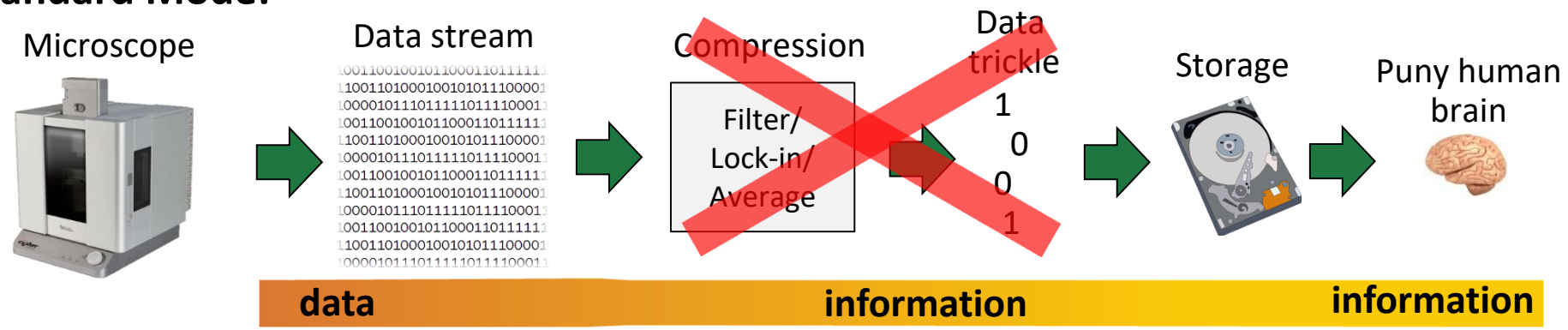
Data Lifecycle



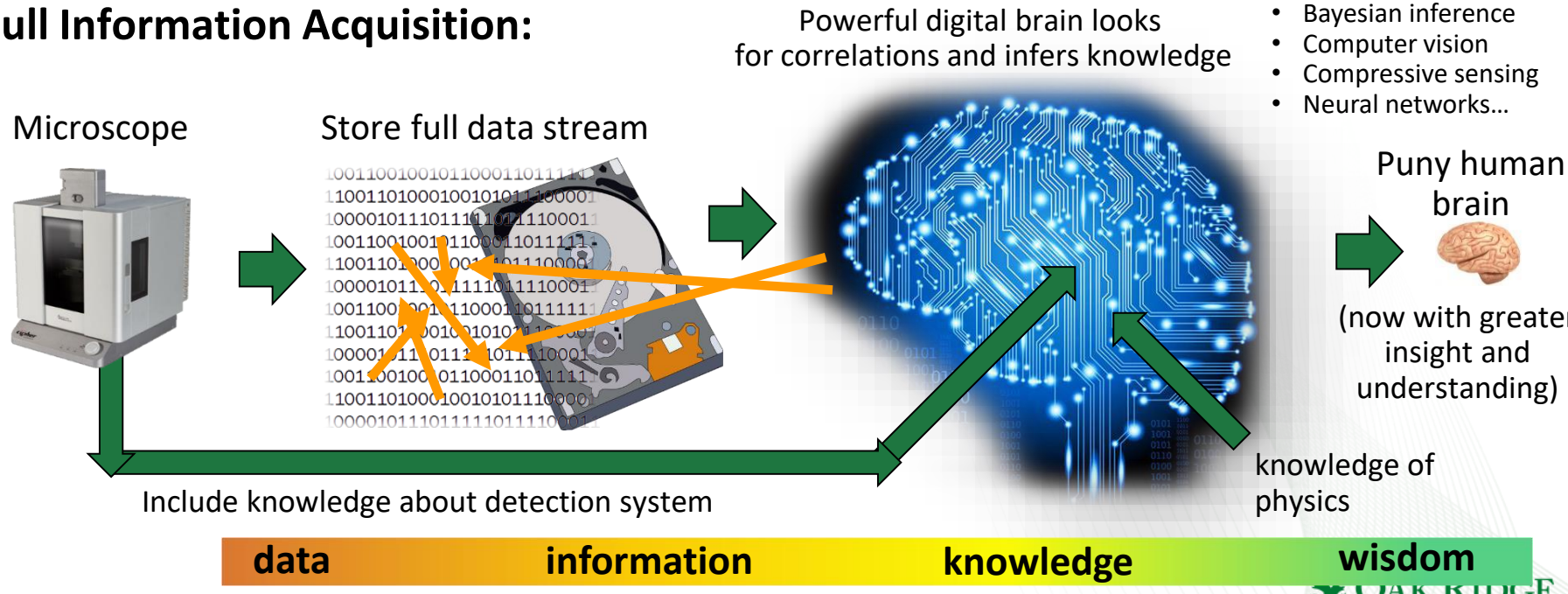
Thickness
=
Data volume

Big Data & Information Transfer in Microscopy

Standard Mode:

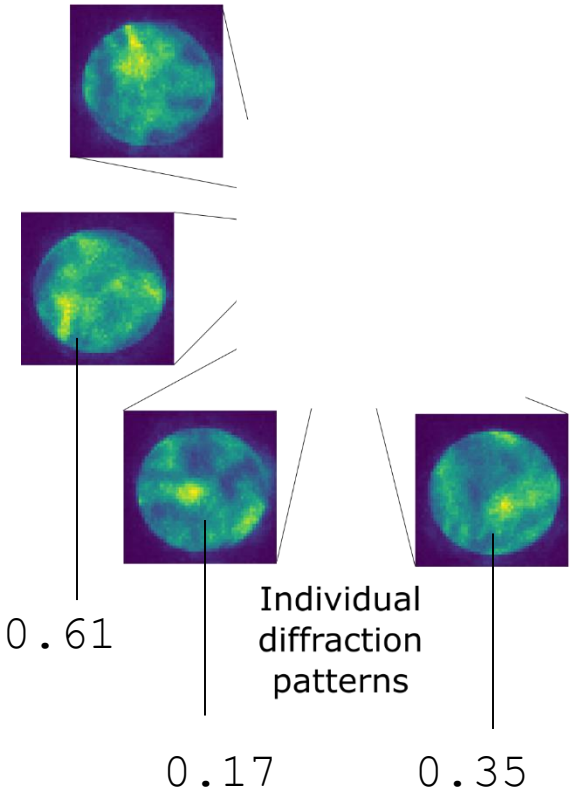


Full Information Acquisition:



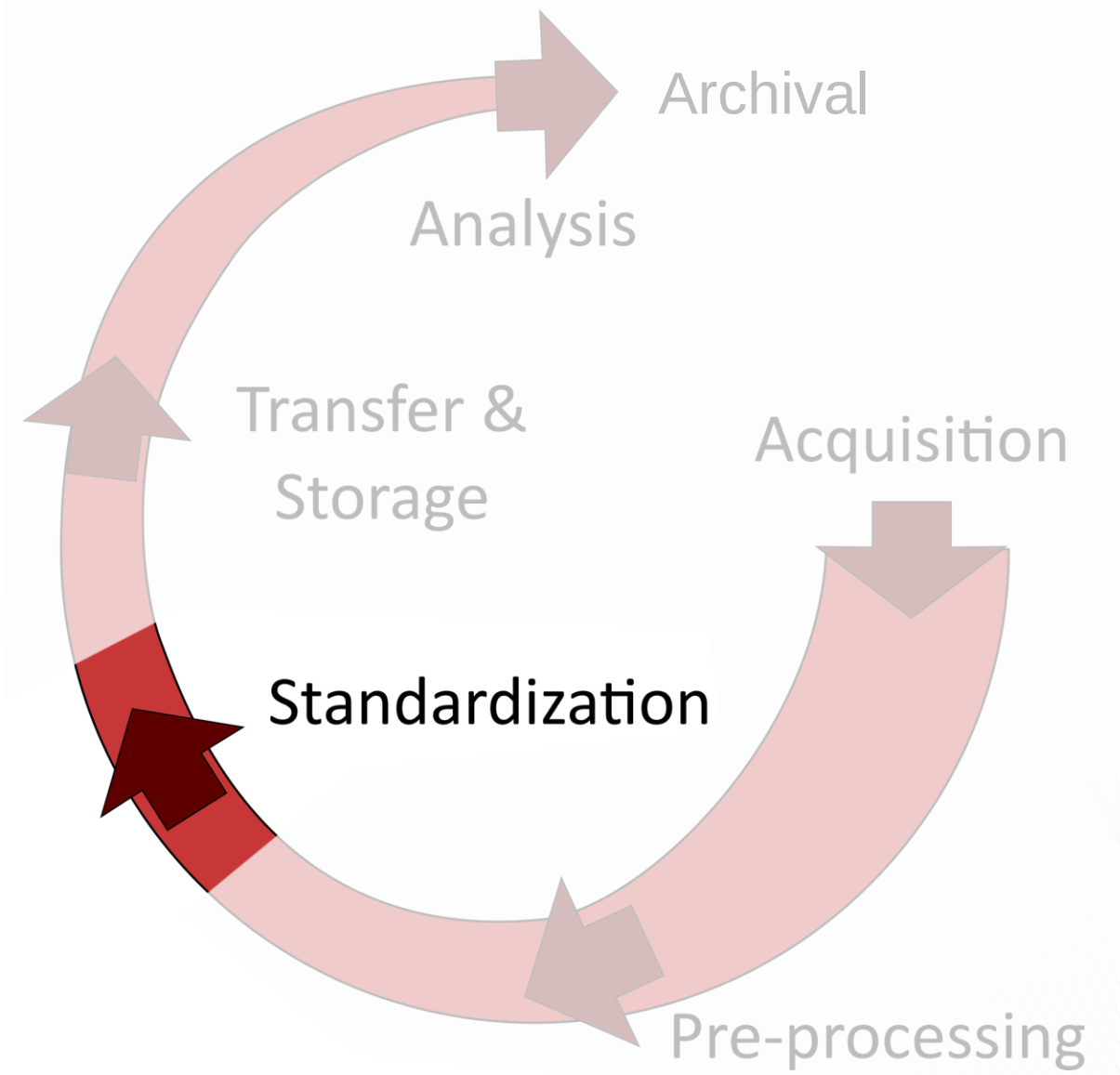
(full) information Acquisition in 4D STEM

Multivariate statistical analysis techniques applied the raw 4D Scanning Transmission Electron Microscopy (STEM) data



Jesse et. al., *Scientific Reports*, 2015

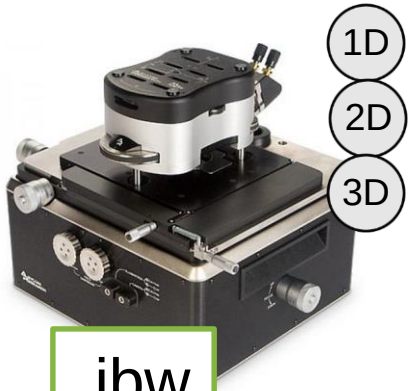
Data Lifecycle



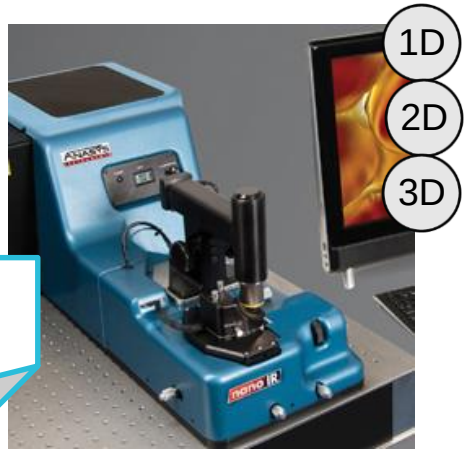
Thickness
=
Data volume

Multitude of File Formats & Data Types

.wdf



.ibw

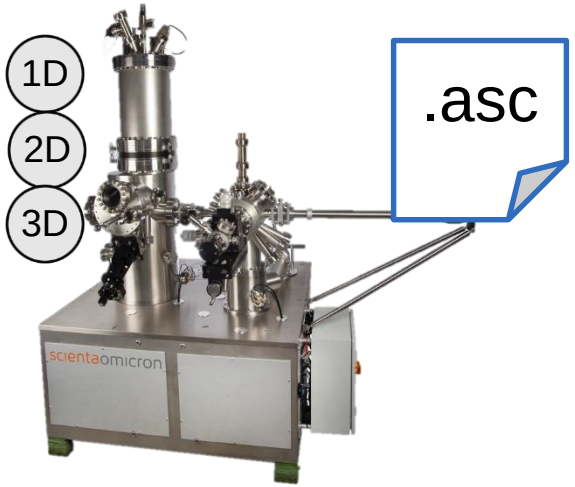


.cdb

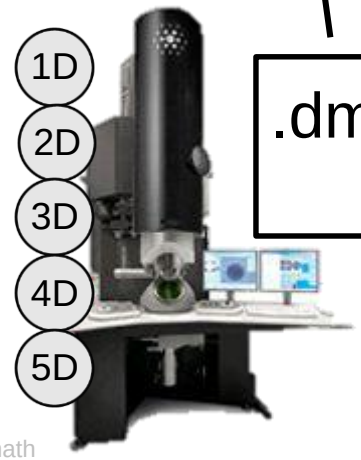
- Proprietary
- Incompatible
- Format-dependent algorithms

≠

- Not suitable for:
  - Sharing
  - Archival



.asc



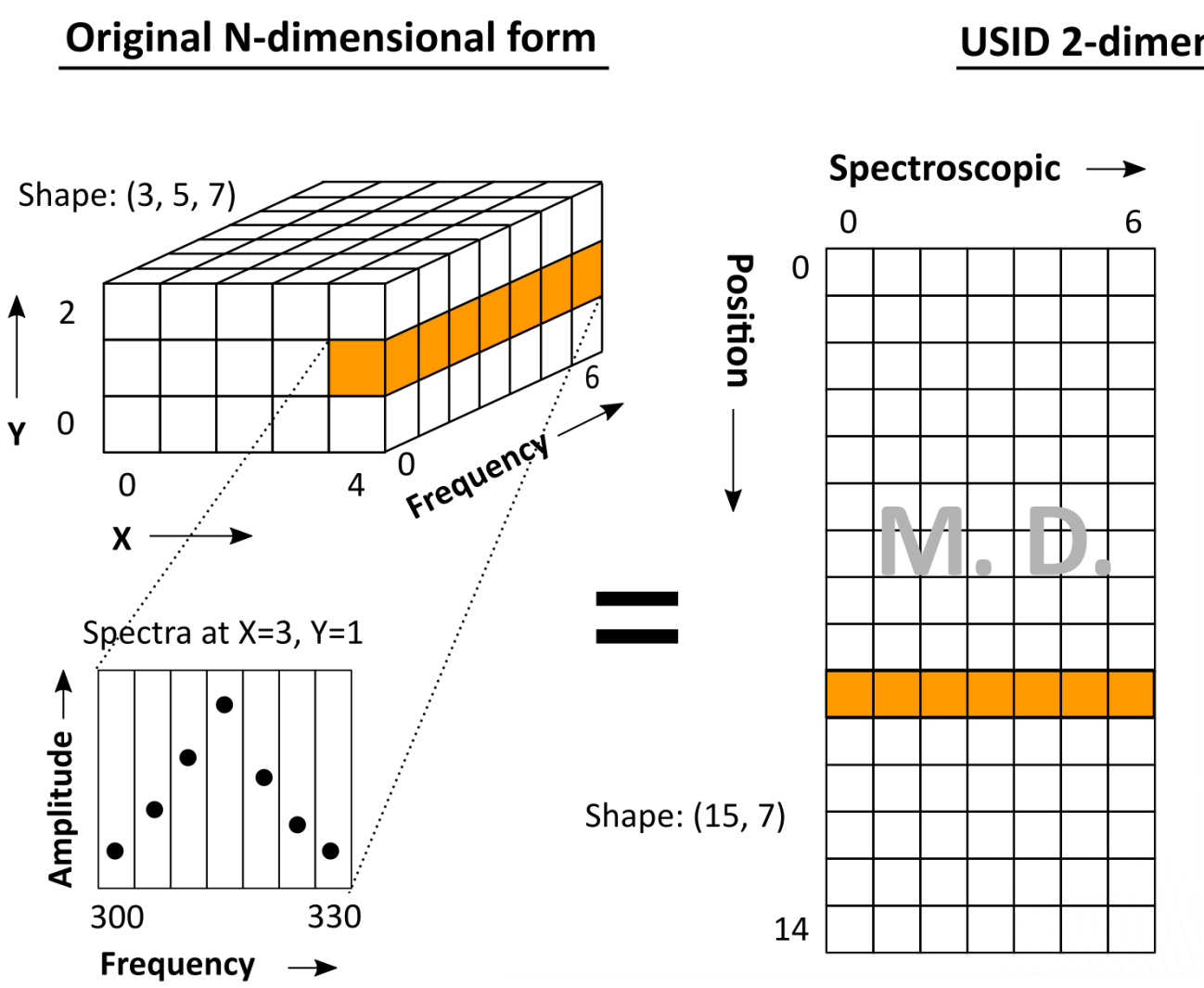
.dm3

.mat

Open Data Models and File Formats

- Collective (industry, academia, journals, funding agencies) agreement and enforcement
- Data Model – Abstract representation of data
- File Format – XML, TXT, HDF5, …
- FAIR data principles – Findable, Accessible, Interoperable, Reusable
- Cohesive community, towards reproducible science
- Many communities already have open standards
  - Climate – NetCDF
  - X-ray / Neutron facilities – NeXus
  - Biological Imaging – OME-TIFF, OME-XML …

Universal Spectroscopic and Imaging Data (USID)

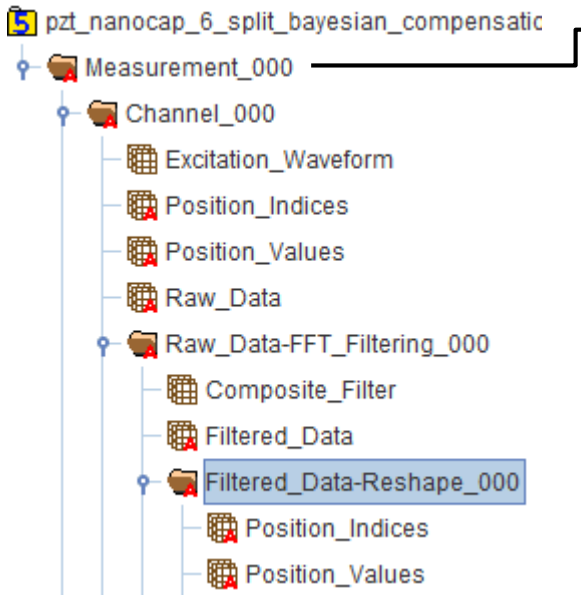


Quantity: Amplitude

Units: V

Hierarchical Data Format (HDF5)

‘File system within file’



Metadata

```
Measurement_000 (2088, 4)
   Group size = 1
   Number of attributes = 43
      BE_actual_scan_time_[s] = 0.004
      BE_amplitude_[V] = 4
      BE_auto_smoothing = auto smoothing on
      BE_band_edge_trim = 0.14614
      BE_band_smoothing_[Hz] = 2560.5
      BE_band_width_[Hz] = 60000
      BE_bins_per_band = 0
      BE_center_frequency_[Hz] = 370000
      BE_phase_variation = 1
      BE_points_per_BE_wave = 0
      BE_repeats = 8
      BE_signal_type = chirp-sinc hybrid
      BE_time/pixel_[s] = 0.004
      File_date_and_time = 06-Feb-2015 11:46
      File_file_name = BELine
```

NeXus

.mat

MATLAB

netCDF

GEMINI OBSERVATORY

- Open, free
- Easily accessible – C, C++, python, Java, …
- Parallel read / write, HPC & cloud compatible
- Already de-facto standard in many communities
- Facilitates provenance tracking and reproducibility

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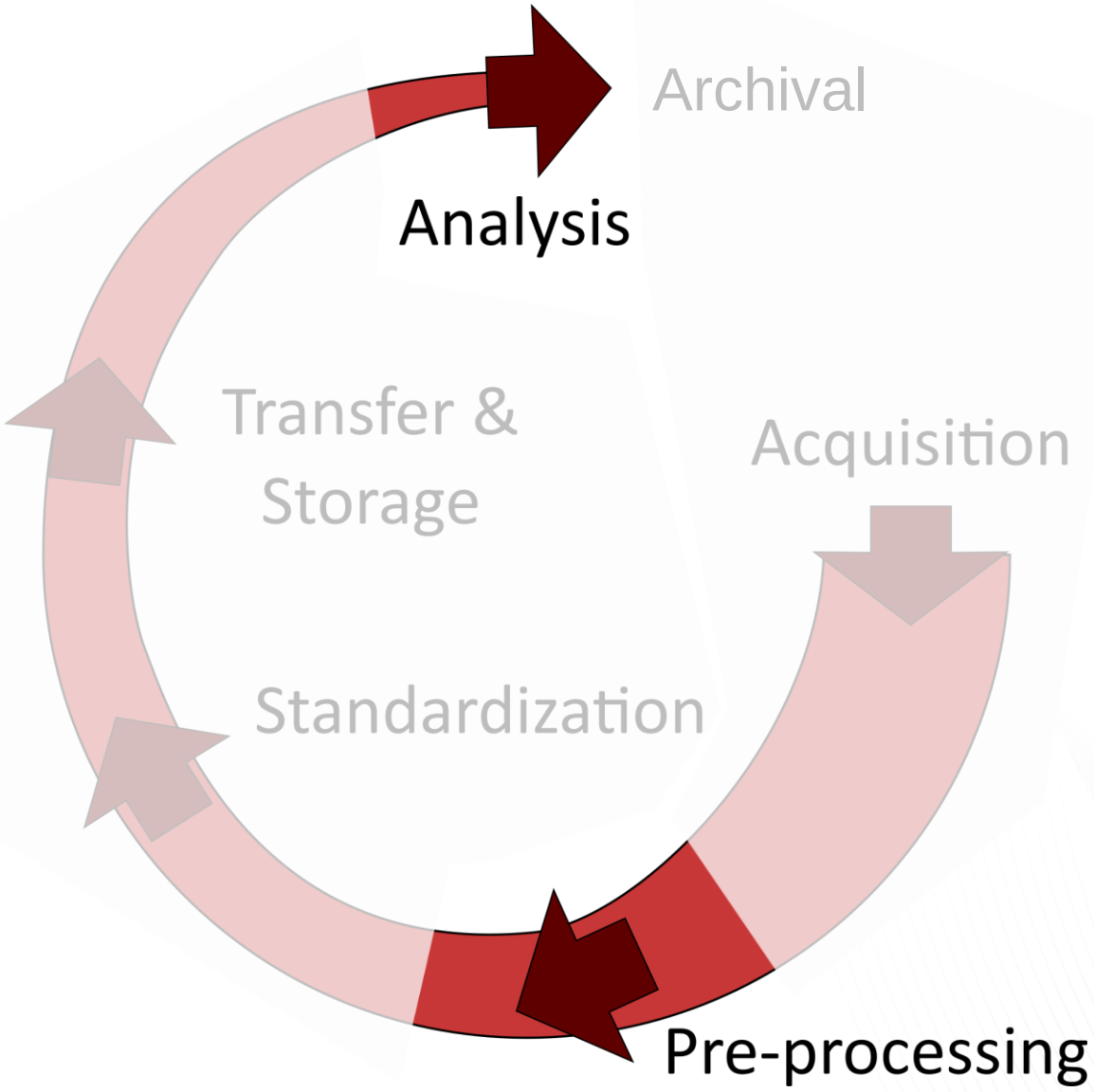
Data Lifecycle



Thickness
=
Data volume

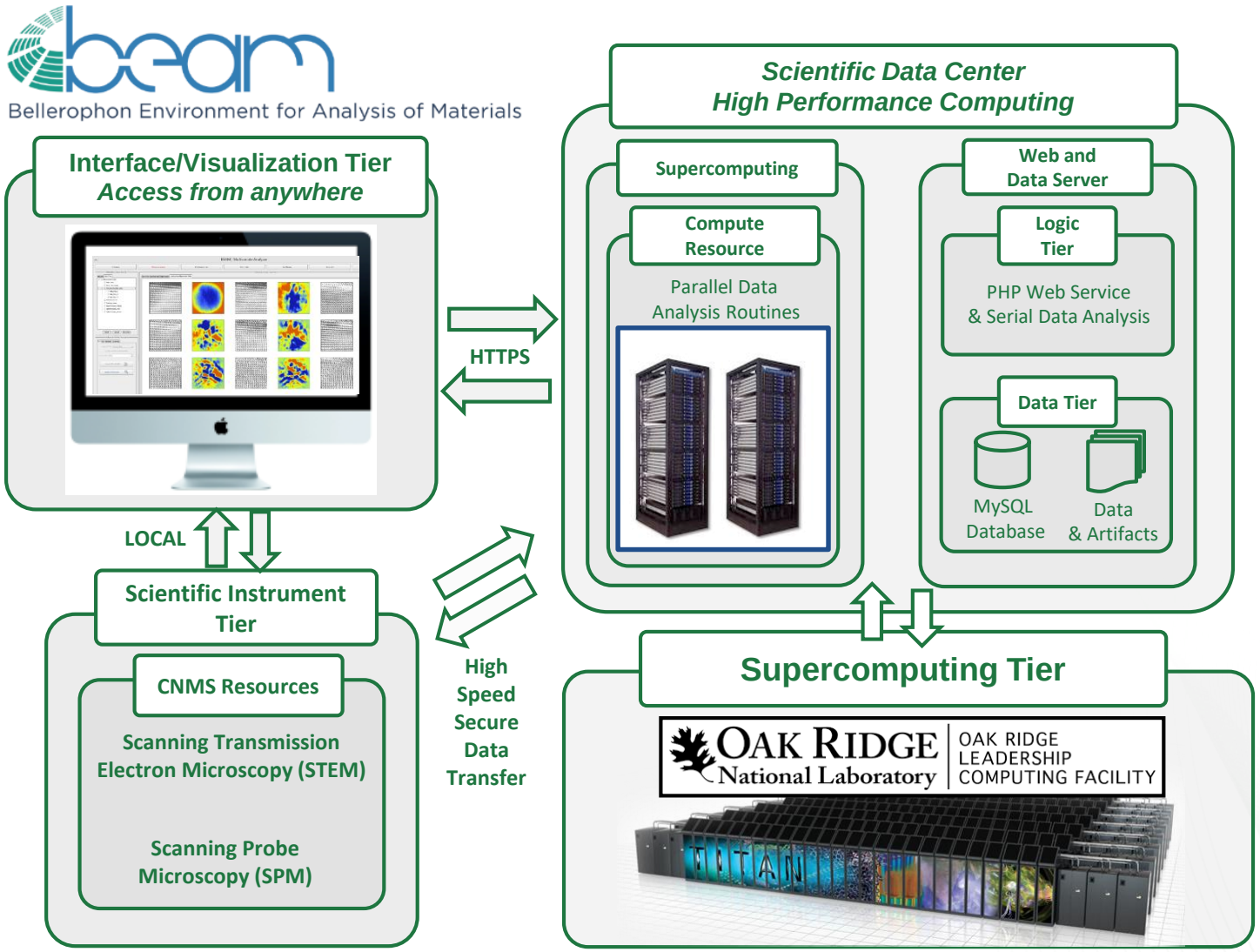
Challenges with Scientific Software

- Proprietary software
  - Closed-source
  - Typically inadequate / not possible to expand features
  - Not portable beyond instrument computer
  - Not scalable beyond a few cores on one node
  - Expensive licenses
- Users
  - Do not have access to software
  - Typically not comfortable with scripting / programming
  - Training on software / user-friendliness

Two-prong (inverse) Software Strategy

Mode	Exploratory / Development	Production
Compute Resource	Instrument-local Workstation  Cloud compute 	High-performance computing cluster 
Who?	Domain scientists	Collaboration with computational facility
Algorithms	Simpler but approximate	Complex but accurate

Instrument-to-HPC Workflows



Many other examples:

- Xi-CAM & CAM-link (LBL)
- ADARA (ORNL)
- Triquetrum
- …

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

Python for Scientific Research

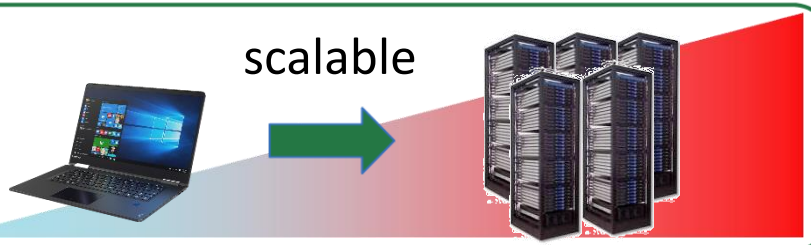
Very easy to learn + code

Numerous, **powerful** libraries for science

scikit learn

NumPy

SciPy



Scripts to cohesive, collaborative packages

Interoperability with other languages

open source™

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

Cross-platform

MacOS™

All for a princely sum of …. **$0!**

The Astropy Project

sunpy
A Community Python Library for Solar Physics

biopython

NIPY

pycroscopy

See Jake Vanderplas' Pycon 2017 Keynote talk:
http://www.youtube.com/watch?v=ZyjCqQEUa8o&t=19m20s

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Towards Open & Reproducible Science

Aim – ALL scientific journal papers accompanied with:

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

Jupyter notebook associated with paper

Visualizing Filtering Results

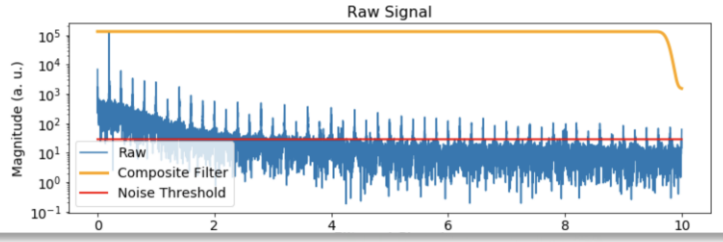
Run the next cell to see what the IV curves look like for the chosen filter parameters. If the current set of filter parameters do not work as well, change the parameters in the previous cell and try again.

Once the results look good, proceed to filter the entire dataset

In [7]:
```
# Test filter on a single line:
row_ind = 50
filt_line, fig_filt, axes_filt = px.processing.gmode_utils.test_filter(h5_main[row_ind], filte
r_parms, samp_rate,
                                                                       show_plots=True, use_rai
nbow_plots=False)
fig_filt.savefig(os.path.join(other_figures_folder, 'FFT_filter_on_line_{}.png'.format(row_ind
)), format='png', dpi=300)

raw_row = np.reshape(h5_main[row_ind], (-1, pts_per_cycle))
filt_row = filt_line.reshape(-1, pts_per_cycle)

fig, axes = px.plot_utils.plot_loops(single_AO, [raw_row, filt_row], dataset_names=['Raw', 'Fi
ltered'],
                                     line_colors=['r', 'b'], x_label='Bias (V)', title='FFT Fi
ltering',
                                     plots_on_side=3, y_label='Current (nA)',
                                     subtitles='Row: ' + str(row_ind) + ' Col:')
fig.savefig(os.path.join(other_figures_folder, 'Example_filtered_loops_from_line_{}.png'.forma
t(row_ind)), format='png', dpi=300)
```



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)

Oak Ridge National Laboratory
Leadership Computing Facility

10.13139/OLCF/1410993

Download

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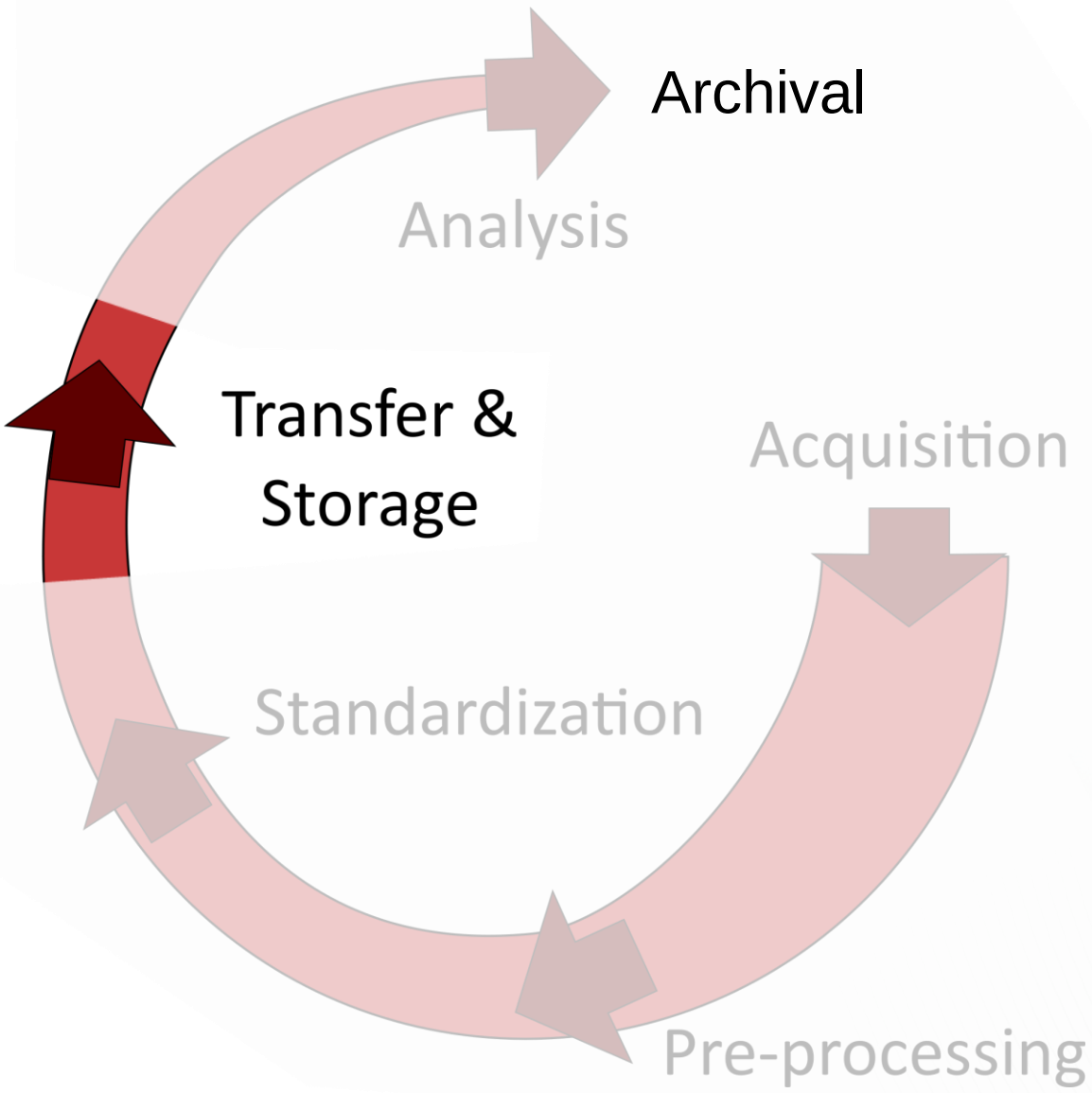
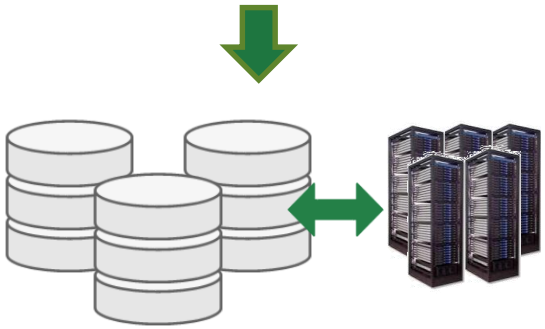
Data Lifecycle



Thickness
=
Data volume

Where should data live?

- Centralized repository
- Failure-resistant, redundant-backup
- **Close to compute** resource(s)
- Old / rarely used data can be archived (e.g. tape)



Archival

Storage Space

Access to Compute

Data Transfer to Centralized Repository

Instrument

Instrument

Instrument

Simple, reliable, fast, transfers for large files

Cloud Compute

globus server

globus server

Network Attached Storage

+

Data Transfer Node* (DTN)

Dedicated fiber line

HPC

Hybrid

SSD

HDD

Speed

PCIe NVME SSD

* Image is not of an actual DTN

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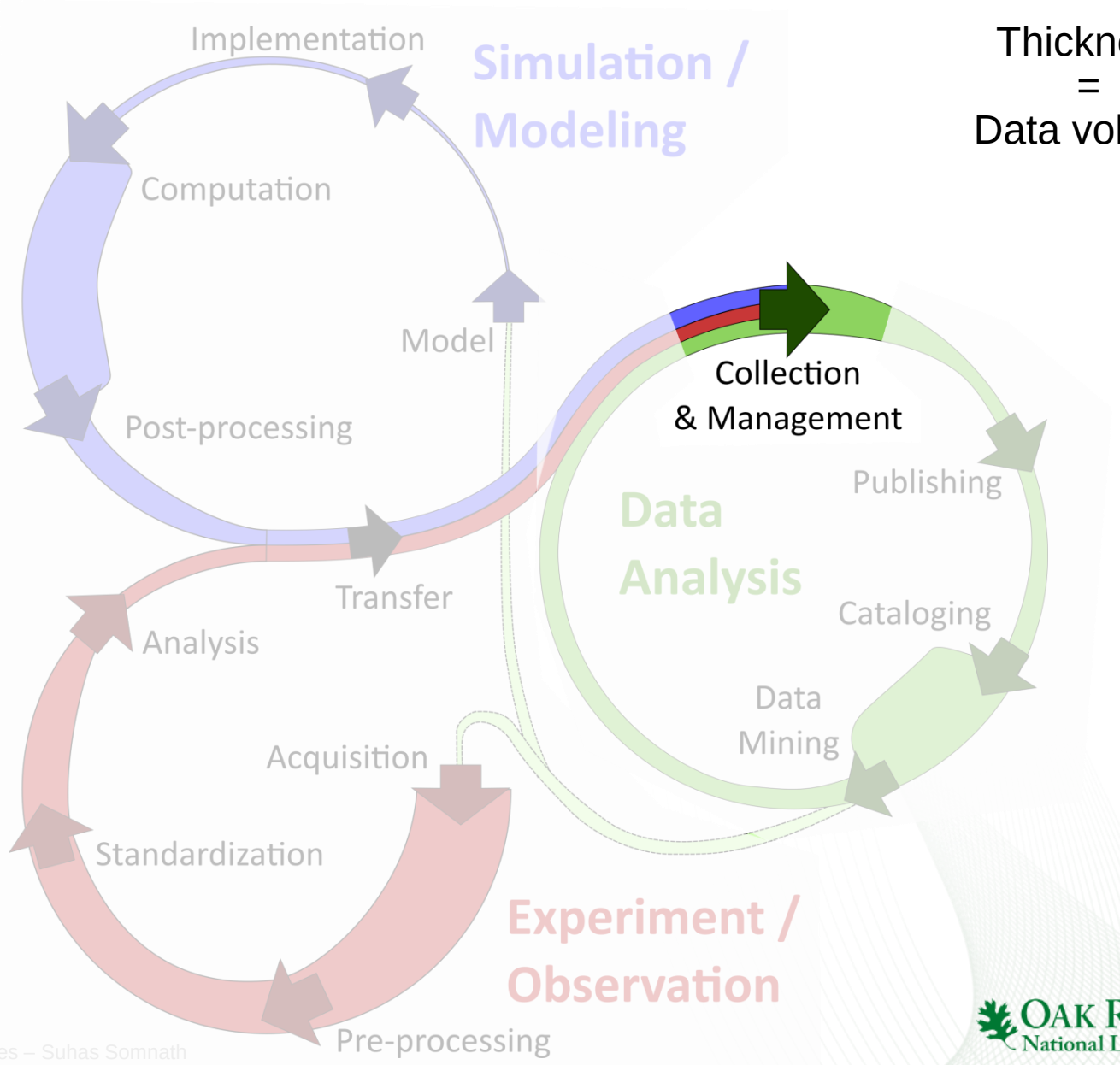
Scalable Data Efforts at ORNL

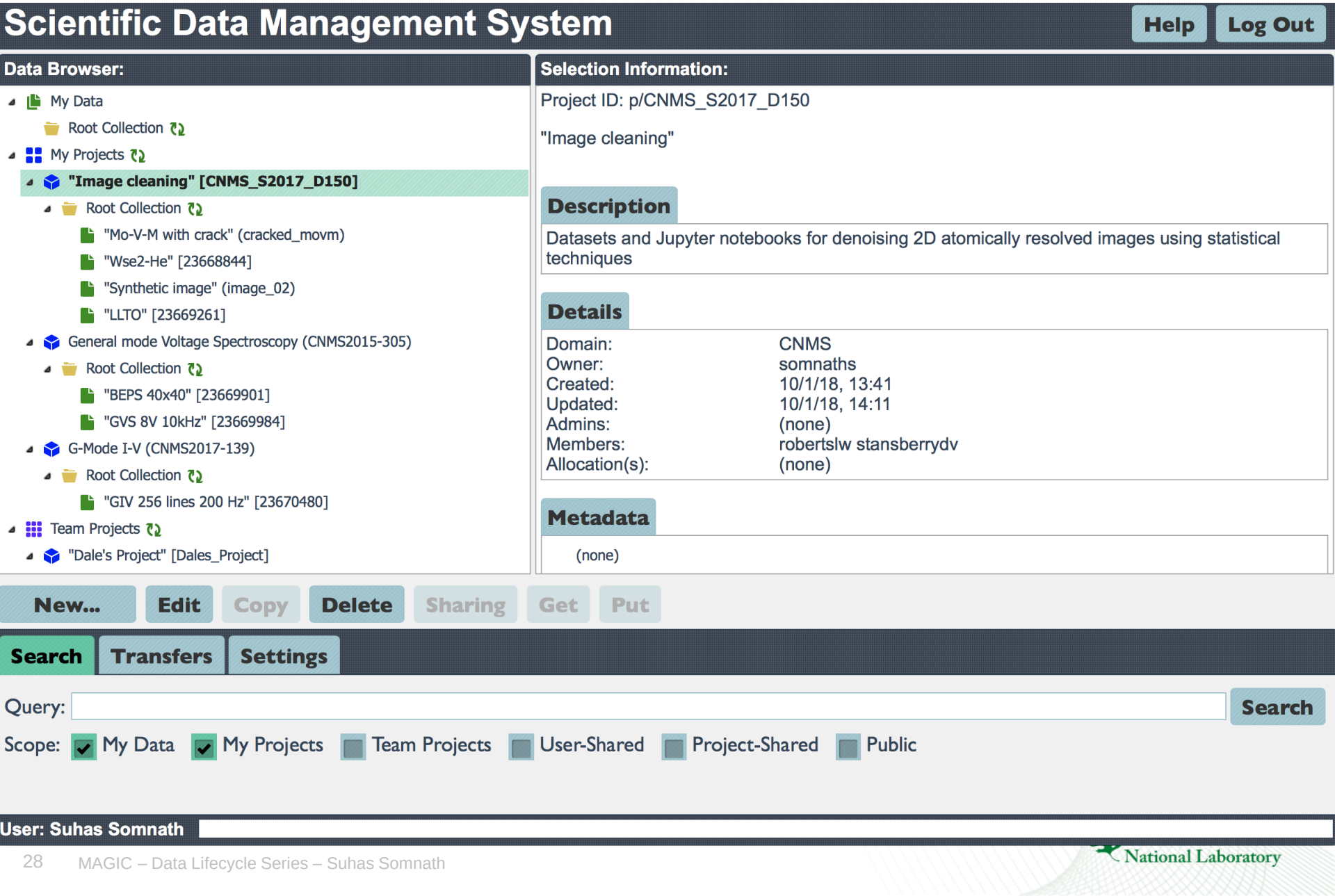


Thickness
=
Data volume

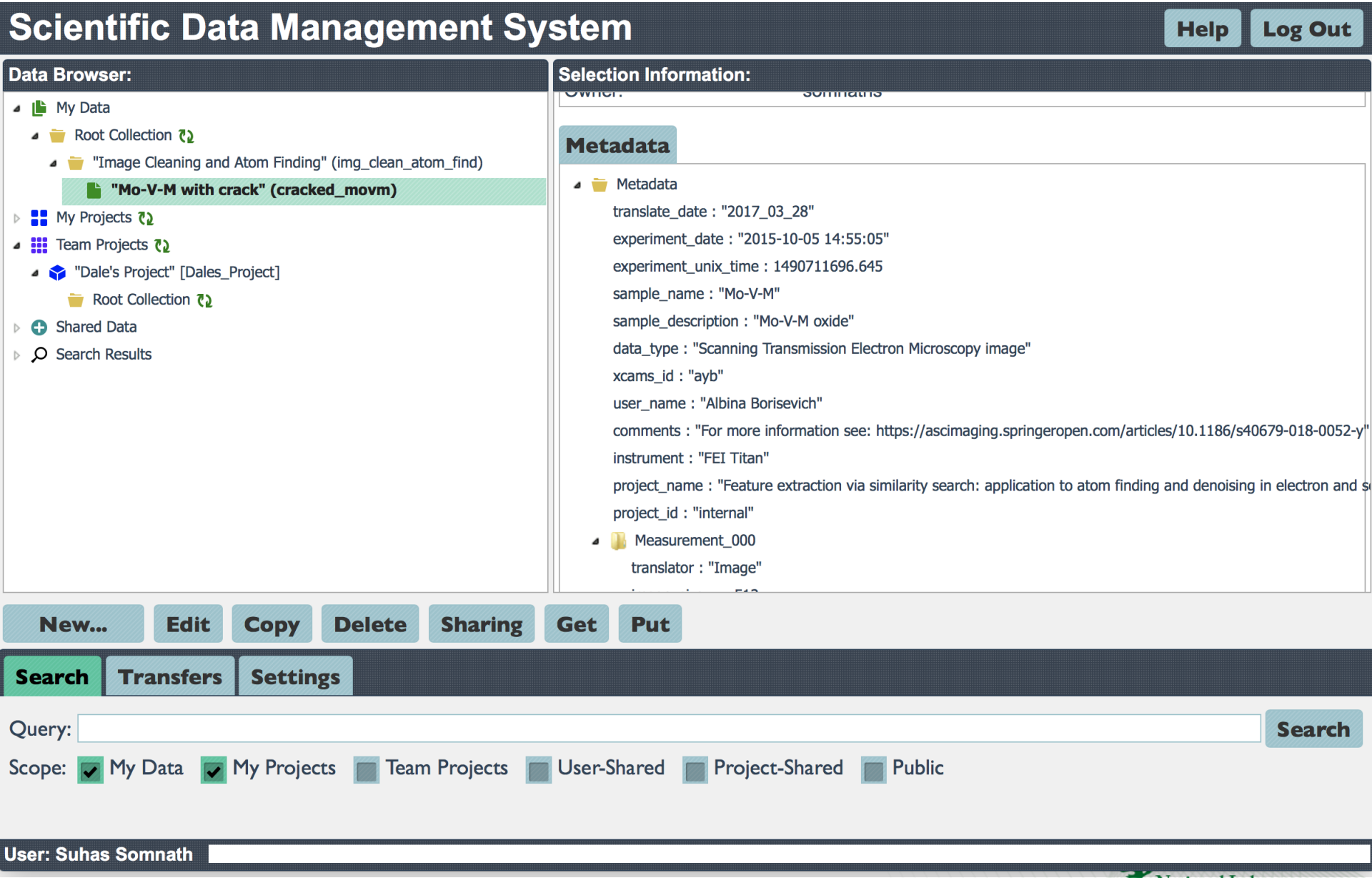
Imagine iTunes for Scientific Data

- Organize data by projects (albums)
- Search via metadata (artist, title, genre, …)
- Make collections (playlists) of datasets
- Access data from any computer
- Publish your own data (songs / album)
- Collaboratively work on projects
- Limit what your siblings can see / listen to
- Simple sign-in like Apple ID
- Fetch data through a standardized interface whether it is coming from one record label or another (CDs, cassette..).
- Quick and robust streaming from / to anywhere

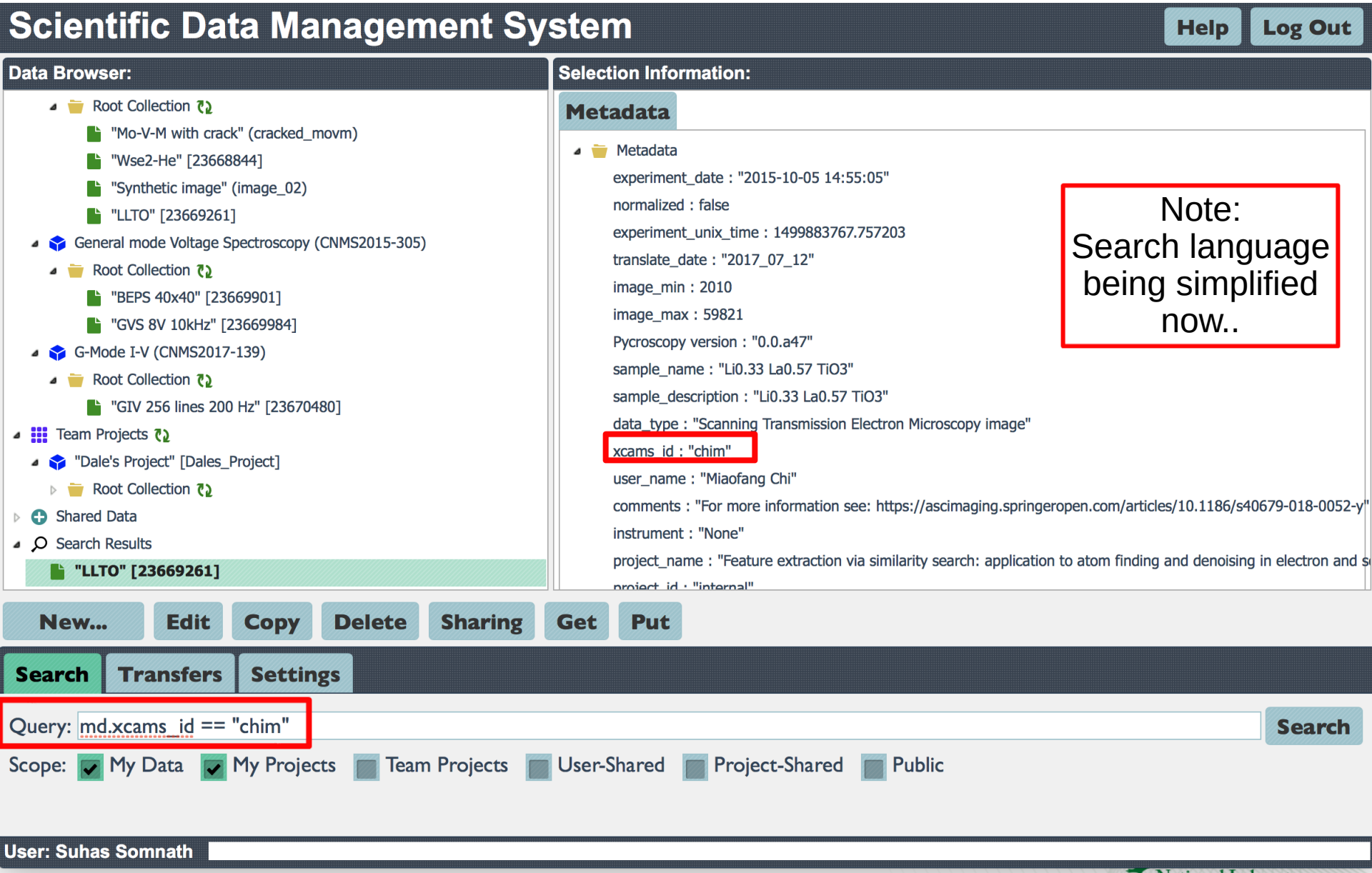
DataFed – a Scientific Data Management System



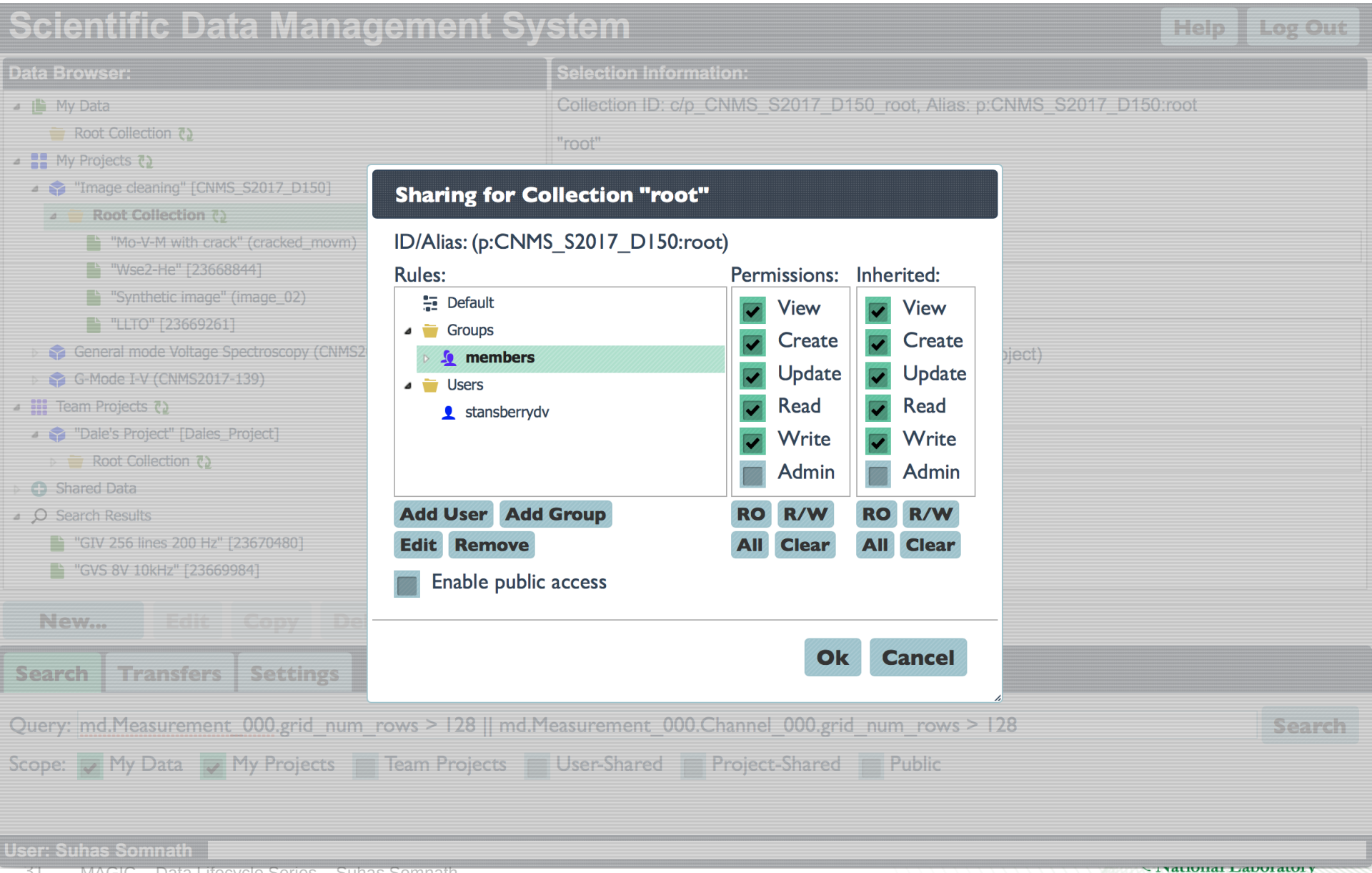
Rich metadata associated with data



Search by metadata



Granular Access Control / Sharing

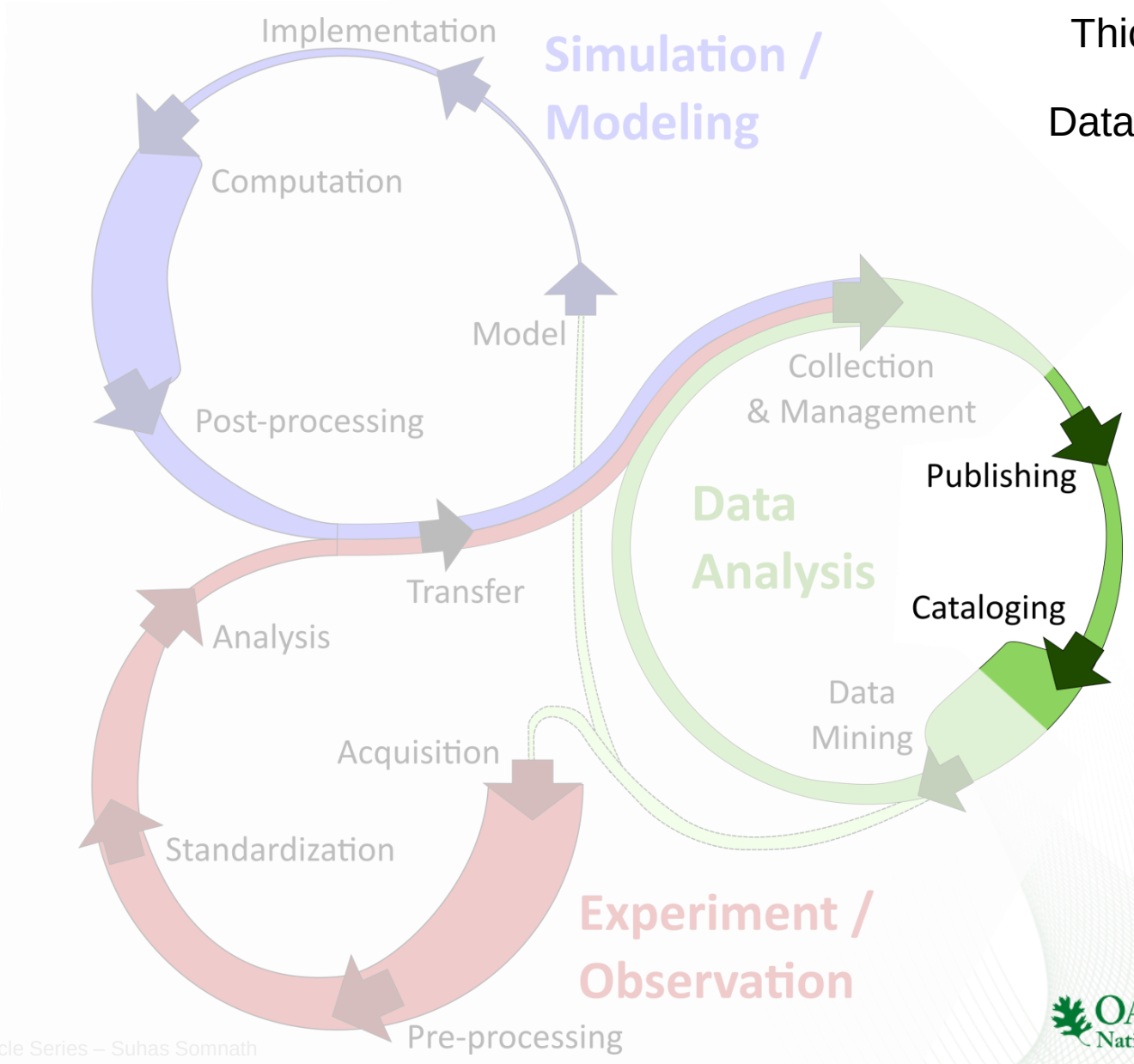


DataFed – a Scientific Data Management System

- **Granular access control / sharing**
- **Search by metadata**
- **Federated identity via Globus**
- Uniform interface for accessing data + caching –
  - Tier 1 (scratch), 2 (network file system), 3 (archive)
- Robust and easy data movement via Globus
- Data dissemination – publish DOI + archive
- Web + command-line interfaces
- Interfaces with compute / data analytics

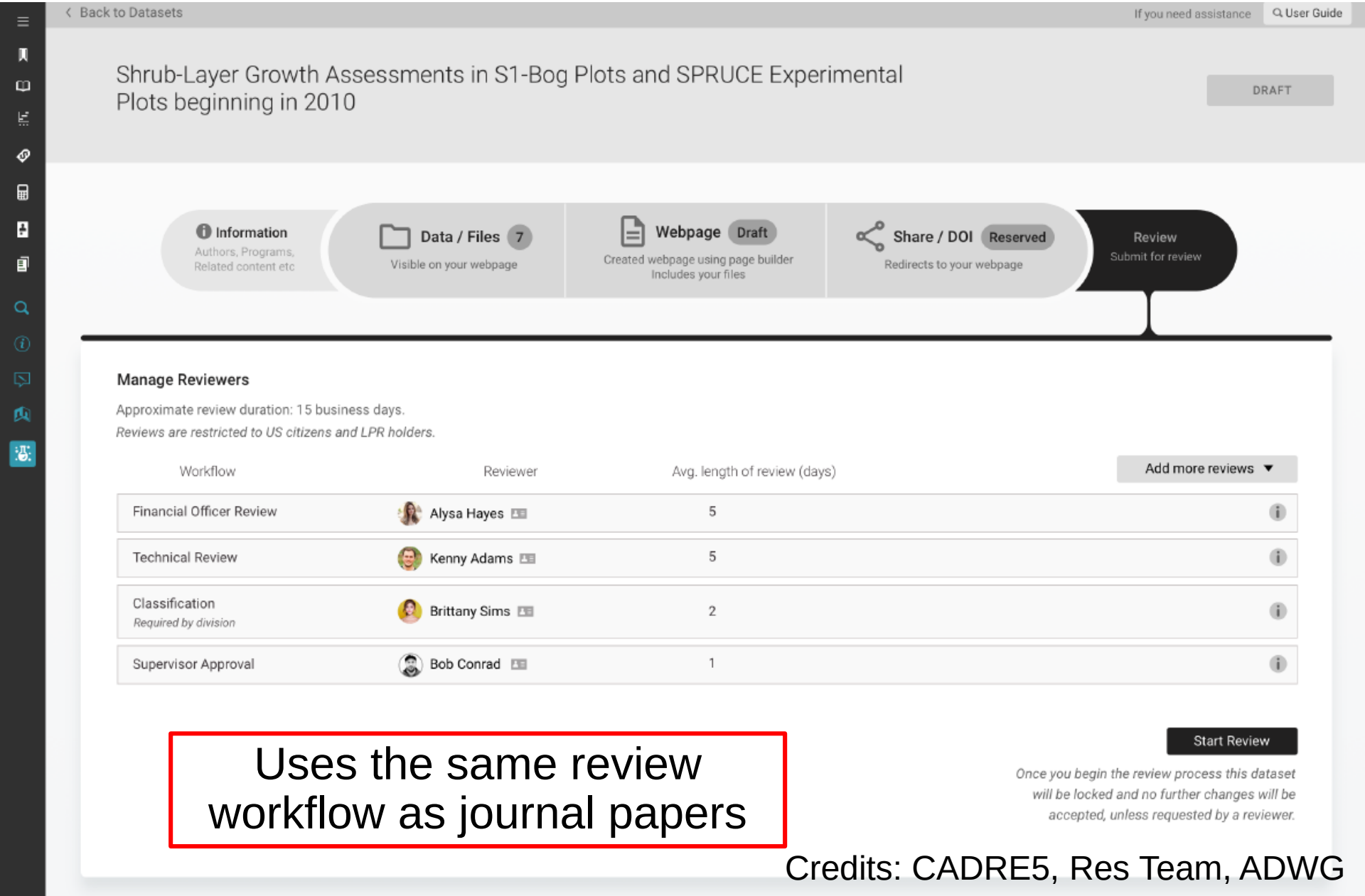
Source: Dale Stansberry (ADWG / NCCS)

Scalable Data Efforts at ORNL



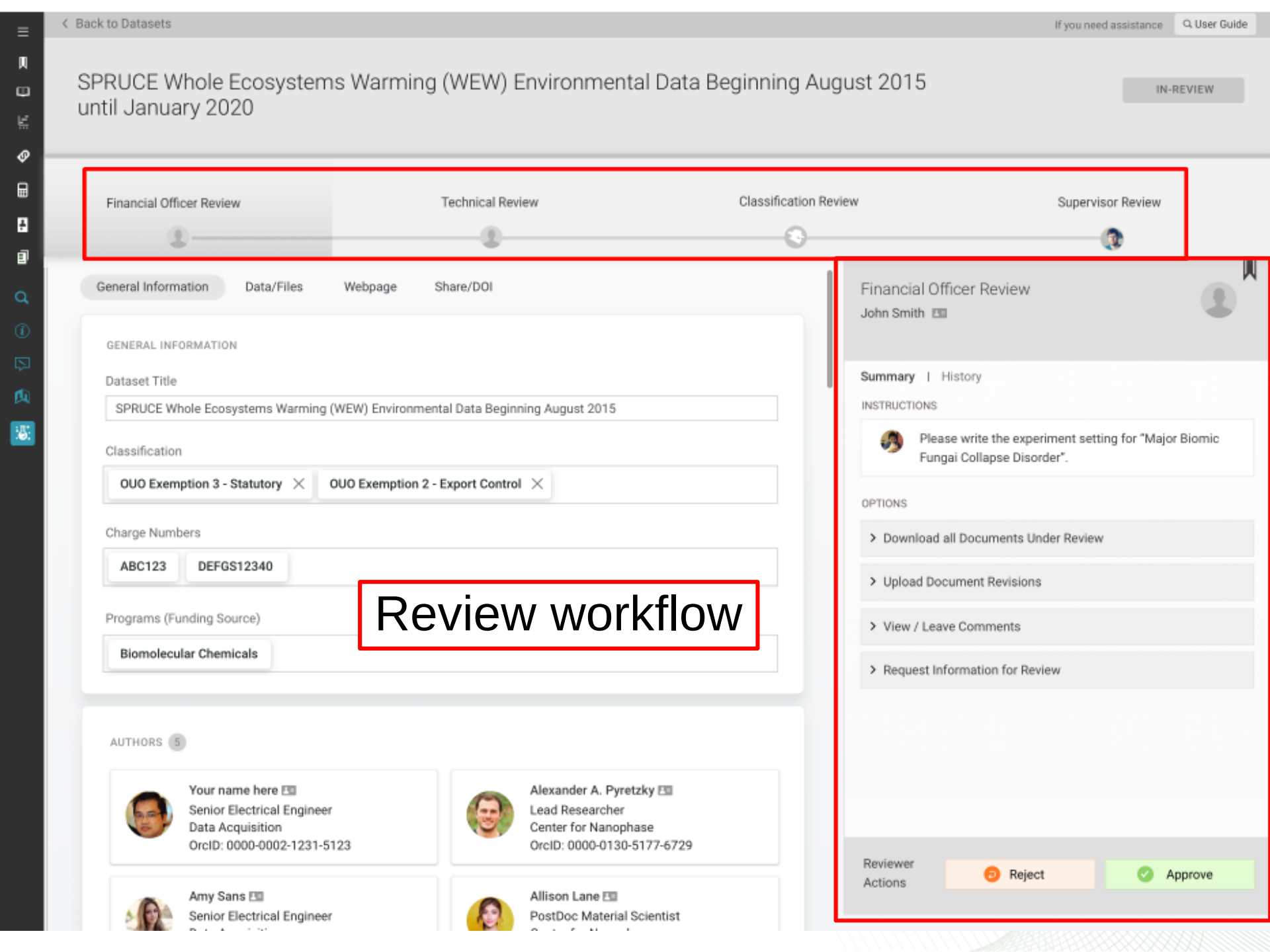
Thickness
=
Data volume

Prototype of Data Publishing

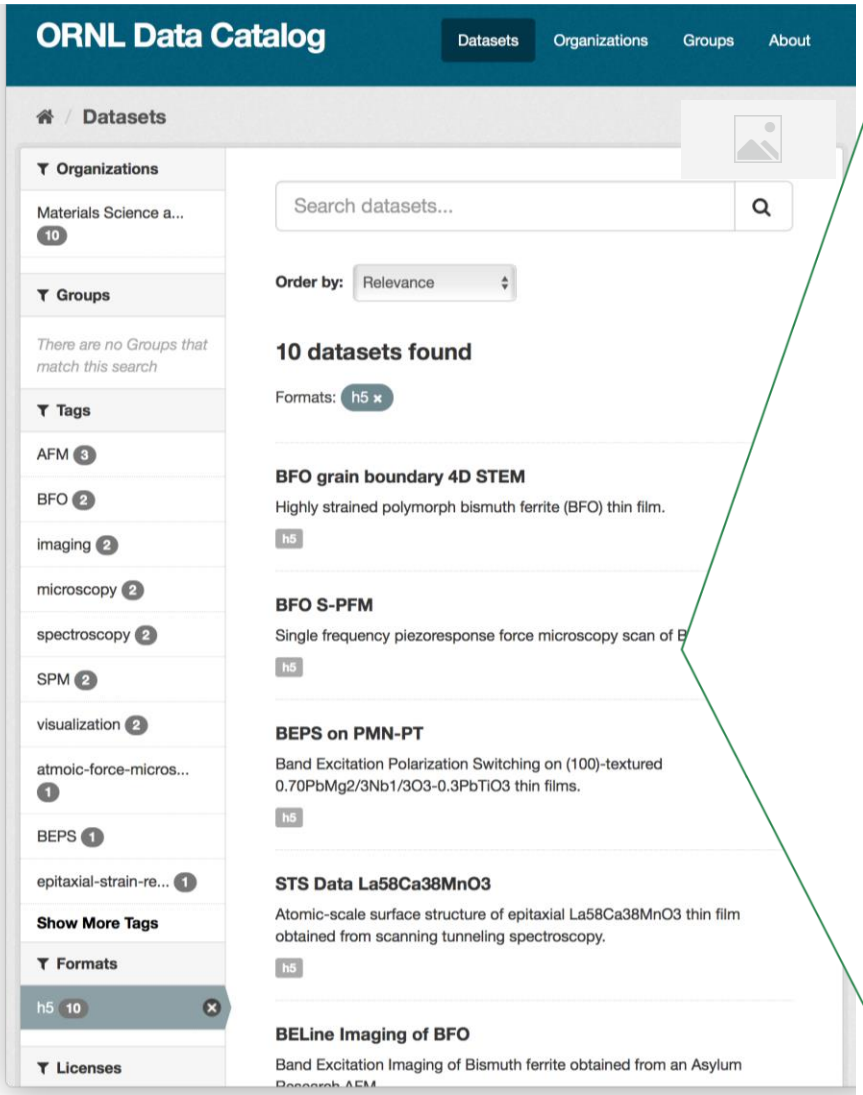


Uses the same review workflow as journal papers

Credits: CADRE5, Res Team, ADWG


Back to Datasets
If you need assistance
User Guide
SPRUCE Whole Ecosystems Warming (WEW) Environmental Data Beginning August 2015 until January 2020
IN-REVIEW
Financial Officer Review
Technical Review
Classification Review
Supervisor Review
General Information
Data/Files
Webpage
Share/DOI
GENERAL INFORMATION
Dataset Title
SPRUCE Whole Ecosystems Warming (WEW) Environmental Data Beginning August 2015
Classification
OUO Exemption 3 - Statutory
OUO Exemption 2 - Export Control
Charge Numbers
ABC123
DEFGS12340
Programs (Funding Source)
Biomolecular Chemicals
Review workflow
AUTHORS 5
Your name here
Senior Electrical Engineer
Data Acquisition
OrcID: 0000-0002-1231-5123
Alexander A. Pyretzky
Lead Researcher
Center for Nanophase
OrcID: 0000-0130-5177-6729
Amy Sans
Senior Electrical Engineer
Allison Lane
PostDoc Material Scientist
Financial Officer Review
John Smith
Summary | History
INSTRUCTIONS
Please write the experiment setting for "Major Biomic Fungai Collapse Disorder".
OPTIONS
Download all Documents Under Review
Upload Document Revisions
View / Leave Comments
Request Information for Review
Reviewer Actions
Reject
Approve

Prototype of ORNL Data Catalog



Additional Info

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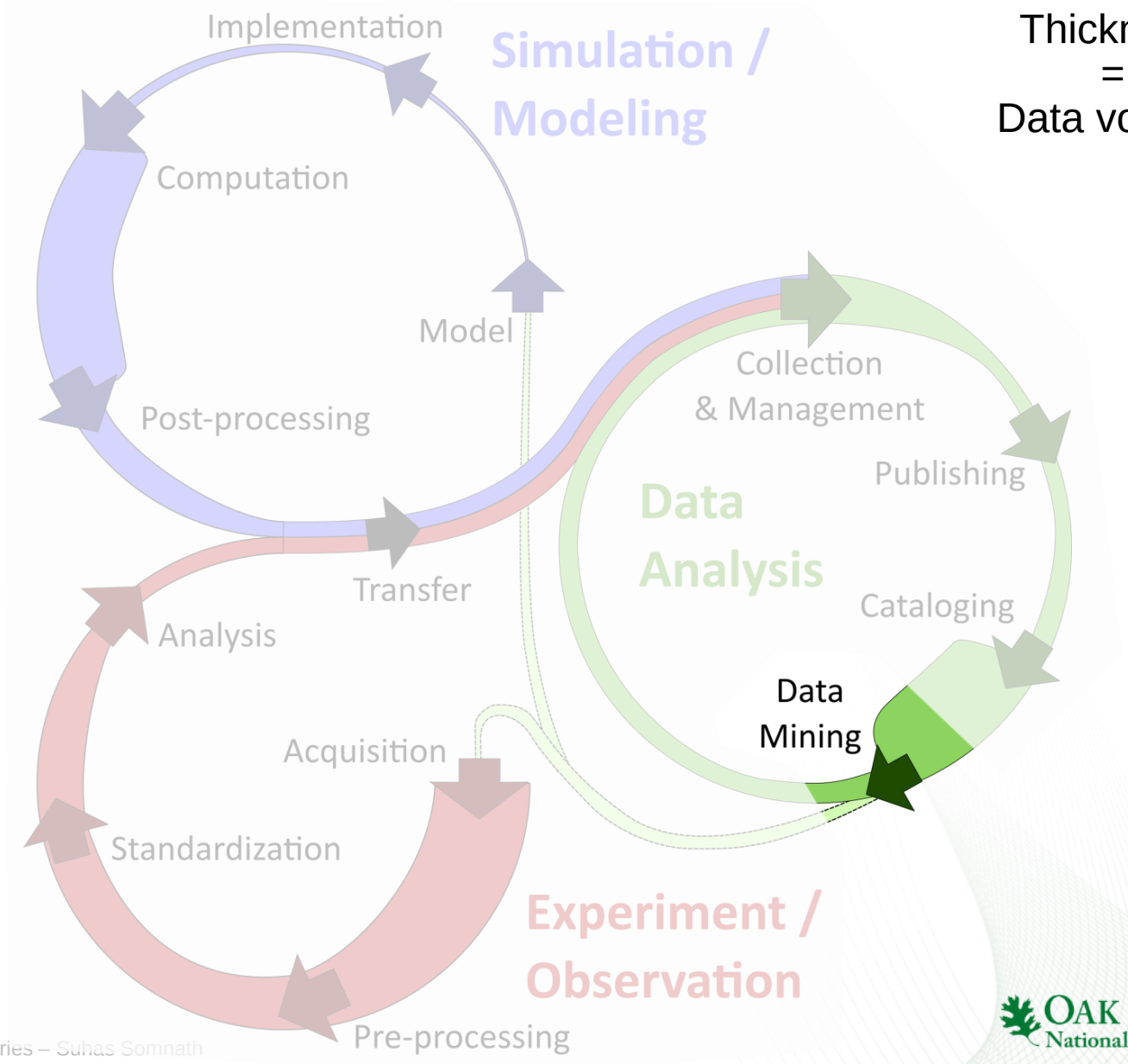
experiment_unix_time	1490711696.645
instrument	FEI Titan
project_id	internal
project_name	Feature extraction via similarity search: application to atom finding and denoising in electron and scanning probe microscopy imaging
sample_description	Mo-V-M oxide
sample_name	Mo-V-M
translate_date	2017_03_28
user_name	Albina Borisevich

Credits - Shubhank Gahlot, Whitney Nelson

Scalable Data Efforts at ORNL



Thickness
=
Data volume

Scalable Machine Learning

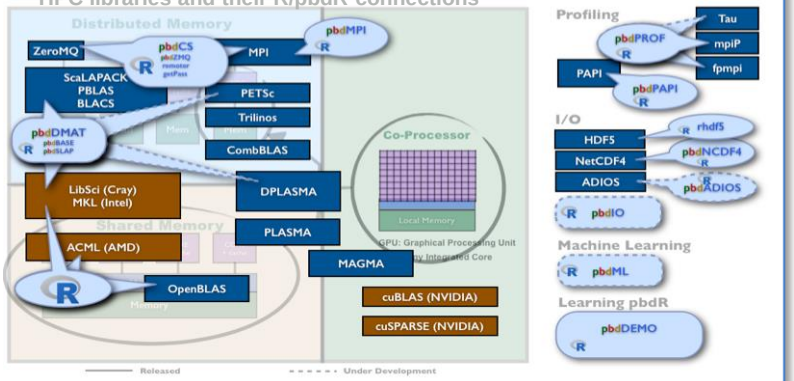
Programming with BIG Data in R

pbdR
Programming with Big Data in R

- Engage parallel math libraries at scale
- R language unchanged
- New distributed concepts
- New profiling capabilities
- New interactive SPMD parallel
- In-situ distributed capability
- In-situ staging capability via ADIOS

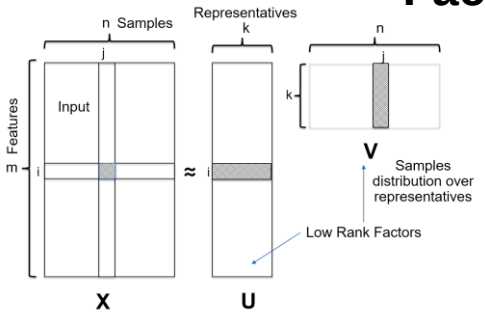
http://pbdr.org

HPC libraries and their R/pbdR connections



Schmidt, Chen, Matheson, and Ostrouchov (2016). Programming with BIG Data in R: Scaling Analytics from One to Thousands of Nodes, ***Big Data Research***

Non-negative Matrix Factorization



Titan – Dense Matrix, Low Rank 50, 100 Iterations, 12,650 Nodes, 202,500 Cores,

Matrix Size	Algos	NMF Time (in Secs)
2.7million x 2.7 million	MU	554
	HALS	197.75
	ANLS/ BPP	219.8
3.03 million x 3.03 million	MU	554
	HALS	197.75
	ANLS/ BPP	219.8

Acknowledgement: Ramki Kannan, ORNL

H2O.ai

DASK-ML

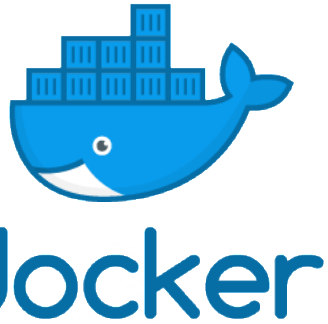
scikit-cuda

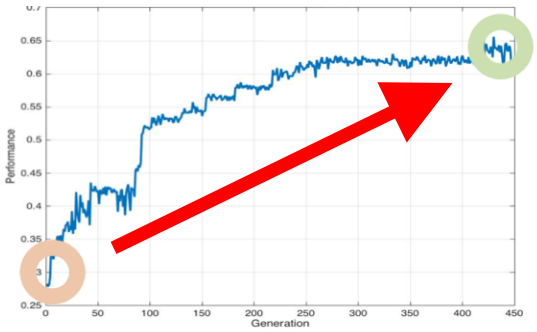
NVIDIA RAPIDS

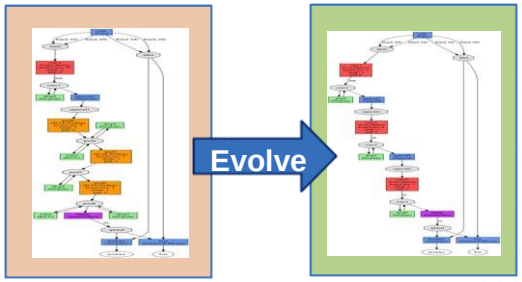
OAK RIDGE National Laboratory

Scalable Deep Learning

Horovod:
Distributed Deep Learning Framework



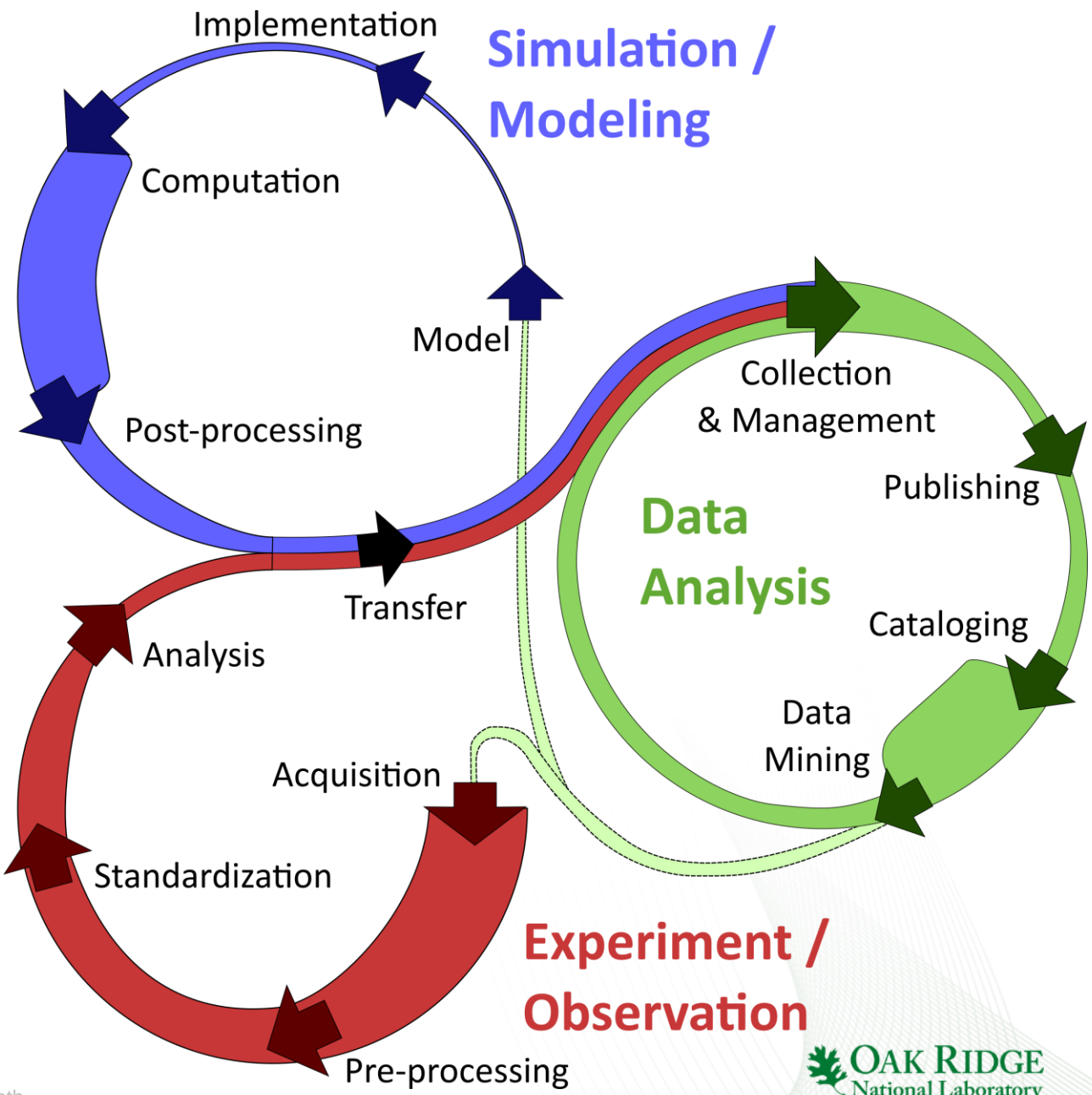




Multi-node Evolutionary Neural Networks for Deep Learning (MENNDL)

Summary

somnaths@ornl.gov



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