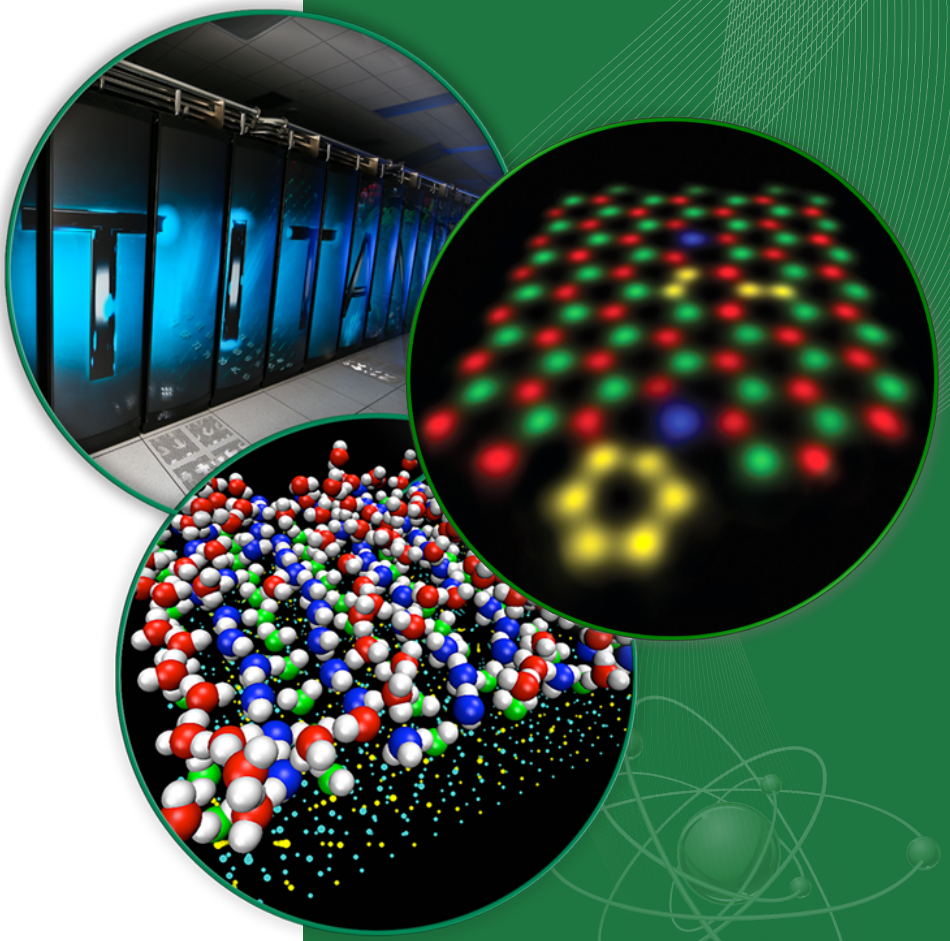
BEAM: An HPC Analysis Pipeline for Nanophase Materials Science



Eric Lingerfelt
Software Engineer

BEAM Software Architect
& Lead Developer

Computer Science Research Group
ORNL Computer Science
and Mathematics Division

OLCF User Meeting
May 25, 2016

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

OAK RIDGE National Laboratory

Computational Challenges at CNMS

- Scientific insight is increasingly dependent on the ability to efficiently integrate and analyze complex multi-dimensional, multi-modal data
- Analysis of data from experimental techniques at CNMS are designed to probe complementary ranges of time, space, and energy
  - Unfortunately, CNMS users cannot do this today without months of effort, much of which is driven by manual analysis and visual inspection of data
- Multi-modal experiments
  - Scanning Transmission Electron Microscopy (STEM)
  - Scanning Tunneling Microscopy (STM)
  - Scanning Probe Microscopy (SPM)
  - Neutron Scattering
  - Simulations
    - Electronic Structure
    - Ab Initio dynamics
    - Molecular dynamics (MD)

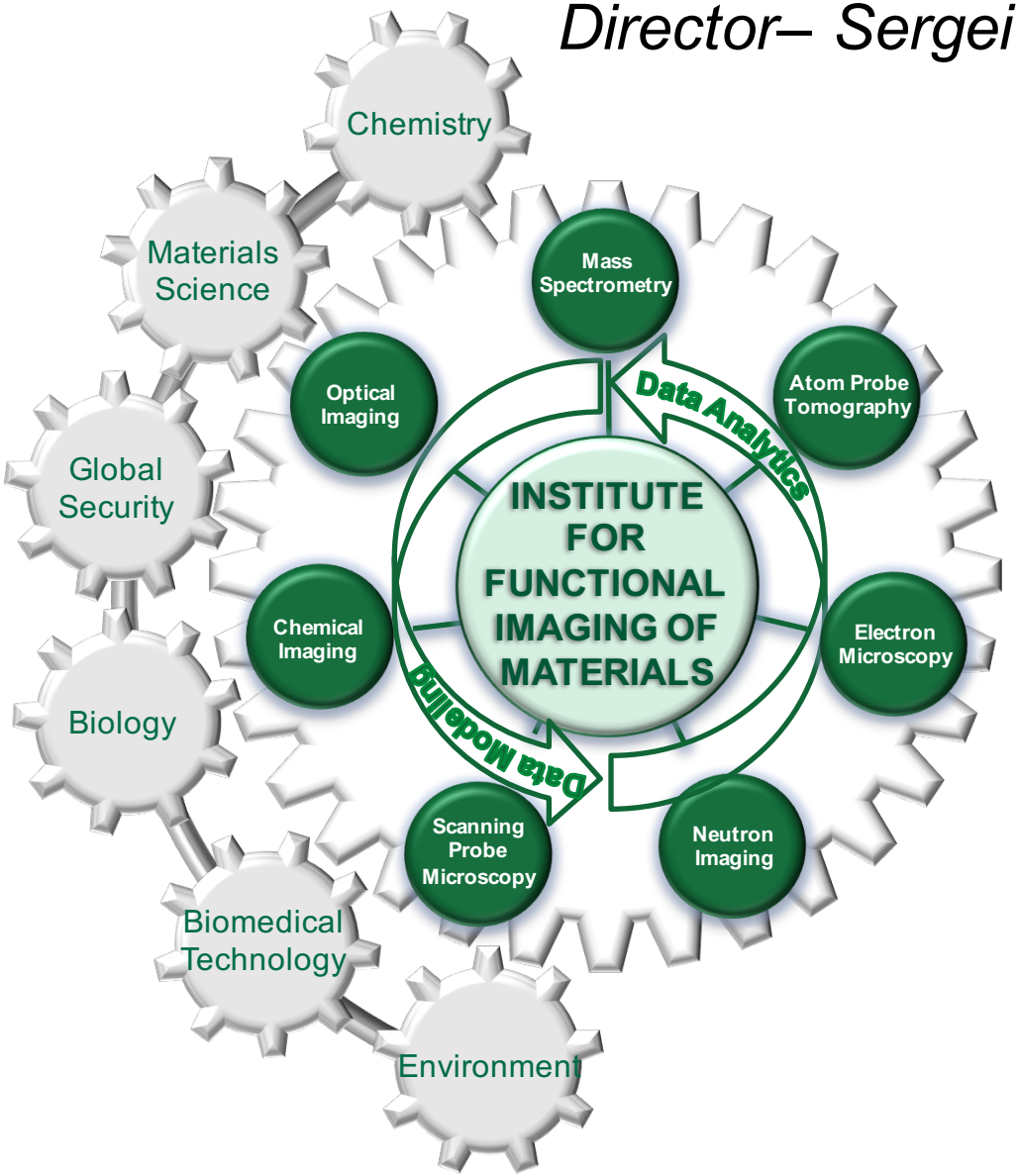
High Dimensional Imaging Data at CNMS

Technique	Dimensionality	Target data set	Target data size
Band Excitation PFM (BE-PFM)	3D, space and ω	(256×256)×64	32 MB
Switching spectroscopy PFM (SS-PFM)	3D, space and voltage	(64×64)×128	4 MB
Time relaxation PFM (TR-PFM)	3D, space and time	(64×64) ×128	4 MB
AC sweeps	4D, space, ω, voltage	(64×64)×64×256	512 MB
BE Polarization Switching (BEPS)	4D, space, ω, voltage	(64×64)×64×128	256 MB
BE thermal	4D, space, ω, temperature	(64×64)×64×256	512 MB
Time relaxation BE (TR-BE)	4D, space, ω, time	(64×64)×64×64	64 MB
First order reversal curves (FORC) BEPS	5D, space, ω, voltage, voltage	(64×64)×64×64×16	2 GB
Time relaxation on sweep, BE	5D, space, ω, voltage, time	(64×64)×64×64×64	16 GB
FORC Time BE	6D, space, ω, voltage, voltage, time	(64×64)×64×64×16×64	128 GB (Lower resolution realized)
FORC IV BEPS	5D, space, ω, voltage, cycle	(64×64)×64×64×16	4 GB
FORC IV and FORC IV-Z	4D, space, voltage, cycle	(64×64)×64×20	200 MB
Time-resolved Kelvin Probe Force Microscopy (KPFM)	3D, space, time	$(60\times20)\times1\cdot10^{6}$	8 MB
Open loop (OL) BE KPFM	4D, space, ω, voltage	(256×256)×32×16	256 MB
General-mode PFM (G-PFM)	3D, space and voltage	$(256\times256)\times1.6\cdot10^{4}$	4 GB
G-mode Voltage Spectroscopy (G-VS)	ND, Space, voltage	$(256\times256)\times1.6\cdot10^{6}$	400 GB (In Development)

A. Belianinov et al. "Big data and deep data in scanning and electron microscopies: deriving functionality from multidimensional data sets", Advanced Structural and Chemical Imaging, 1(1), pp.1-25.

Institute for Functional Imaging of Materials

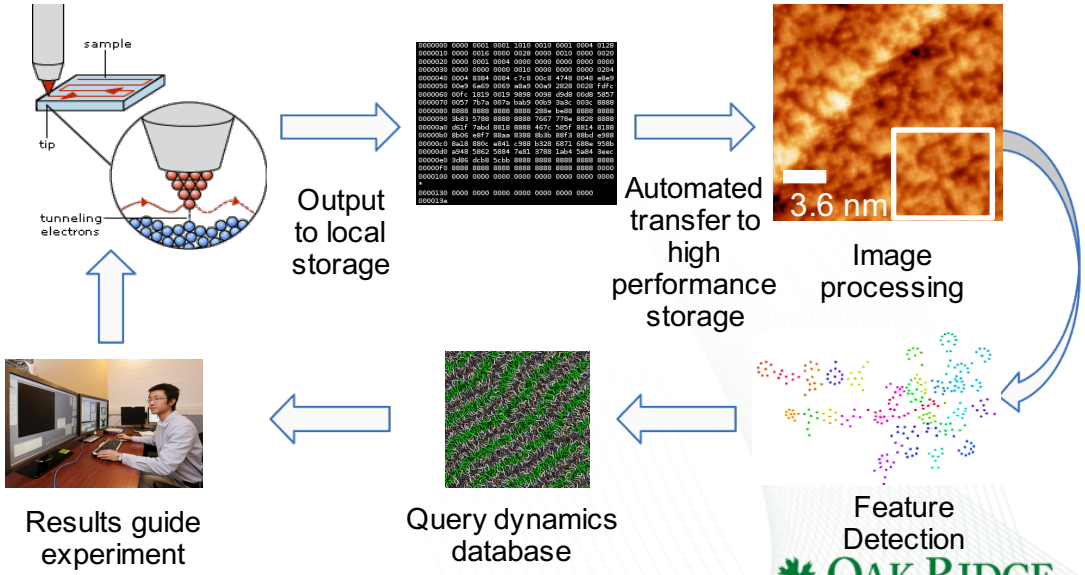
Director– Sergei Kalinin



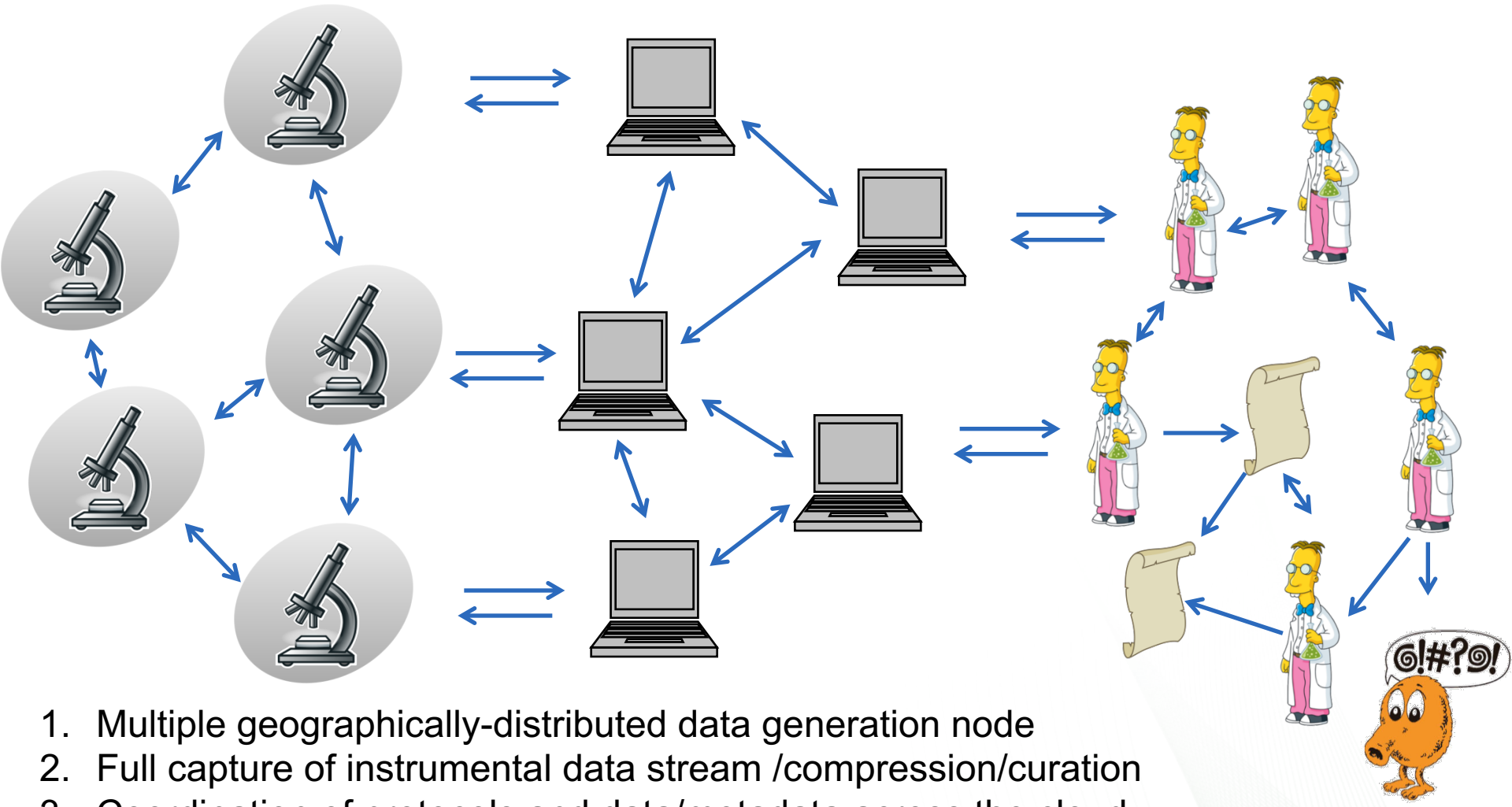
- Bridge physical imaging with theory via big data and data analytics to design new materials
- Leverage unique ORNL strengths in
  - Physics and chemistry on the atomic scale in real space
  - Mesoscale structure and functional probing
  - Big data and predictive theories: Biggest computation effort

Workflow System Requirements

- Robust analysis in near real-time
  - Fixed time-window to conduct the experiment at national facilities requires feedback in near-real time to drive the next step in the experiment
- Robust analysis at multiple scales that is accessible to any one with any computational background
  - Easily utilize DOE HPC compute and data resources to efficiently integrate and analyze complex multi-modal data with no previous experience as a computer programmer or HPC user.
- Long-term data stewardship
  - Unbroken chain of custody
  - Maintain data integrity
  - Link to DOI
  - Storage infrastructure
  - Ability to share results down the hallway or around the world

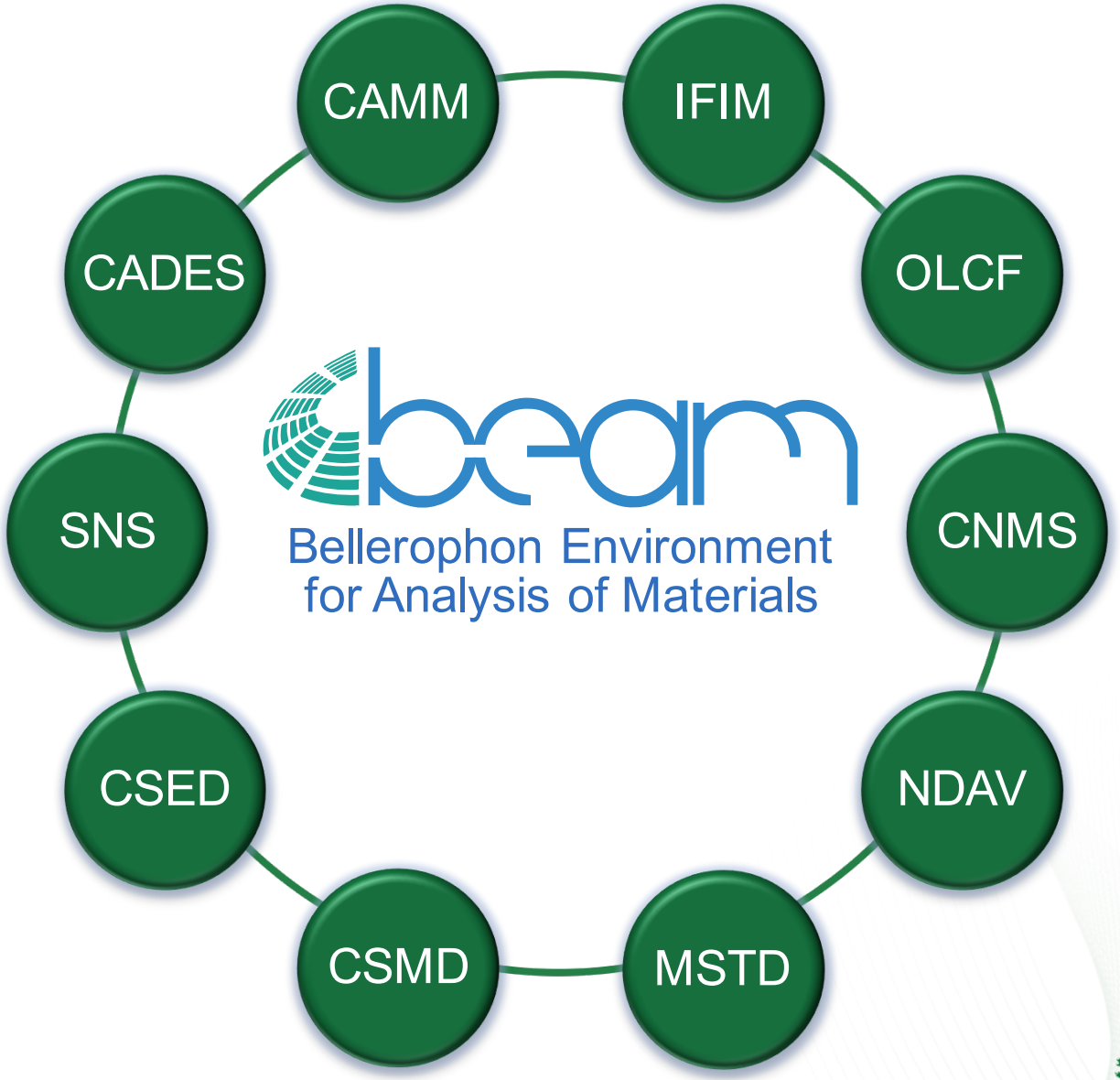


Imaging in the Cloud



1. Multiple geographically-distributed data generation node
2. Full capture of instrumental data stream /compression/curation
3. Coordination of protocols and data/metadata across the cloud
4. Cloud-based processing and dimensionality reduction
5. Community-wide analytics

Integrating DOE Expertise with DOE Resources



BEAM Design Approach

- Provide a flexible environment for advanced analysis of materials imaging
  - Encapsulated end-to-end solution
  - Central, easy-to-use, SaaS portal
  - Provide a mechanism for efficient delivery of modern HPC algorithms developed by mathematicians and computational scientists.
  - Allow authenticated access to data analysis services and remotely stewarded data from anywhere in the world at any time

beam

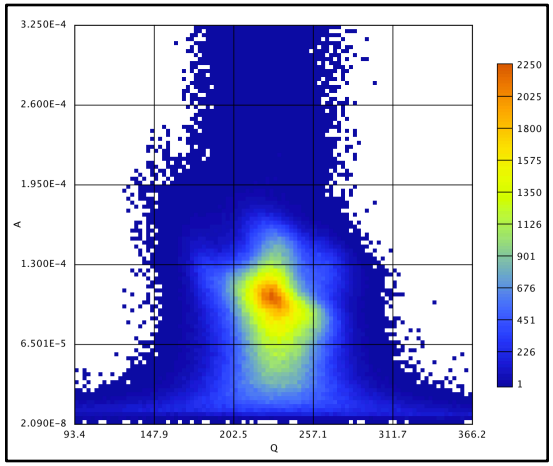
CADES

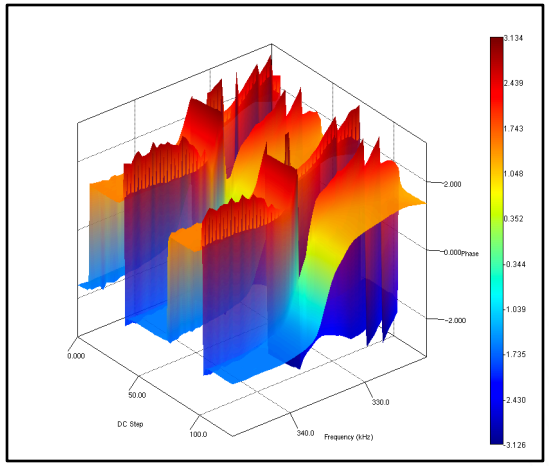
Institute for Functional Imaging of Materials
Oak Ridge National Laboratory

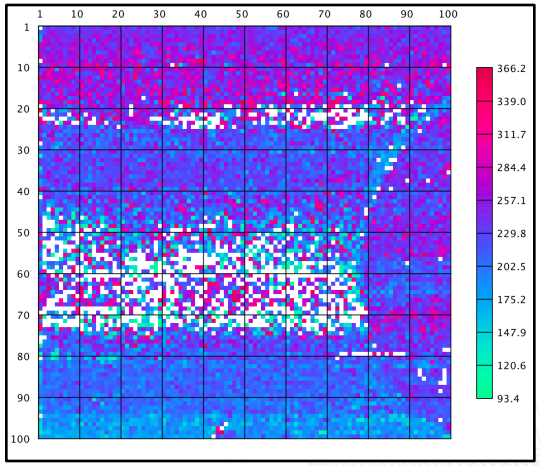
Oak Ridge National Laboratory | Center for Nanophase Materials Sciences

BEAM Design Approach

- Integrate across multiple microscopes and experimental modalities
- Utilize OLCF and CADES compute and data storage resources seamlessly
- Provide interactive, customizable data views using state-of-the-art multi-dimensional visualization tools

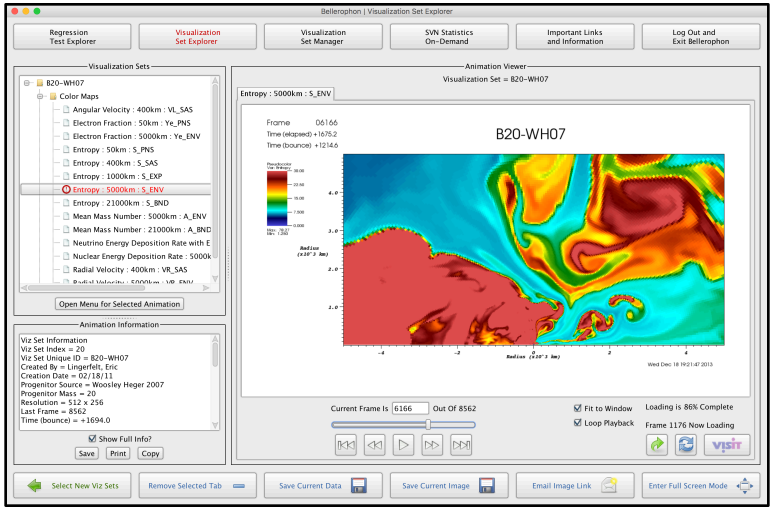


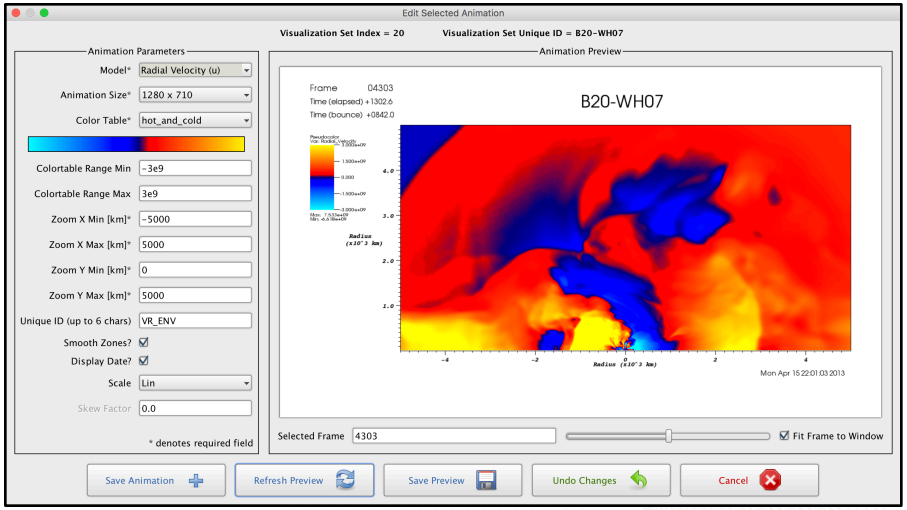




Bellerophon

- Bellerophon is a computational workflow environment for real-time analysis, data & artifact management, and regression testing developed for large-scale HPC simulations (currently migrating to CADES from UTK)
  - In production at ORNL since 2010 for the multi-dimensional, multi-physics core-collapse supernova application *CHIMERA*
  - DB currently includes 40 CCSn models, >100K data files, and ~1150 animations comprised of 1.5 MILLION real-time rendered images under complete management with provenance





E. Lingerfelt & B. Messer. "Bellerophon: A Computational Workflow Environment for Real-time Analysis, Artifact Management, and Regression Testing of Core-Collapse Supernova Simulations", SC15, Austin, TX.

Accelerating Scientific Discovery in Core-Collapse Supernova Research

THE DEVELOPMENT OF EXPLOSIONS IN AXISYMMETRIC *AB INITIO* CORE-COLLAPSE SUPERNOVA SIMULATIONS OF 12–25 $M_\odot$ STARS

STEPHEN W. BRUENN[1], ERIC J. LENTZ[2,3], W. RAPHAEL HIX[3,2], ANTHONY MEZZACAPPA[2,4], JAMES AUSTIN HARRIS[2], O. E. BRONSON MESSER[5,3], EIRIK ENDEVE[6,2,4], JOHN M. BLONDIN[7], MEREK AUSTIN CHERTKOW[2], ERIC J. LINGERFELT[6,3], PEDRO MARRONETTI[8], KONSTANTIN N. YAKUNIN[2,3,4]

Gravitational Wave Signatures of *Ab Initio* Two-Dimensional Core Collapse Supernova Explosion Models for 12–25 $M_\odot$ Stars

Konstantin N. Yakunin[1,2,3], Anthony Mezzacappa[1,2], Pedro Marronetti[4], Stephen W. Bruenn[5], W. Raphael Hix[1,3], Eric J. Lentz[1,2,3,6], O. E. Bronson Messer[1,4,7], J. Austin Harris[1], Eirik Endeve[1,8], John M. Blondin[9], and Eric J. Lingerfelt[3,7]

AXISYMMETRIC *AB INITIO* CORE-COLLAPSE SUPERNOVA SIMULATIONS OF 12–25 $M_\odot$ STARS

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Two- and Three-Dimensional Multi-Physics Simulations of Core Collapse Supernovae: A Brief Status Report and Summary of Results from the "Oak Ridge" Group

Anthony Mezzacappa,[1,2] Stephen W. Bruenn,[3] Eric J. Lentz,[1,2,4] W. Raphael Hix,[1,4] O. E. Bronson Messer,[4,5] J. Austin Harris,[1] Eric J. Lingerfelt,[6] Eirik Endeve,[1,6] Konstantin N. Yakunin,[2] John M. Blondin,[7] and Pedro Marronetti[8]

Neutrinos and Supernovae

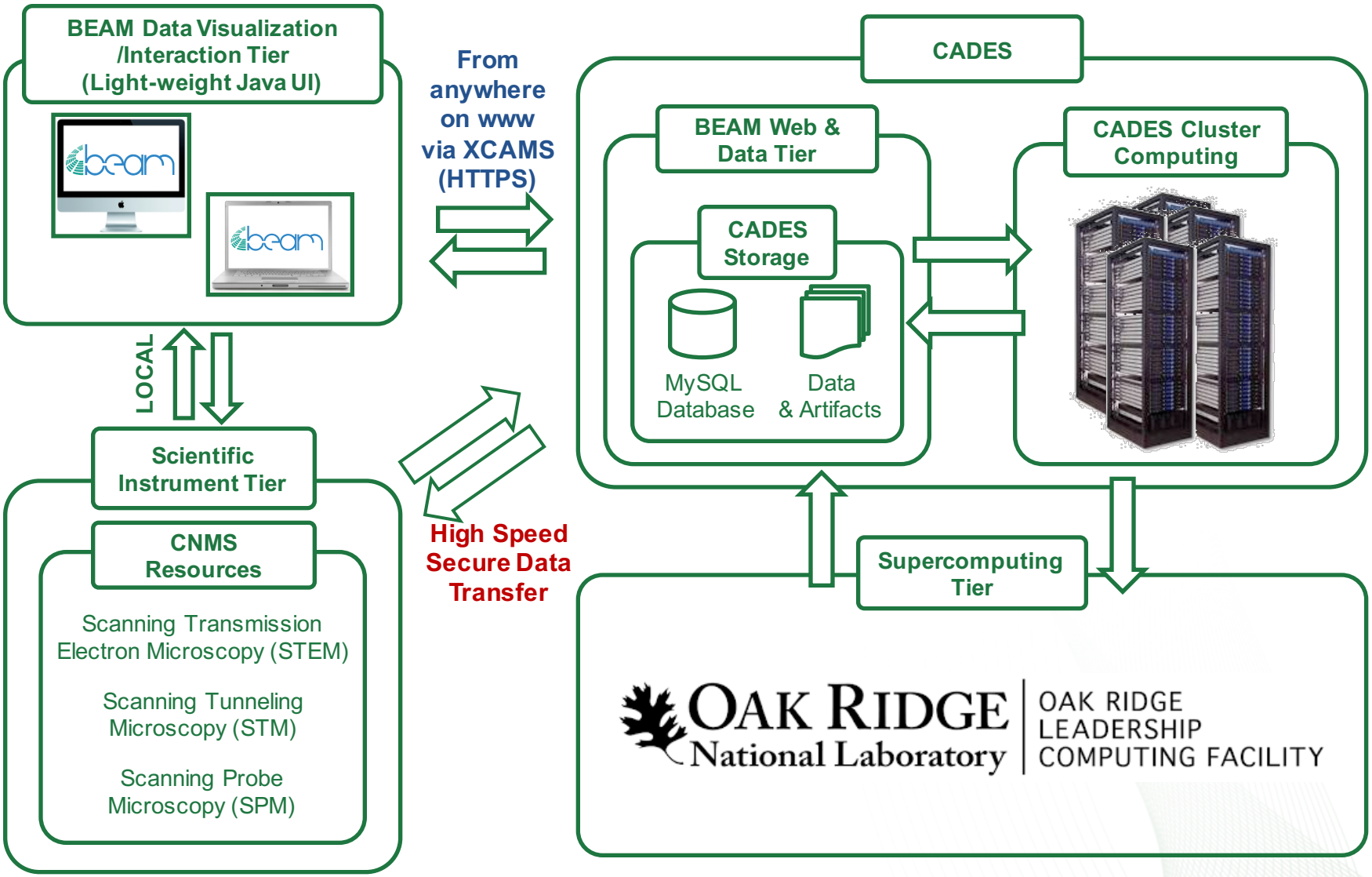
Stephen W Bruenn[1], Eric J. Lentz[3,2,4], Eric J. Lingerfelt[5], Anthony Mezzacappa[2,3,5], W. Raphael Hix[2,3], John N. Blondin[6], O. E. Bronson Messer[7,3], Pedro Marronetti[1]

Leveraging the Power of CADES

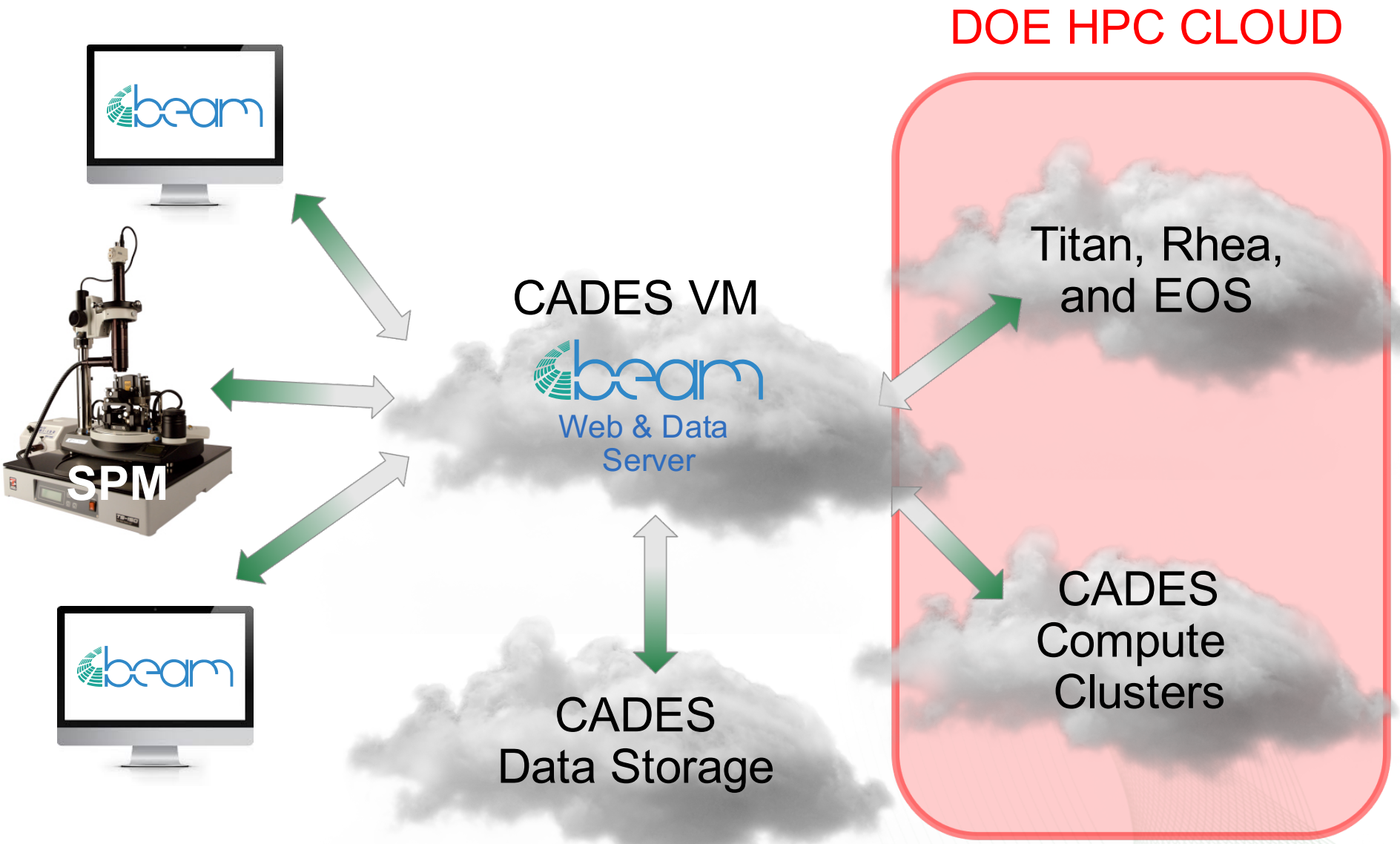
- ORNL Compute and Data Environment for Science
  - Core compute and data services required by major science facilities, large projects, small teams, and single principal investigators
  - Both data infrastructure and compute & data science expertise with and among many projects
  - A rich set of services coupled with experts in data science and domain scientists

- How does BEAM use CADES?
- Infrastructure as a Service (IaaS) provides VM, software, and database support
- On demand cluster computing capability
  - BEAM is currently integrated with a 128 core machine
- CNMS is currently completing installation of a new compute cluster in CADES
  - Cray CS400 with 768 cores and 4TB of RAM
- High performance data storage
  - 100TB for BEAM users available FY16

Distributed Multi-tier Architecture



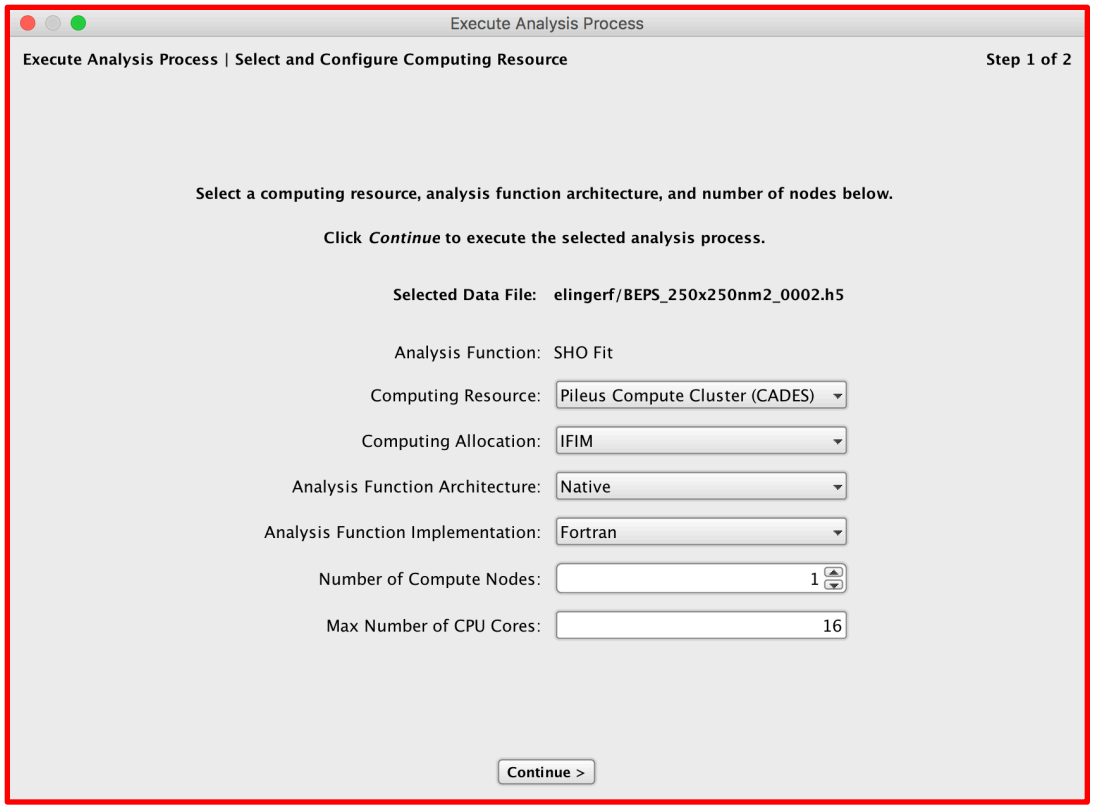
Distributed *Cloud-based* Architecture



Utilization of OLCF Resources by Facility User

- Skill set requirements
  - Fluent in Linux OS commands and shell scripting in a terminal
  - Fluent in compilers and platform dependent libraries and software
  - Be knowledgeable of OLCF user policies concerning data management
  - Learn how to move data in and out of the OLCF
  - Learn how to configure, monitor, and execute parallel jobs using Titan's MOAB / Torque scheduler
- Steps for successful job execution at OLCF
  - Apply for an allocation of CPU hours (or join an existing allocation)
    - ***OLCF DD Award 2016: CADES / OLCF Computational Workflows for Materials Science***
  - Log into Titan using a terminal
  - Compile your code using the preferred environment
  - Write PBS scripts to
    - Move data into and out of OLCF using a Data Transfer Node (DTN)
    - Execute program in parallel across compute nodes
    - Visualize results

“Push Button” Execution of HPC Workflows



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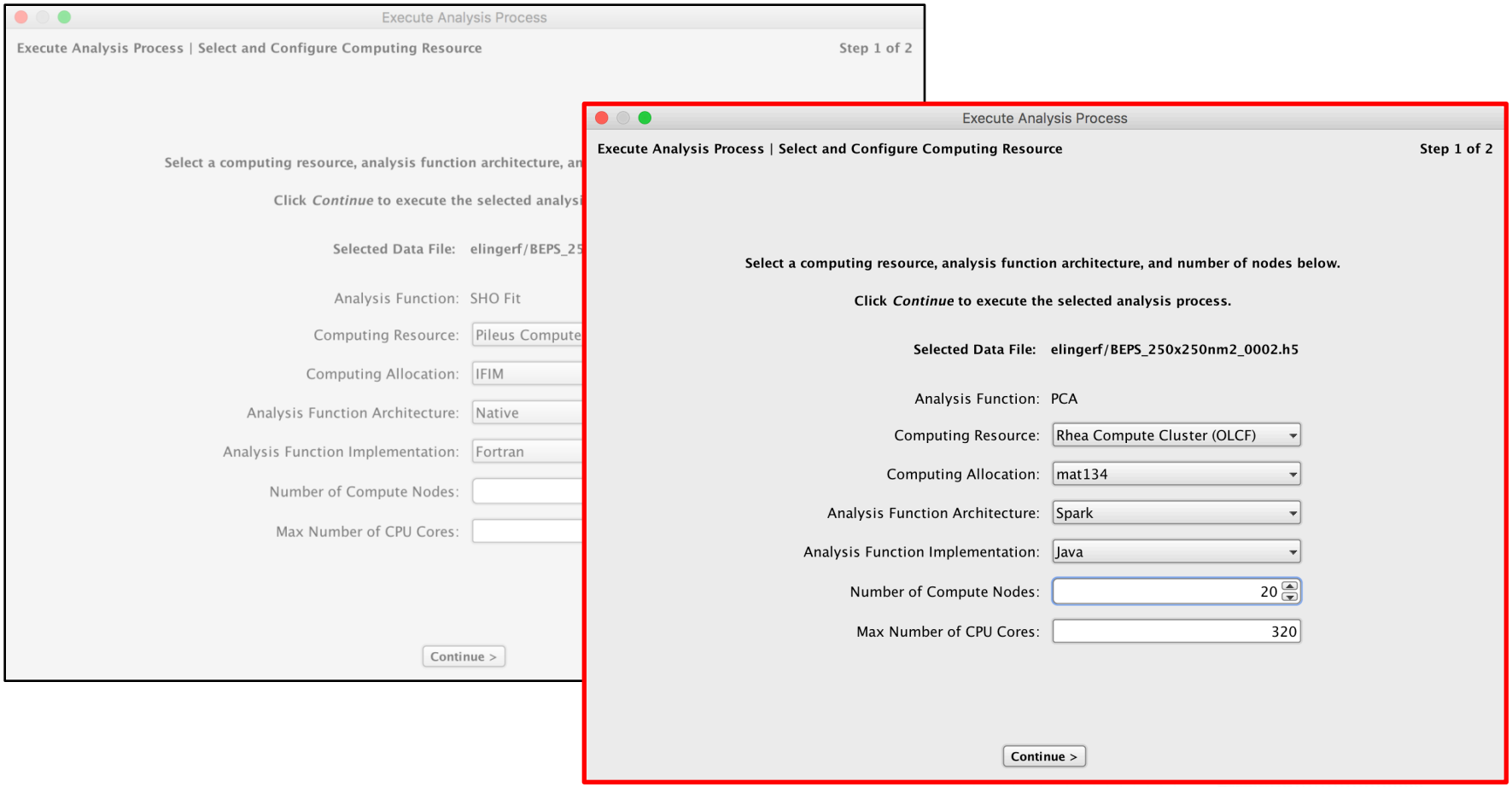

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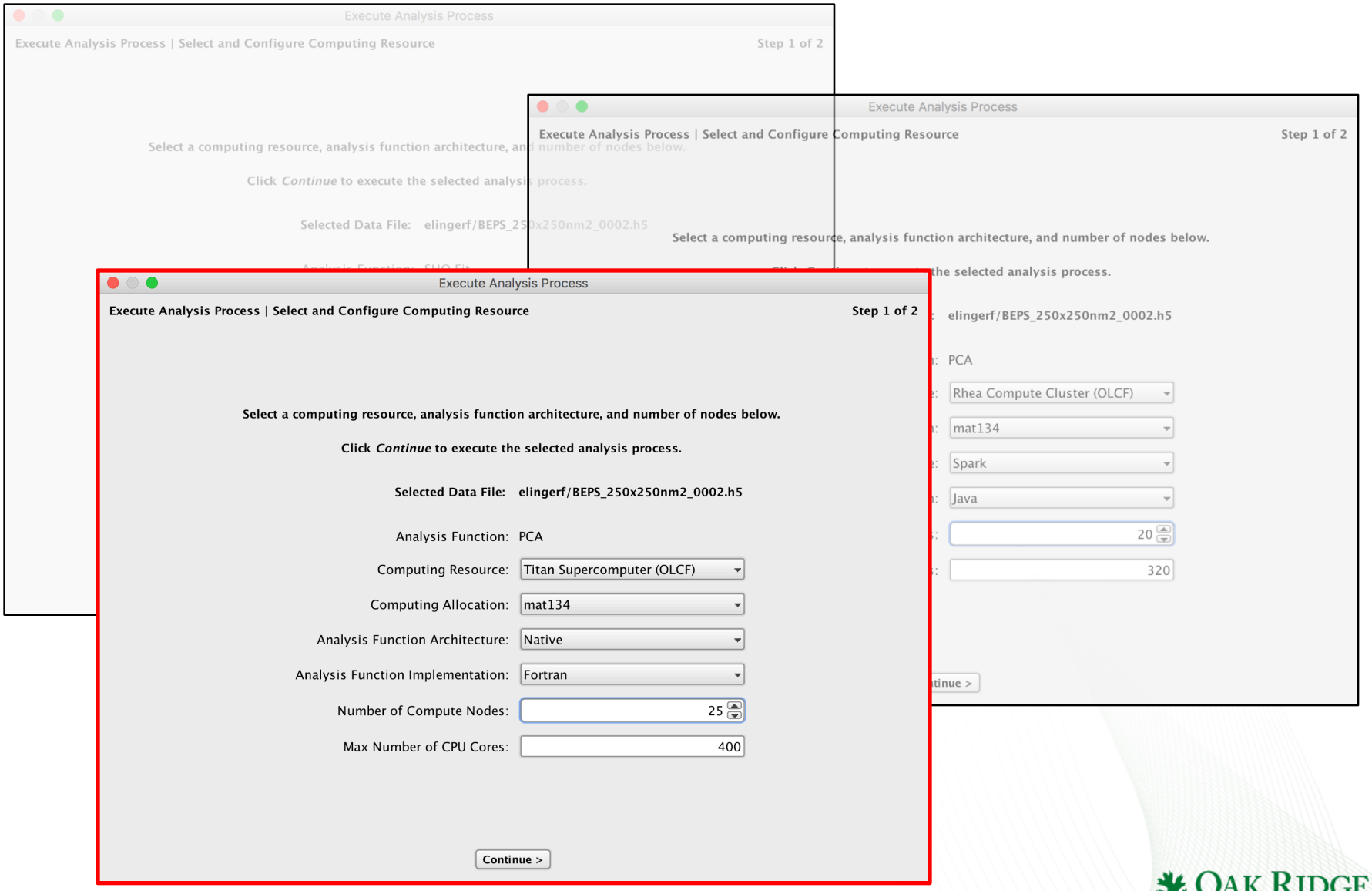


Real-time Monitoring & Override of HPC Workflows

Execute Analysis Process

Execute Analysis Process | Monitor Progress **Step 2 of 2**

The selected analysis process has been completed.

Selected Data File: elingerf/BEPS_250x250nm2_0002.h5

Analysis Function:	SHO Fit	Computing Resource:	Titan Supercomputer (OLCF)
Analysis Function Architecture:	Native	Computing Allocation:	mat134
Analysis Function Implementation:	Fortran	Number of Compute Nodes:	25
Number of CPU Cores Used:	400	Max Number of CPU Cores:	400

Execution Status

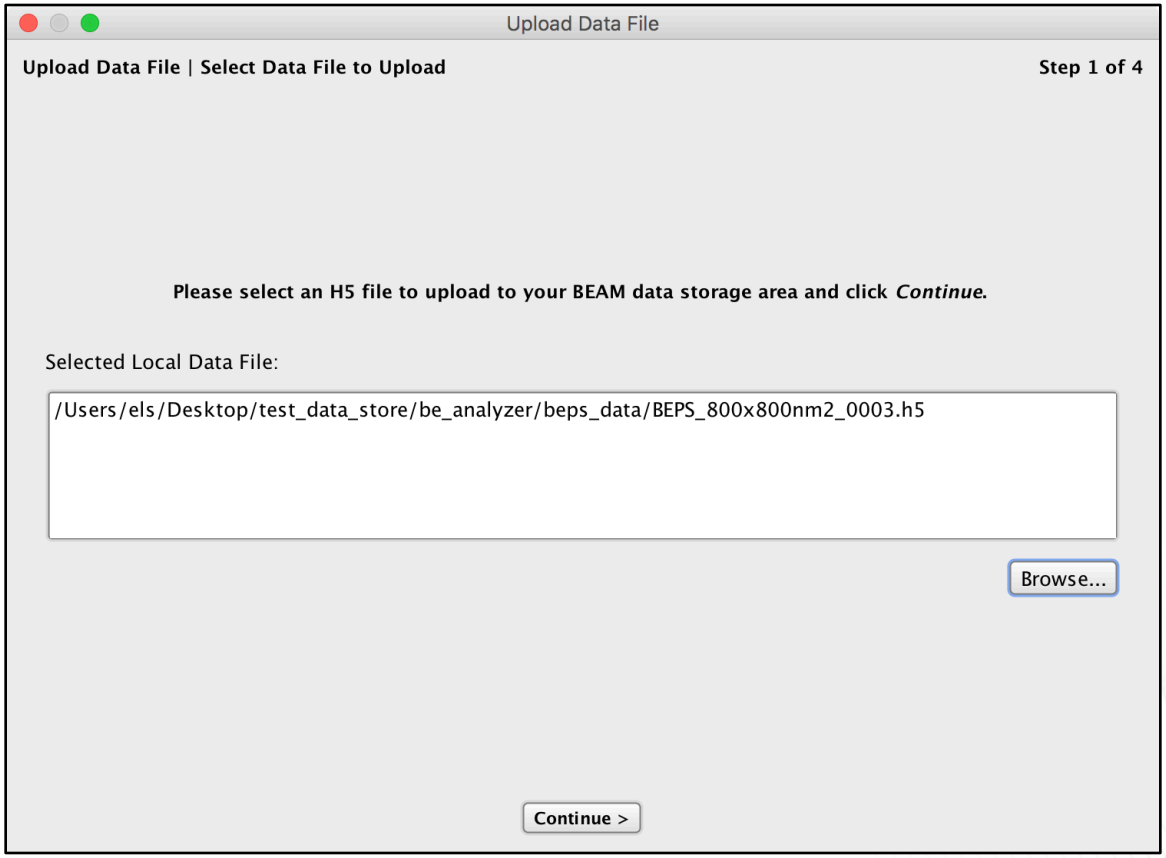
```
05/20/2016 11:31:11 | Setting data movement job on the queue on DTN.
05/20/2016 11:31:14 | The job id 22549 has been assigned for your data movement job on DTN.
05/20/2016 11:31:15 | Downloading data from CADES to OLCF.
05/20/2016 11:31:16 | Data download complete.
05/20/2016 11:31:16 | Setting analysis job on the queue on Titan.
05/20/2016 11:31:16 | The job id 2804953 has been assigned for your data analysis job on Titan.
05/20/2016 11:31:26 | Executing analysis job on Titan.
05/20/2016 11:31:31 | Analysis job complete.
05/20/2016 11:31:31 | Setting data movement job on the queue on DTN.
05/20/2016 11:31:31 | The job id 22550 has been assigned for your data movement job on DTN.
05/20/2016 11:31:32 | Uploading data from OLCF to CADES.
05/20/2016 11:31:36 | Data upload complete.
SHO Fit analysis process completed in 25.001 seconds!
```

View Analysis Results

< Back | Close Execute Analysis Process

Cloud Data Management with BEAM

- Easily transmit data files to your private BEAM storage area in a few simple steps
- Each BEAM data storage area is only accessible by the owner through a secure, encrypted network connection via the Java UI
- Each data file (and its metadata) is uniquely identified in BEAM's database



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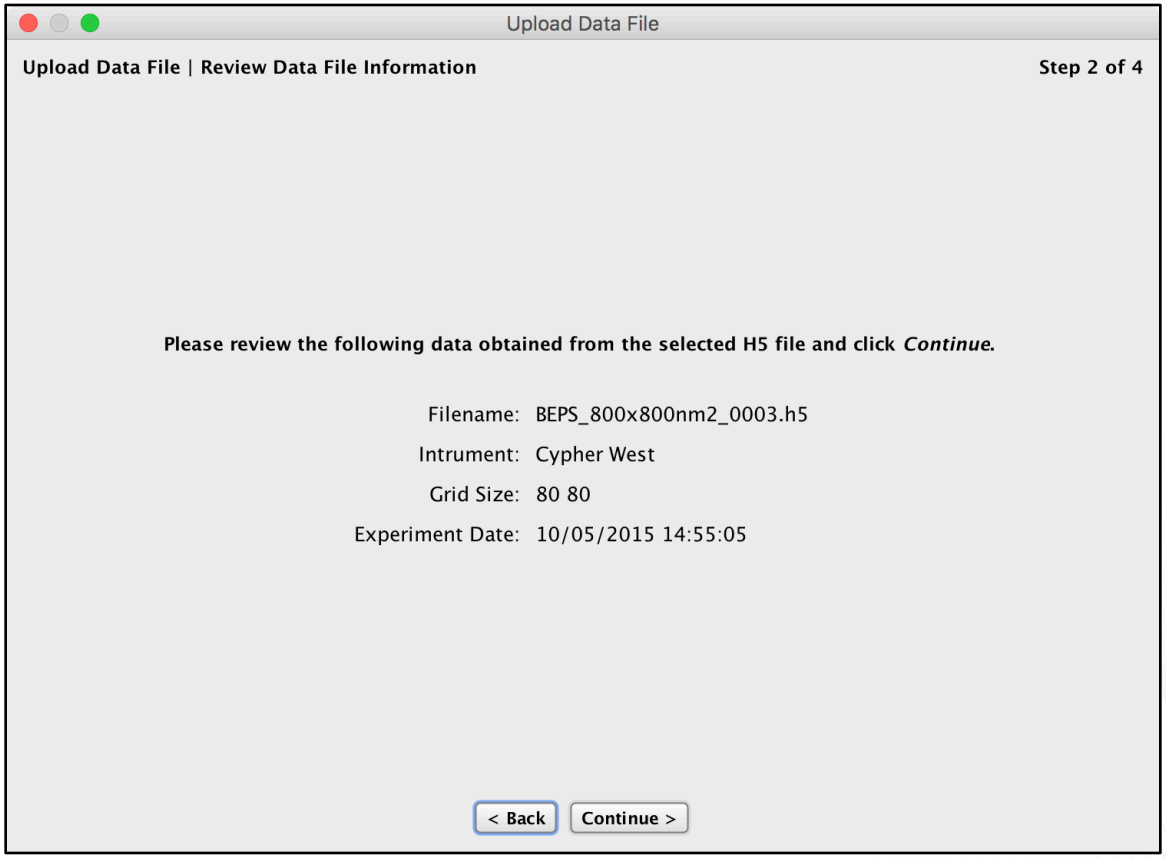

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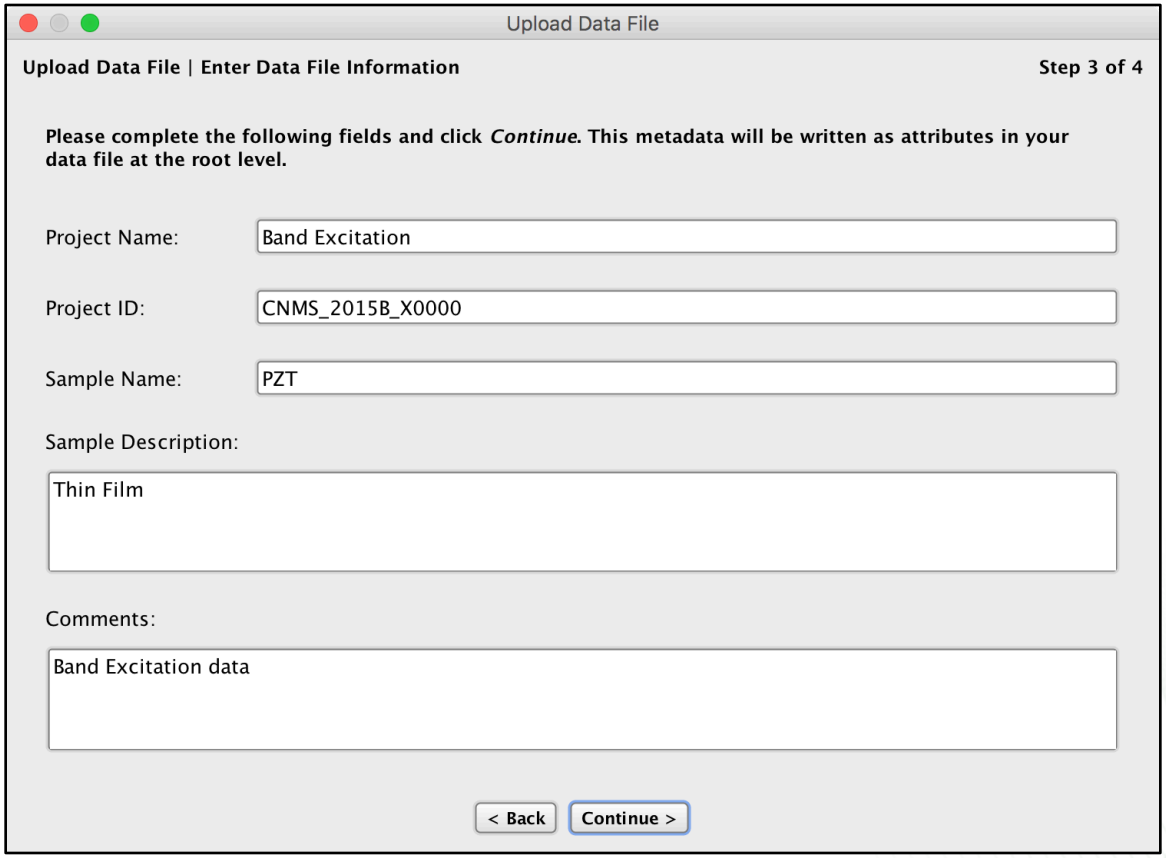

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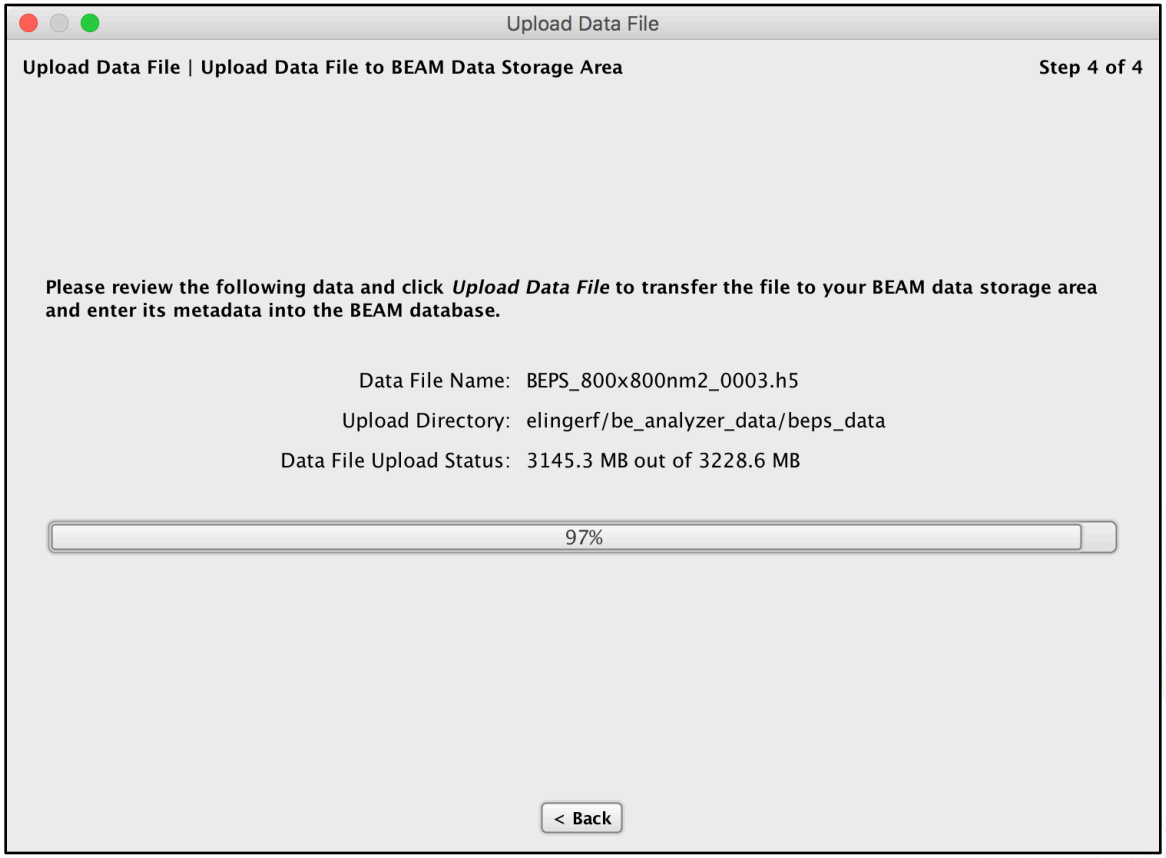
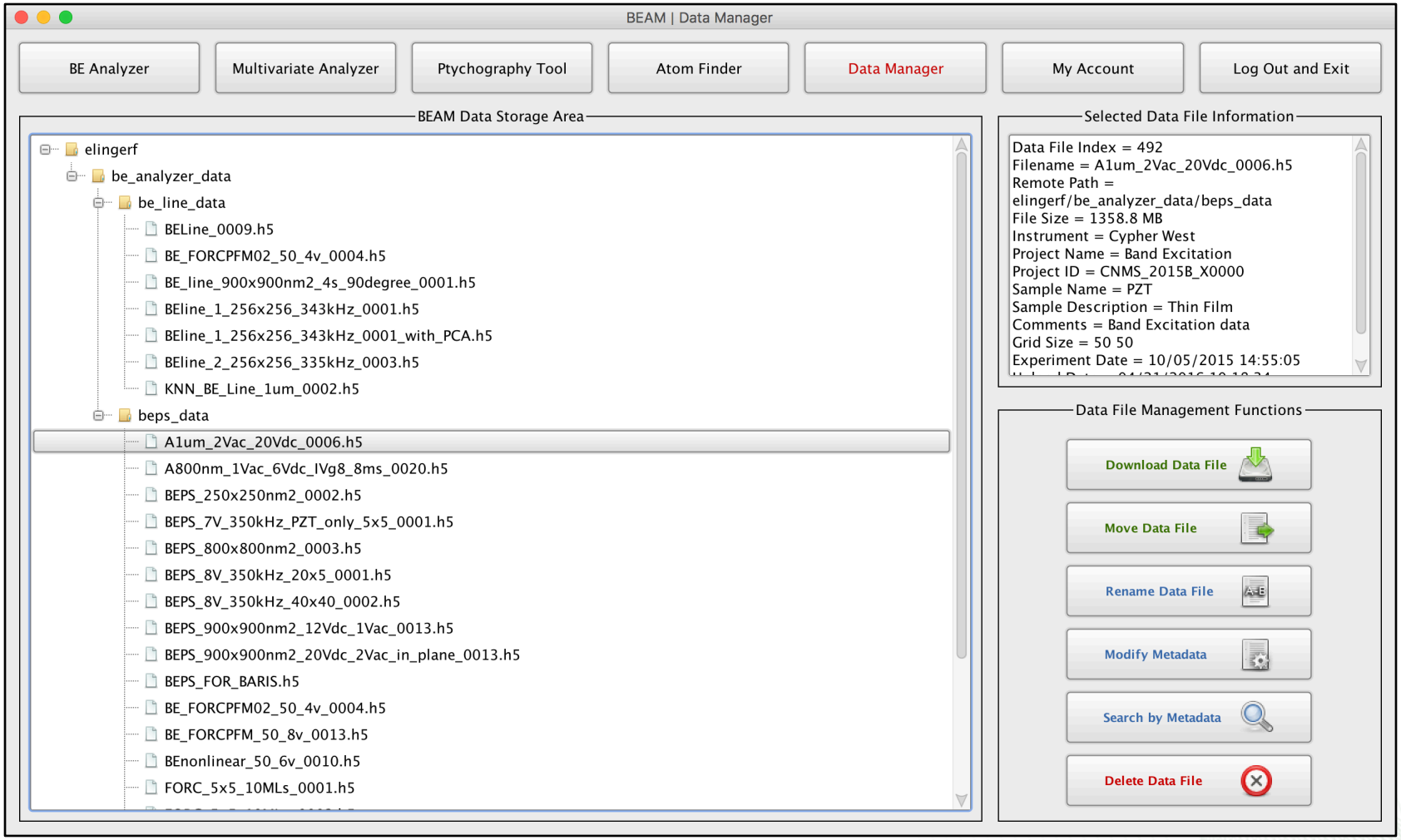


BEAM's *Data Manager* Tool

Manipulate remote directories and files as if they were stored locally



BEAM Workflow Database Object Model

accounts
- username: varchar(20)
- email: varchar(80)
- first_name: varchar(200)
- last_name: varchar(200)
- create_date: datetime
- hash: char(40)
- allocation_indices: text

sessions
- id: char(40)
- username: varchar(20)
- start_time: datetime
- expire_time: datetime
- ip: int
- host: varchar(100)

allocations
- allocation_index: int
- allocation: varchar(40)
- user_facility: enum

analysis_processes
- analysis_process_index: int
- analysis_function_index: int
- data_file_index: int
- allocation_index: int
- id: char(40)
- num_nodes: int
- num_cores: int
- platform_username: text
- input_parameters: text
- create_date: datetime
- end_date: datetime

workflow_updates
- workflow_update_index: int
- analysis_process_index: int
- type: enum
- value: text
- create_date: datetime

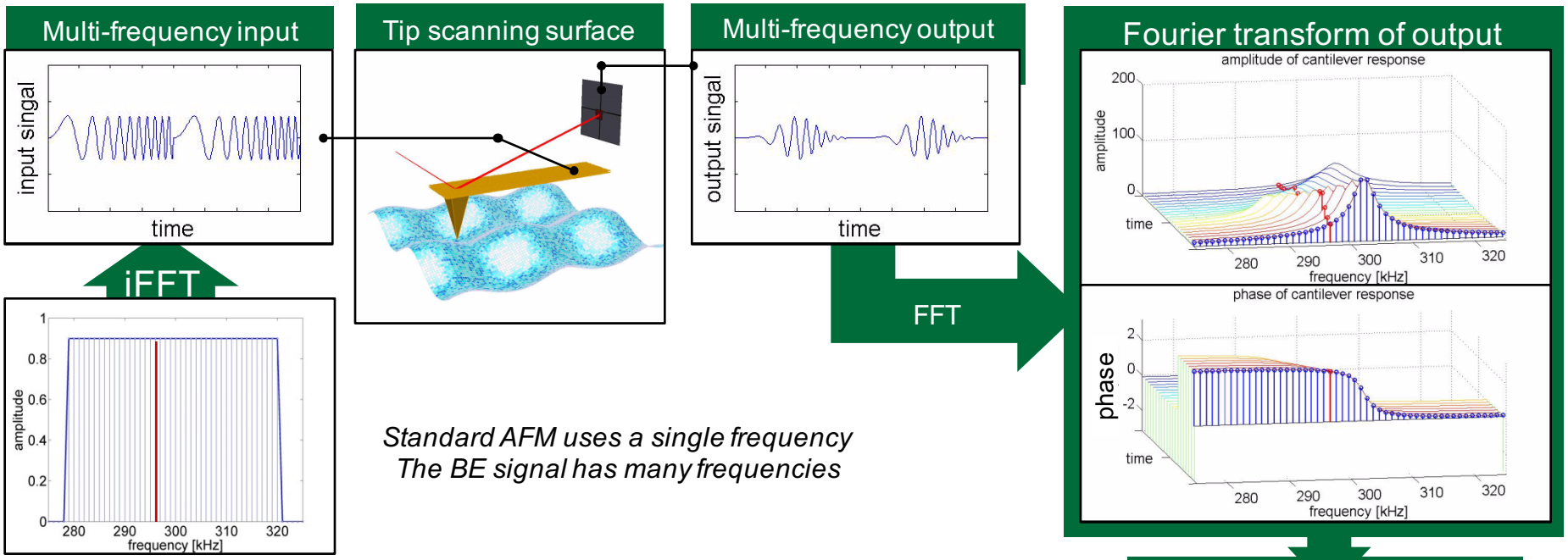
analysis_platforms
- analysis_platform_name: varchar(20)
- host_name: text
- host_key: text
- host_type: enum
- user_facility: enum
- num_nodes_max: int
- num_cores_per_node: int

analysis_functions
- analysis_function_index: int
- analysis_function_type: enum
- analysis_platform_name: varchar(20)
- implementation: enum
- architecture: enum

data_files
- data_file_index: int
- path: text
- name: text
- username: varchar(20)
- data_tool: enum
- instrument: enum
- project_name: text
- project_id: text
- sample_name: text
- sample_desc: text
- comments: text
- grid_size_x: int
- grid_size_y: int
- exp_date: datetime
- upload_date: datetime

Band Excitation (BE) Atomic Force Microscopy 20

Scientists – Stephen Jesse et. al.

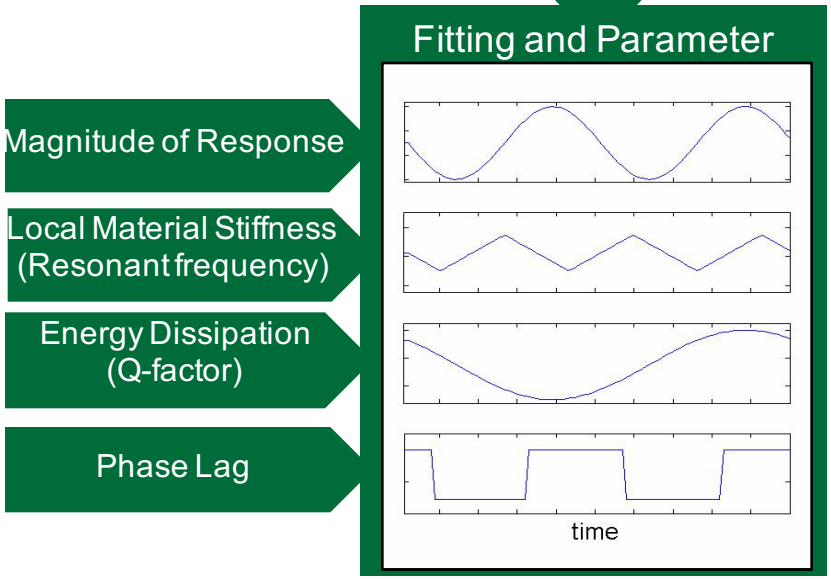


Standard AFM uses a single frequency
The BE signal has many frequencies

The probe/sample is excited by many frequencies to capture complex dynamic interactions between the tip and the surface.

Parallel acquisition of many frequencies results in large data sets that need to be processed.

Fitting is performed on response spectra to extract maps of important material parameters with 10's nm resolution. ***Fitting can sometimes take days to finish.***



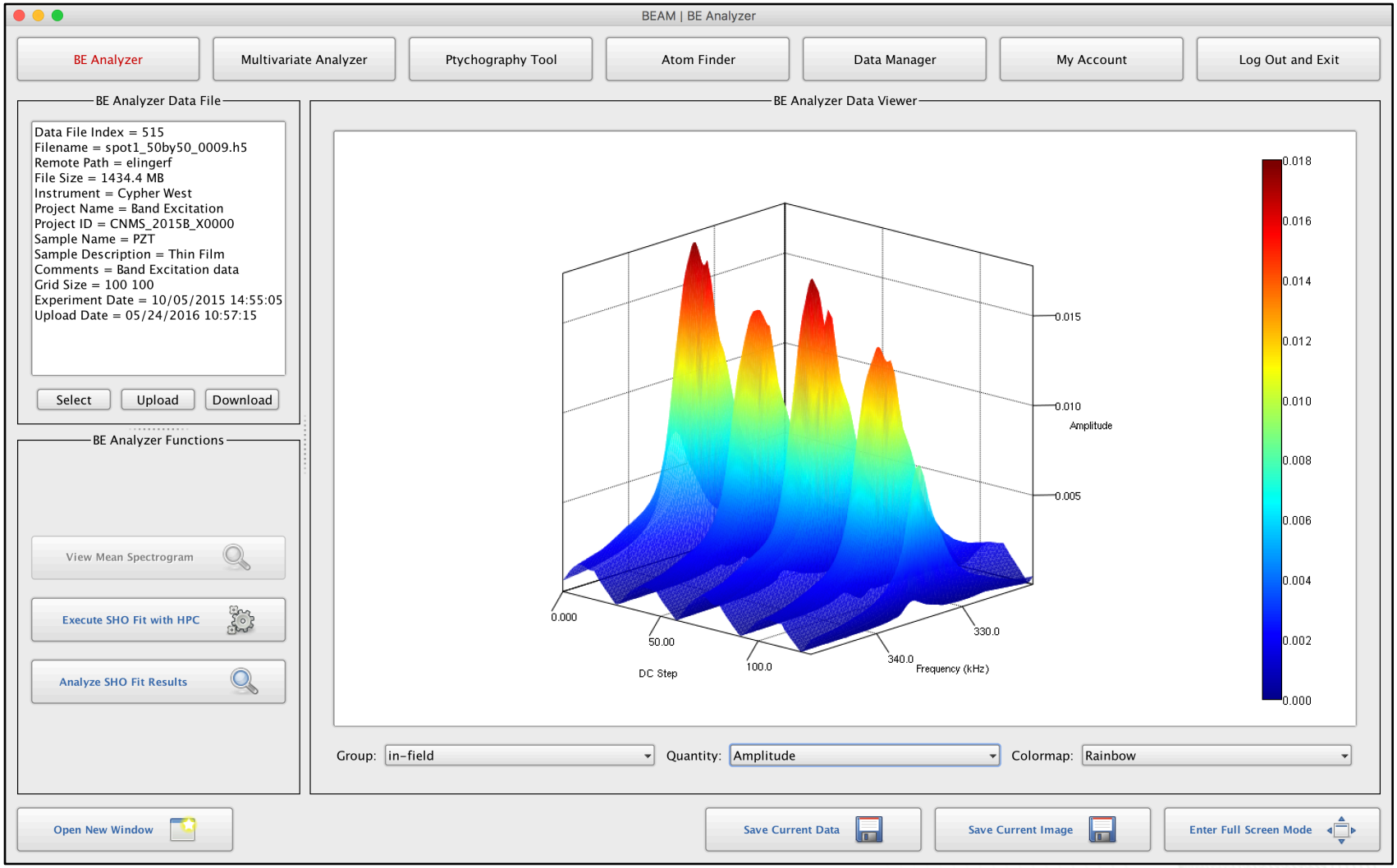
BE Analysis SHO Fitting Algorithm

Mathematician – Eirik Endeve

$$f(\omega; A_0, \omega_0, Q, \varphi) = \frac{A_0\, \omega_0^2\, e^{i\varphi}}{\omega^2 - i\,\omega\,\omega_0/Q - \omega_0^2}$$

- Experimental data fitted to four-parameter model
  - A_0, ω_0, Q, φ
- Levenberg-Marquardt algorithm for least squares minimization of experimental data to model
- Many *independent* minimization problems performed in parallel with Fortran and MPI
- An efficiency increase of 1000x was immediately realized!
- Days to minutes and hours to seconds!

BEAM's *BE Analyzer* Tool



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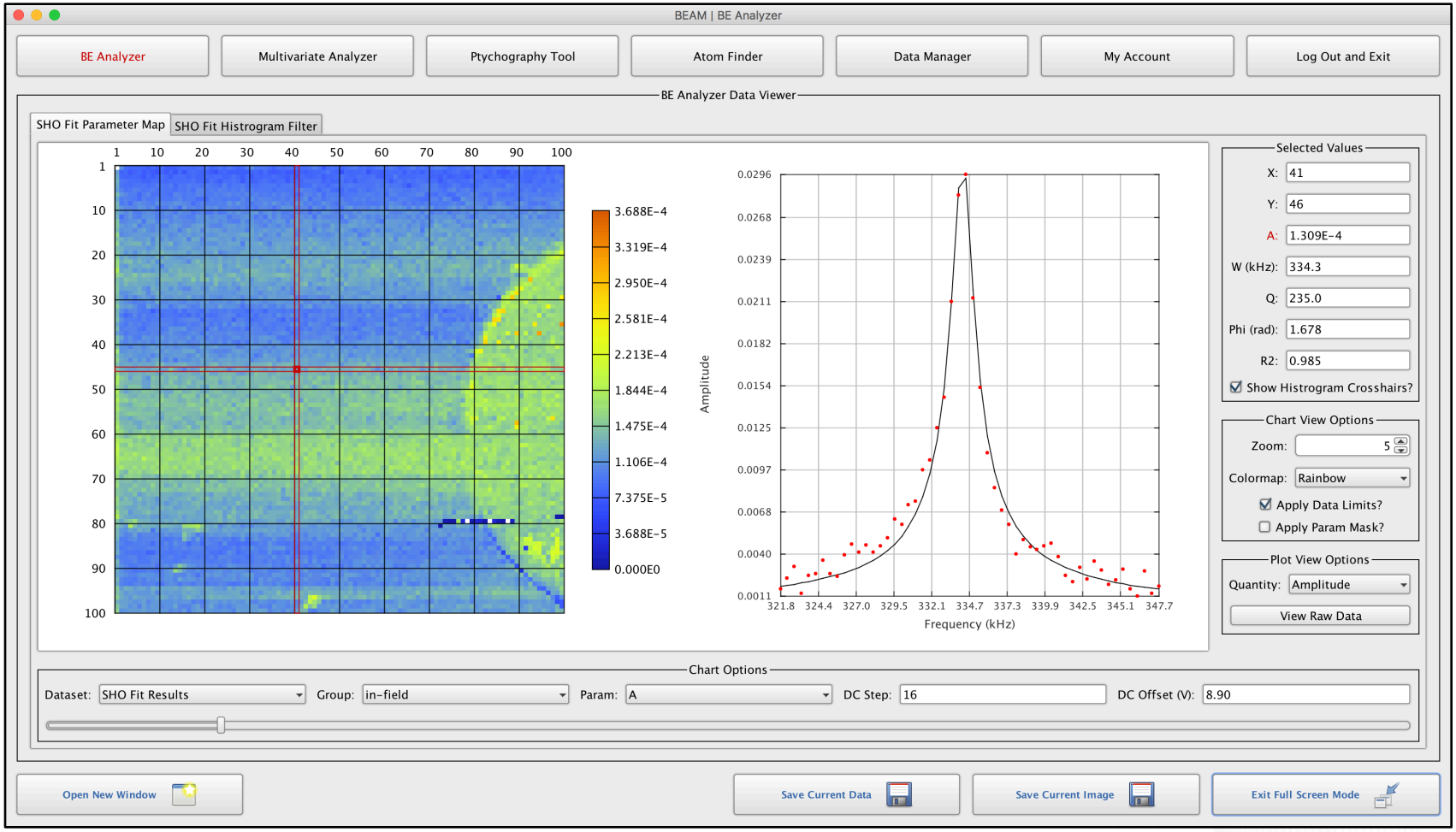
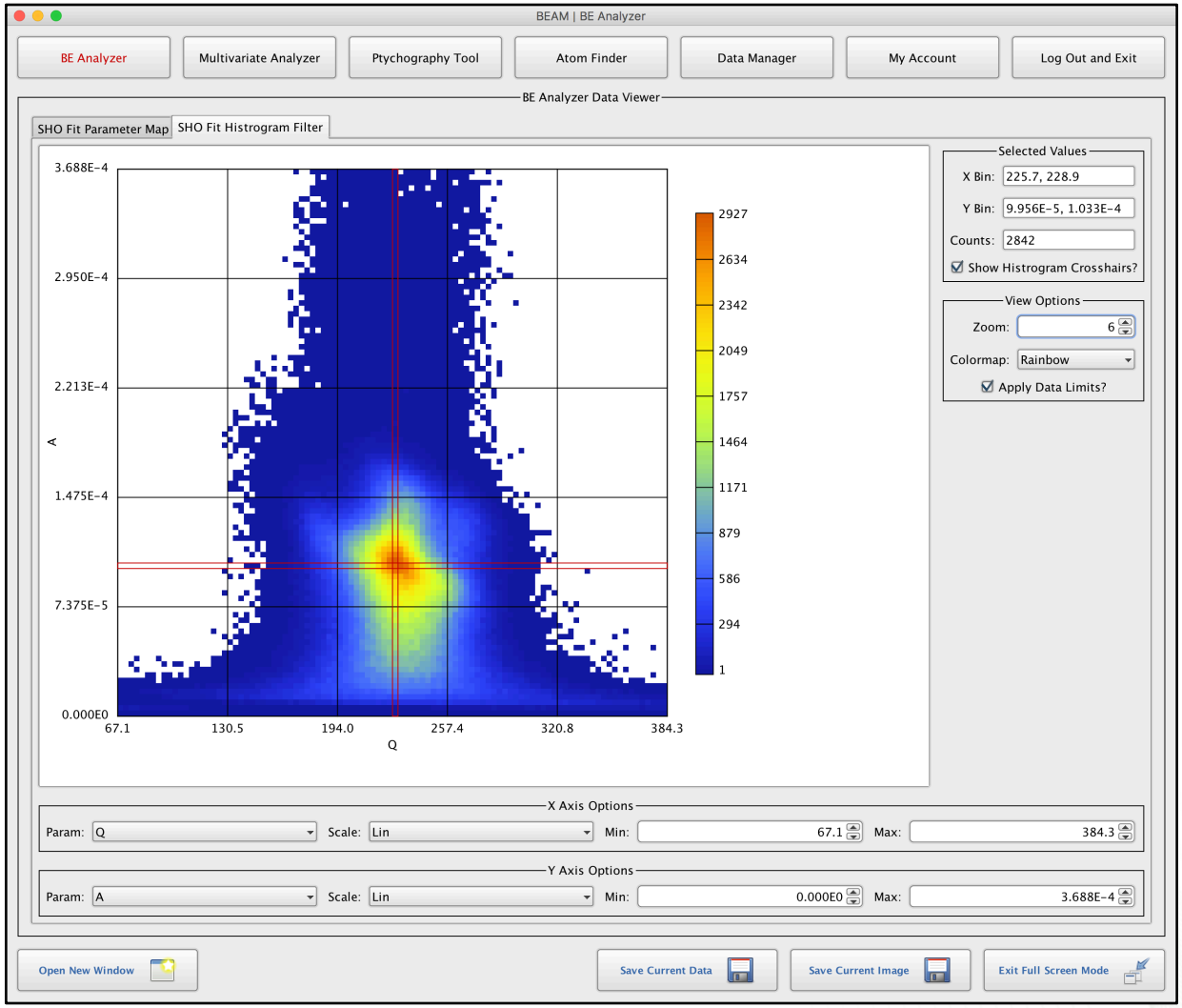


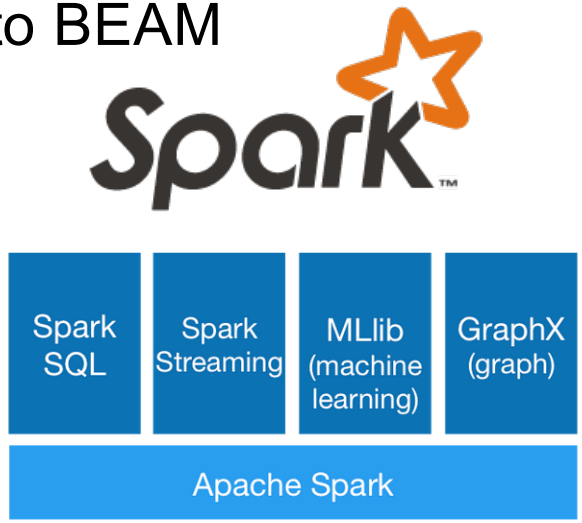
BEAM's *BE Analyzer* Tool



Machine Learning - PCA

Scientists – John Harney, Seung-Hwan Lim
Software Engineer – Dale Stansberry

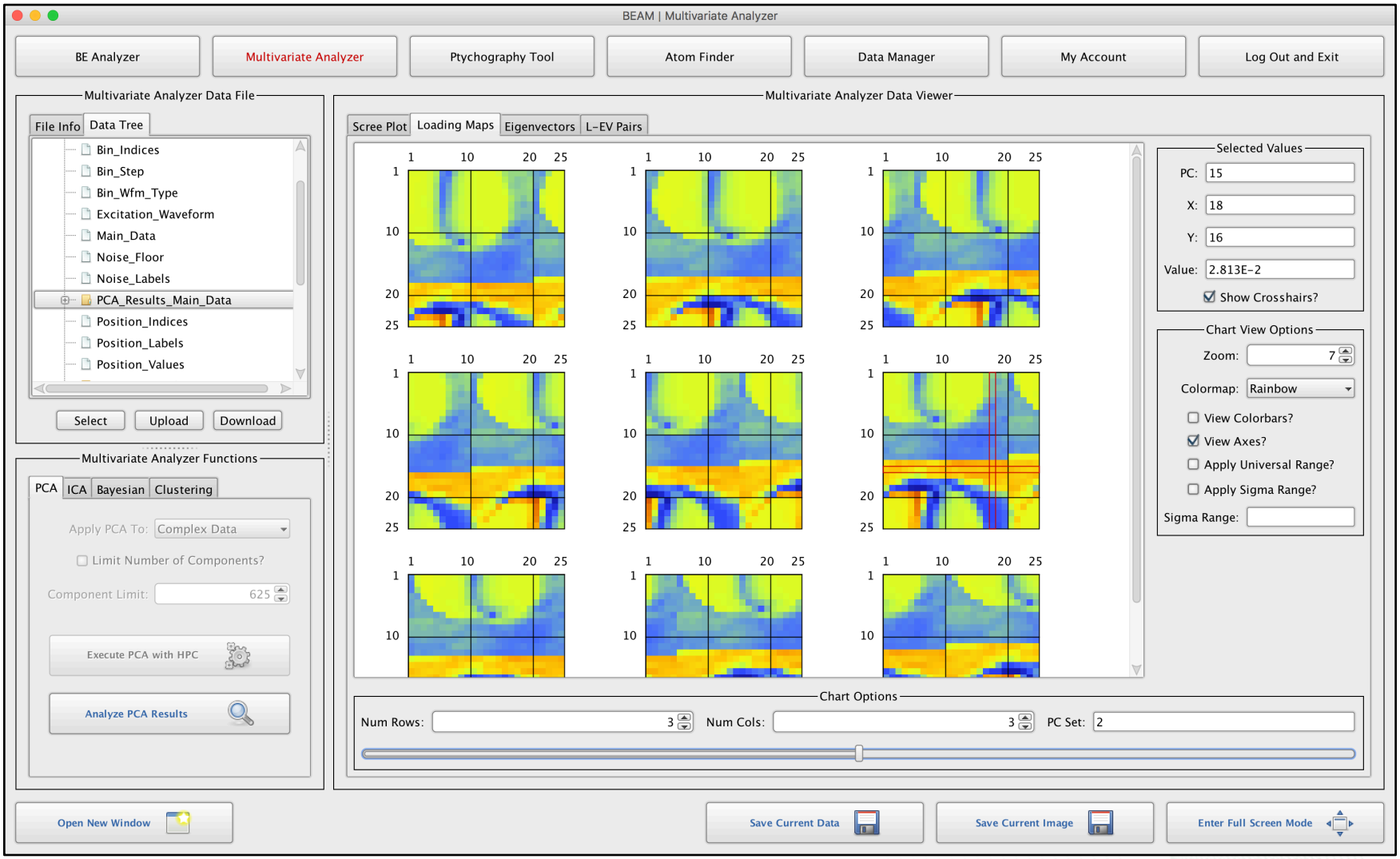
- Working closely with the Advanced Data and Workflow Group
- Integrating Spark On Demand on Rhea into BEAM
- Easy to use "right out of the box"
- Great documentation and support
- Write code in Scala, Java, or Python
- Integration with Java HDF5 IO



Mathematician – Eirik Endeve

- Fortran implementation using MPI and Scalapack
- Available on Titan and EOS through BEAM

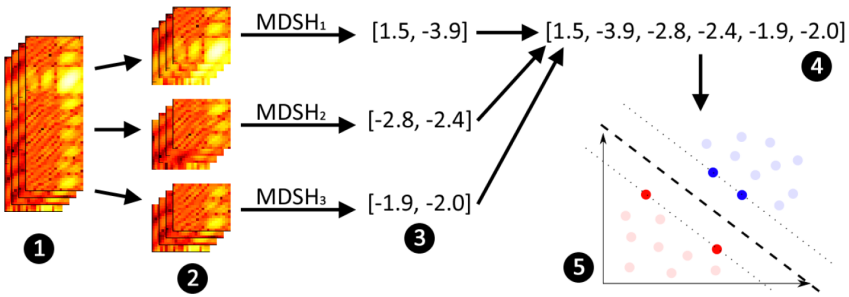
BEAM's *Multivariate Analyzer* Tool



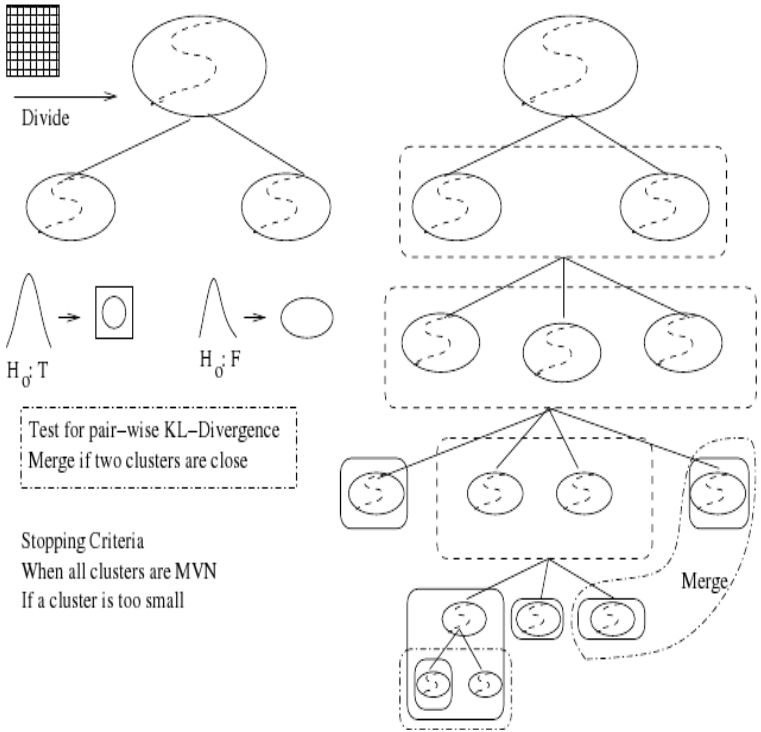
Machine Learning - MDSH-based GX-Means Clustering for Ptychography

Scientist – Chris Symons

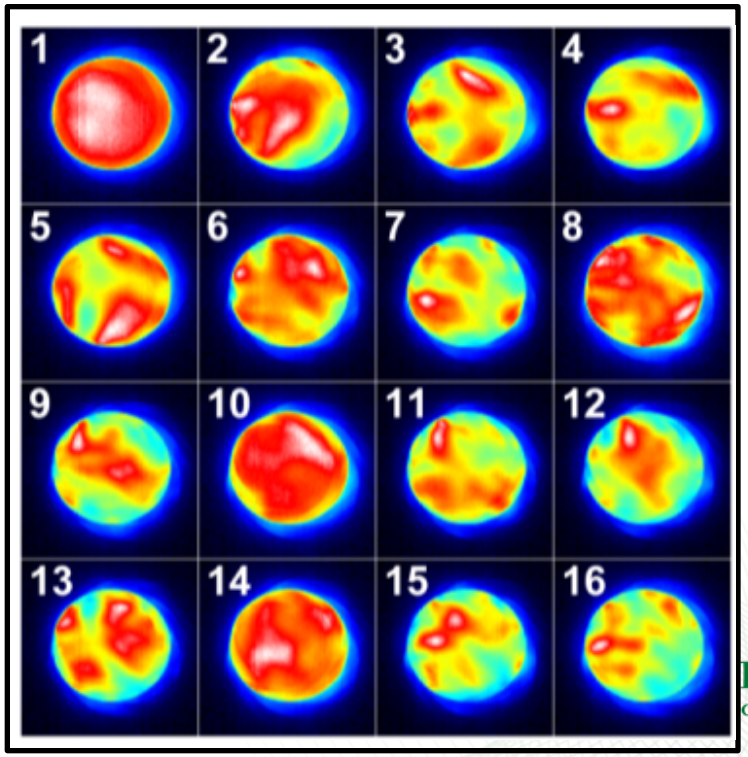
Multi-Dimensional Spectral Hash (MDSH) based dimensionality reduction for ronchigrams to allow fast, accurate clustering of high-dimensional data



GX-Means Intelligent Clustering



Mean Ronchigrams for Each Cluster



Automation of Guided Force-Field Optimization Against Neutron Data with the BEAM Computational Infrastructure at CADES

Scientist – J. Borreguero
Software Engineer – E. Lingerfelt, Mathematician – B. Park
Systems Engineer – N. Grodowitz

Objectives

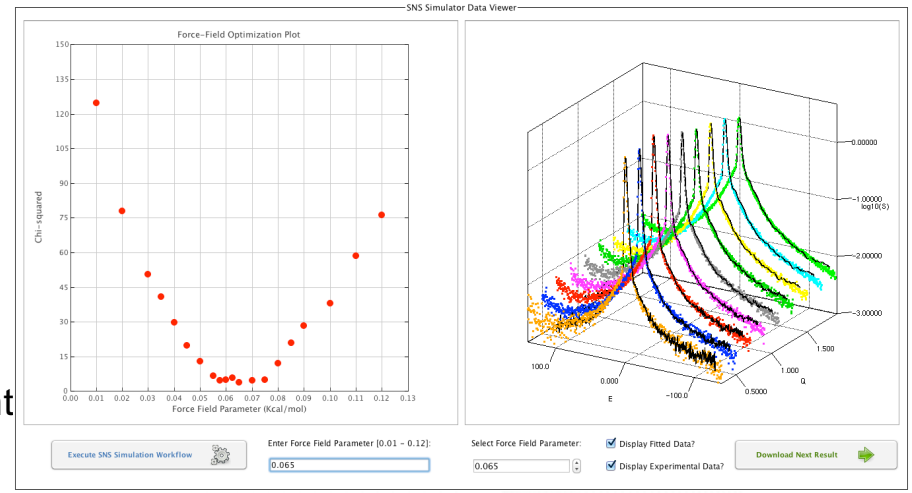
- Automate computational workflows of parameter-refinement of force-fields used in Molecular Dynamics simulations by iterative optimization against Quasi-Elastic Neutron Scattering (QENS) data taken at the BASIS beamline of the Spallation Neutron Source
- Enable interactive 2D and 3D data views of simulation results versus neutron data

Accomplishments

- Guided calculation of neutron scattering functions from the simulated system with the Bellerophon Environment for Analysis of Materials (BEAM)
- Remote job submission, monitoring, and override of HPC resources at CADES with BEAM
- Implementation of interactive 2D and 3D data views using the BEAM XY Plotter and JZY3D with OpenGL

Impact

The optimization workflow empowers the user to rapidly calculate neutron scattering functions from his/her simulation, modify force-field parameters to achieve optimal approximation against experiment, and robustly visualize the results.



The above figure displays the results of 20 guided force-field parameter simulations calculating the optimization of potential energy barrier to methyl rotations in octamethyl silsesqioxane using the BEAM infrastructure at CADES.

SNS SPALLATION NEUTRON SOURCE

CAMM Center for Accelerating Materials Modeling

beam

CADES

BEAM Neutron Science Workflow at CADES

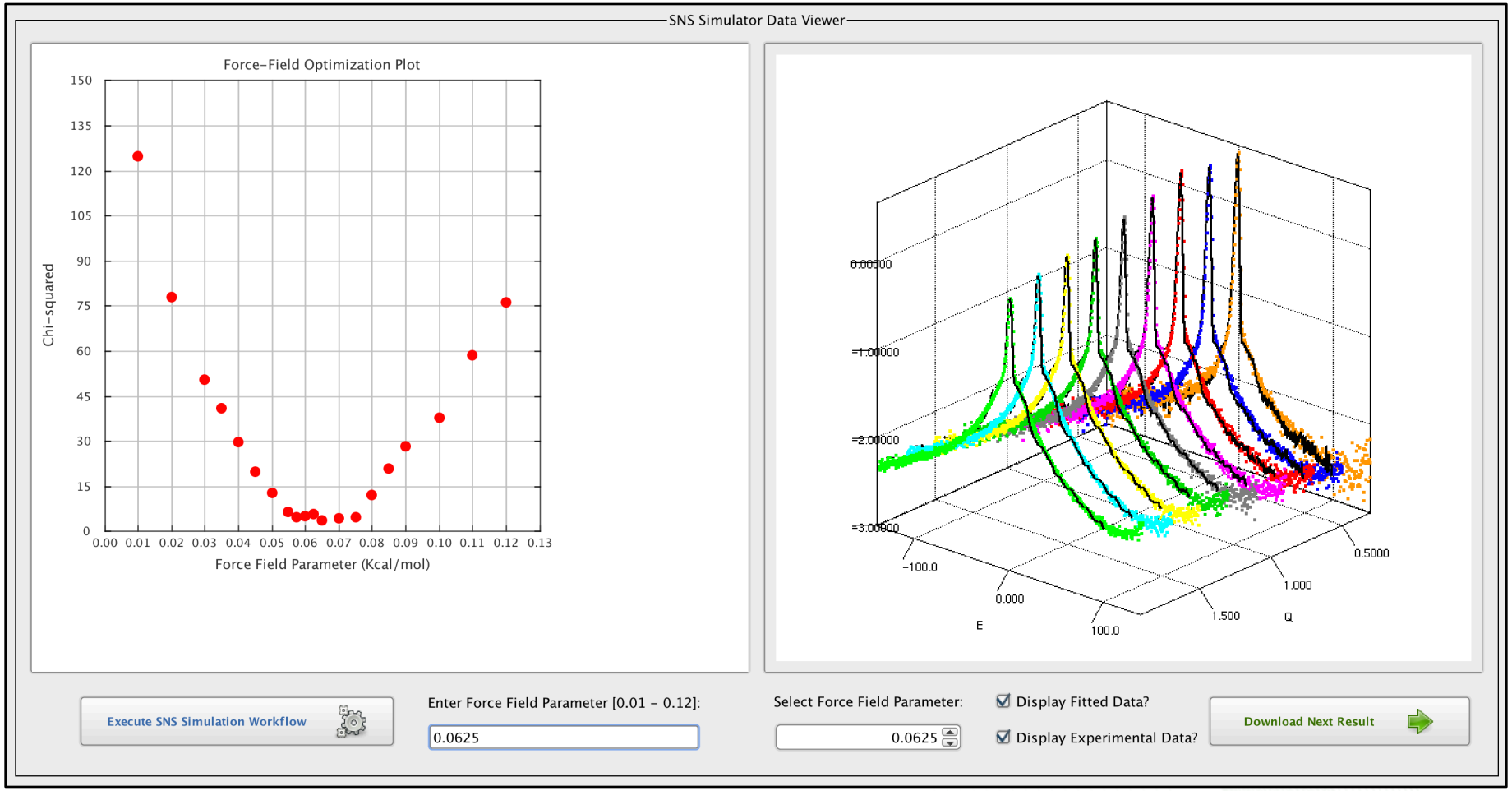
(1) NAMD Scalable Molecular Dynamics

(2) Amber Tools — removal of global rotations and translations

(3) Sassena — calculation of the structure factors

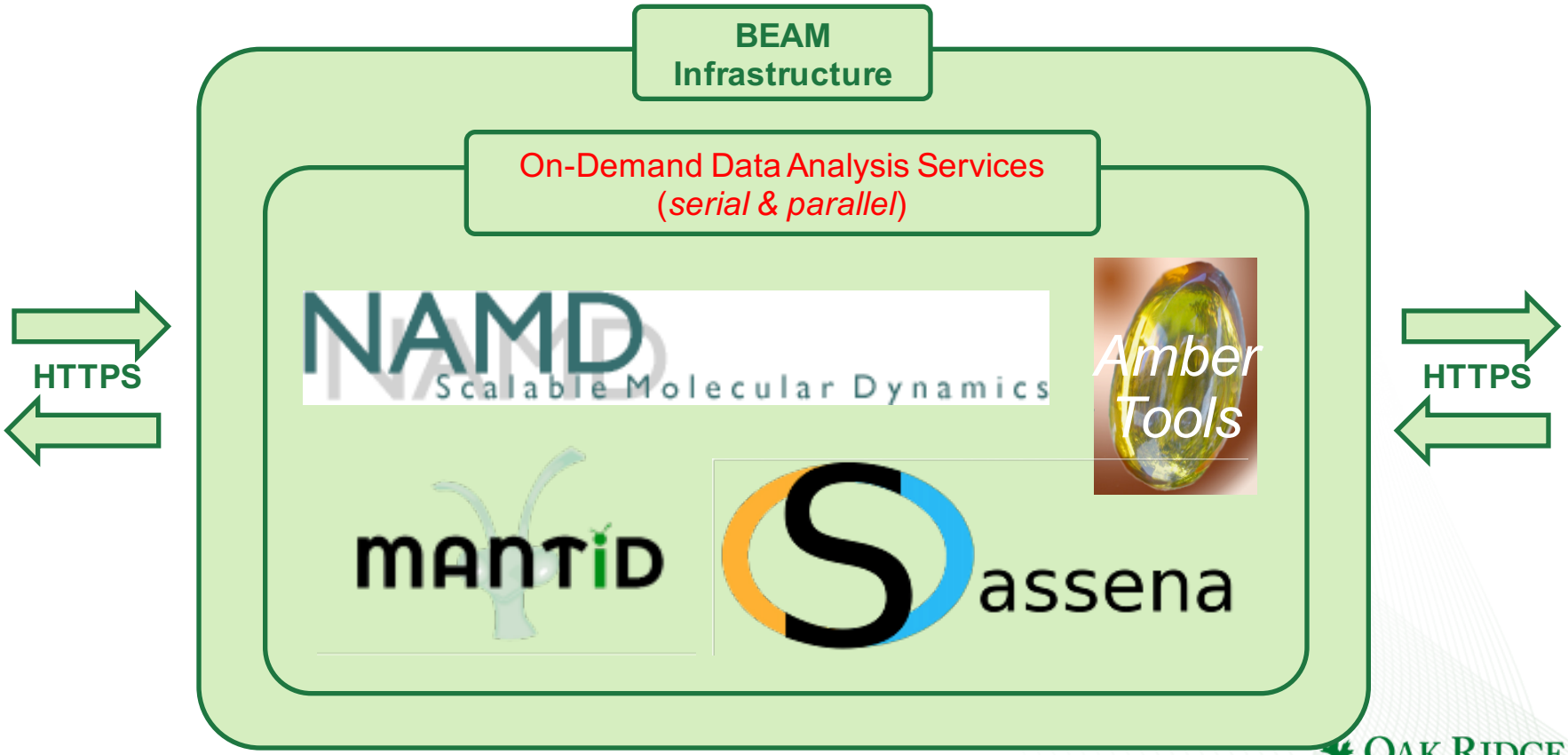
(4) MANTID — fitting against experiment

BEAM Neutron Science Workflow at CADES

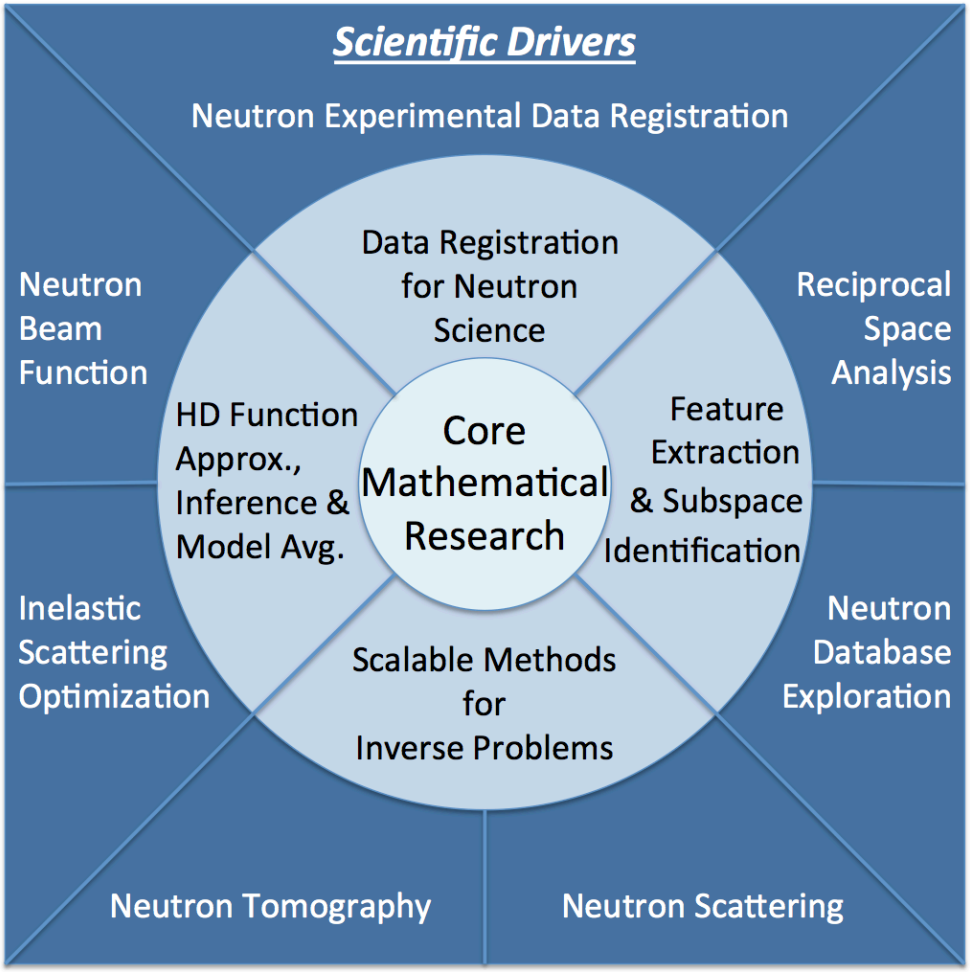


Enable Online NDAV Workflows using BEAM

- Potential to enable automated workflows utilizing multiple software packages and tools
- Leverage capability to initialize, monitor, and override HPC workflows
- Provide a bridge between existing SNS workflows and the OLCF



ACCURATE QUANTIFIED MATHEMATICAL METHODS FOR NEUTRON SCIENCE (*ACUMEN*)



ACUMEN will develop scalable mathematical research that will impact neutron & experimental science at ORNL. Current focus targets:

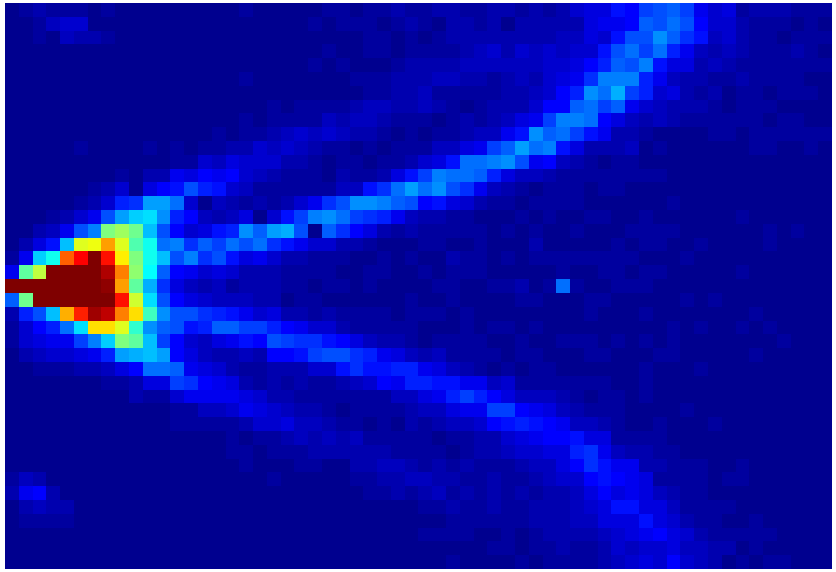
- Neutron Tomography
- Neutron Scattering
- Inelastic Scattering Optimization
- Resolution Function
- Institute involvement and Laboratory investment

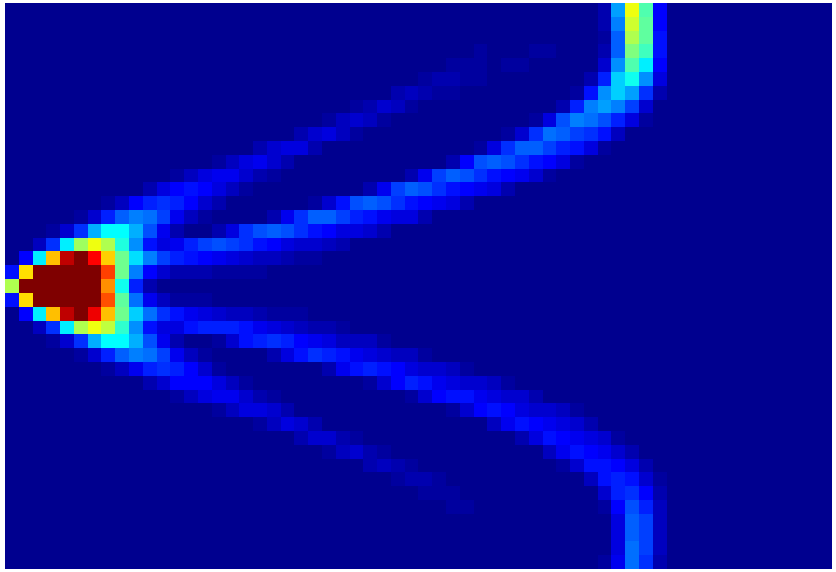
ASCR Funded Project under Dr. Steve Lee.

Inelastic Neutron Scattering

Scientists – Olivier Delaire, Jennifer Niedziela, Dipanshu Bansal
Mathematicians – Rick Archibald, Feng Bao

- Time-of-Flight Neutron Spectrometer used to measure Niobium on TOPAZ as seen on the *top right.*
- S(Q,E) space is four dimensional, forming a large search space to optimize.





- Theoretical phonon calculation using DFT computationally expensive.
- Developed scalable optimization of DFT with probabilistic bounds of solution.
- Whole S(Q,E) spaced optimized *bottom left.*

Inelastic Neutron Scattering

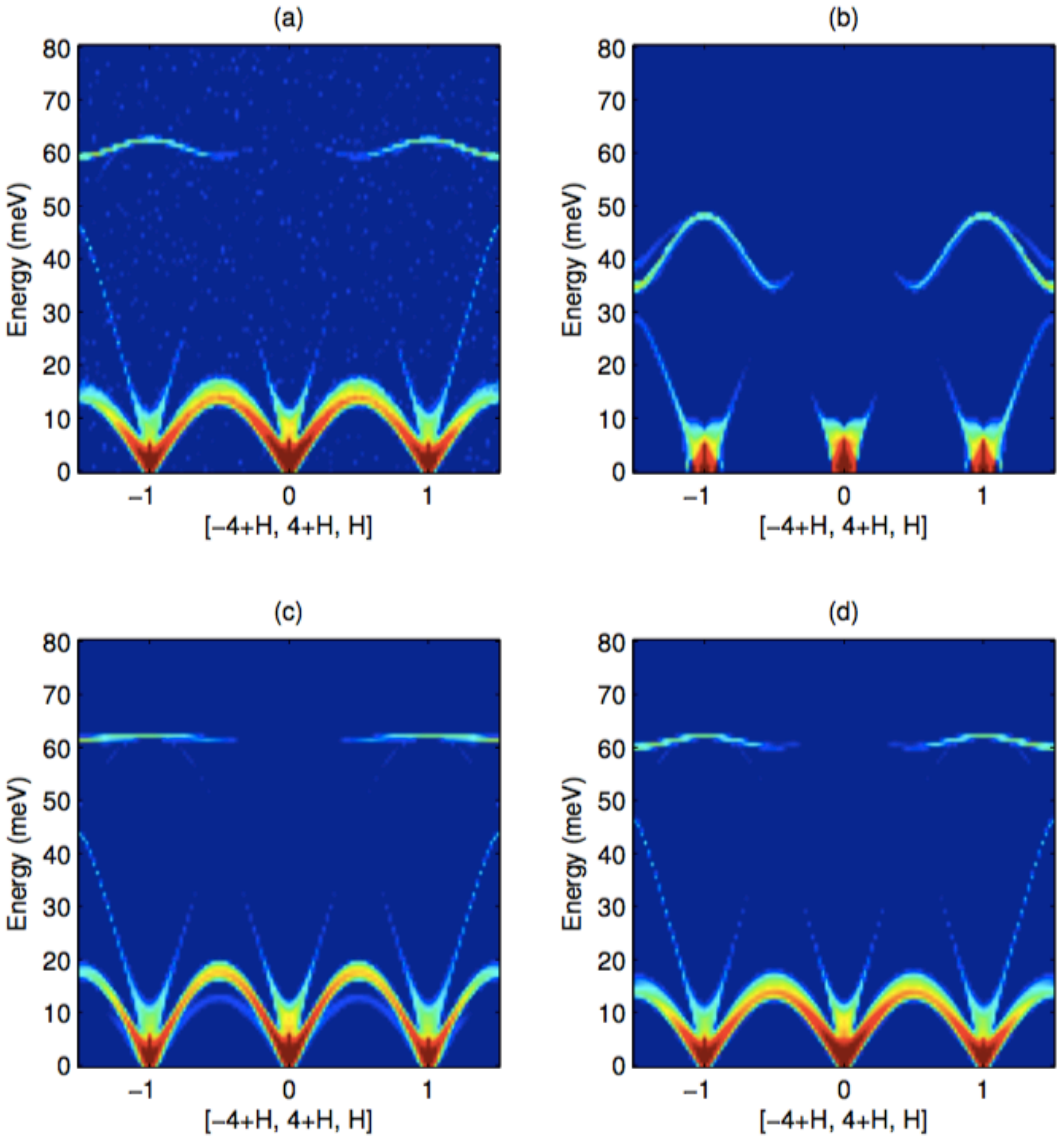
- Inelastic Neutron Scattering dynamics can be given as:

$$I_{\{\Phi\}}(\mathbf{Q},\omega) = S_{\{\Phi\}}(\mathbf{Q},\omega) * R(\mathbf{Q},\omega)$$

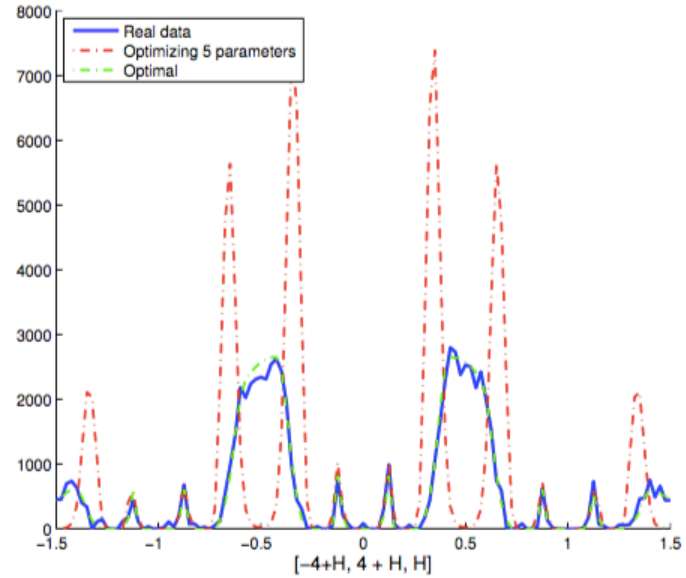
Intensity of scattered neutrons is convolution of the scattering function and the resolution function.

- SIMPHONIES code calculates scattering function from atomic force parameters
- ACUMEN codes are utilized to optimize SIMPHONIES output for comparison to experimental data
- Task is expensive experimentally and computationally
- Plan to install and maintain accessible SIMPHONIES /ACUMEN workflow on CADES and OLCF compute resources

ACUMEN / SIMPHONIES Example – Silicon



Cross-section



(a) Measurement
(b) Initial Conditions
(c) Nearest Neighbors
(d) Final

BEAM Future Roadmap

- Scale to larger data sizes and real-time streaming data flows
- Deployment of a suite of machine learning methods provided as toolkit to users
- Multi-modal data integration and analysis across multiple microscopes and experimental modalities
- Provide expanded capability to execute ensembles of simulations to guide experiments at the SNS and CNMS ("theory-in-the-loop")
- Continue development of intuitive user-friendly workflows and custom dashboards and software tools for large-scale integrated data analytics, computational modeling, and collaboration
- Implement, integrate, and deliver HPC workflow, data management, and analysis capabilities as an open science platform at CADES and the OLCF!