

Applied Mathematics and Neutrons

ACUMEN

Rick Archibald
Oak Ridge National Laboratory

**Neutron Day Seminar Series:
Data and Instrument Software**

**SNS
March 24, 2017**

Motivation – Computation Facilities

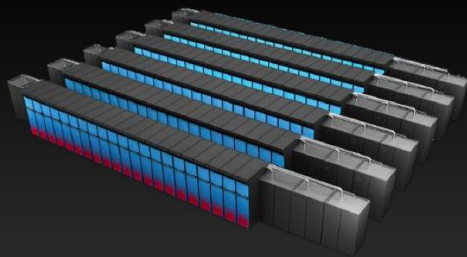
Titan at Oak Ridge

World's Top Open Science Computing Research Facility

18,000 Tesla GPUs

20+ PetaFlops

~90% of flops from GPUs



2x Faster, 3x More Energy Efficient
than Current #1 (K Computer)

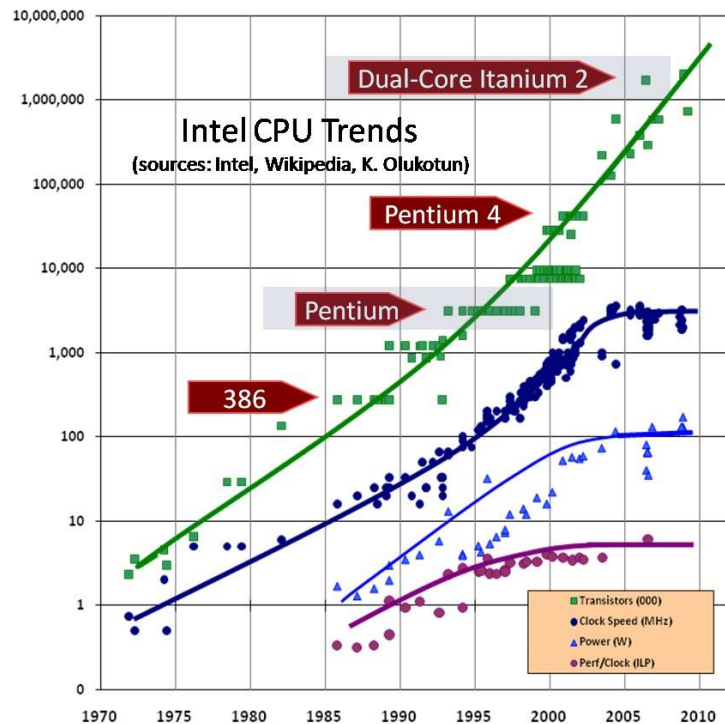
TITAN VS SUMMIT

Compute System Comparison



ATTRIBUTE	TITAN	SUMMIT
Compute Nodes	18,688	~3,400
Processor	(1) 16-core AMD Opteron per node	(Multiple) IBM POWER 9s per node
Accelerator	(1) NVIDIA Kepler K20x per node	(Multiple) NVIDIA Volta GPUs per node
Memory per node	32GB (DDR3)	>512GB (HBM+DDR4)
CPU-GPU Interconnect	PCI Gen2	NVLINK (5-12x PCIe3)
System Interconnect	Gemini	Dual Rail EDR-IB (23 GB/s)
Peak Power Consumption	9 MW	10 MW

The Free Lunch Is Over: A Fundamental Turn Toward Concurrency in Software



Motivation – Experimental Facilities



One of the highest steady-state neutron flux research reactor in the world

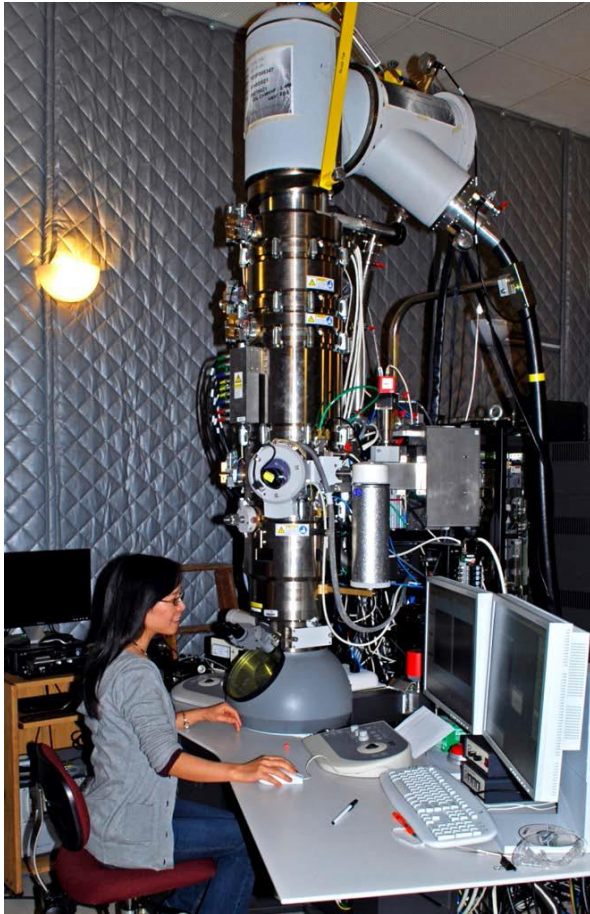


Spallation Neutron Source

*World's most powerful
accelerator-based
neutron source*



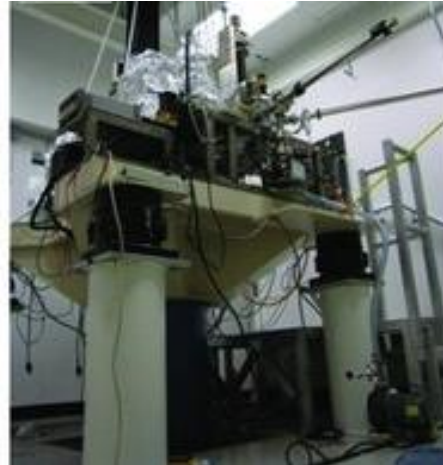
Motivation – Experimental Facilities



CNMS

Center for Nanophase
Materials Sciences

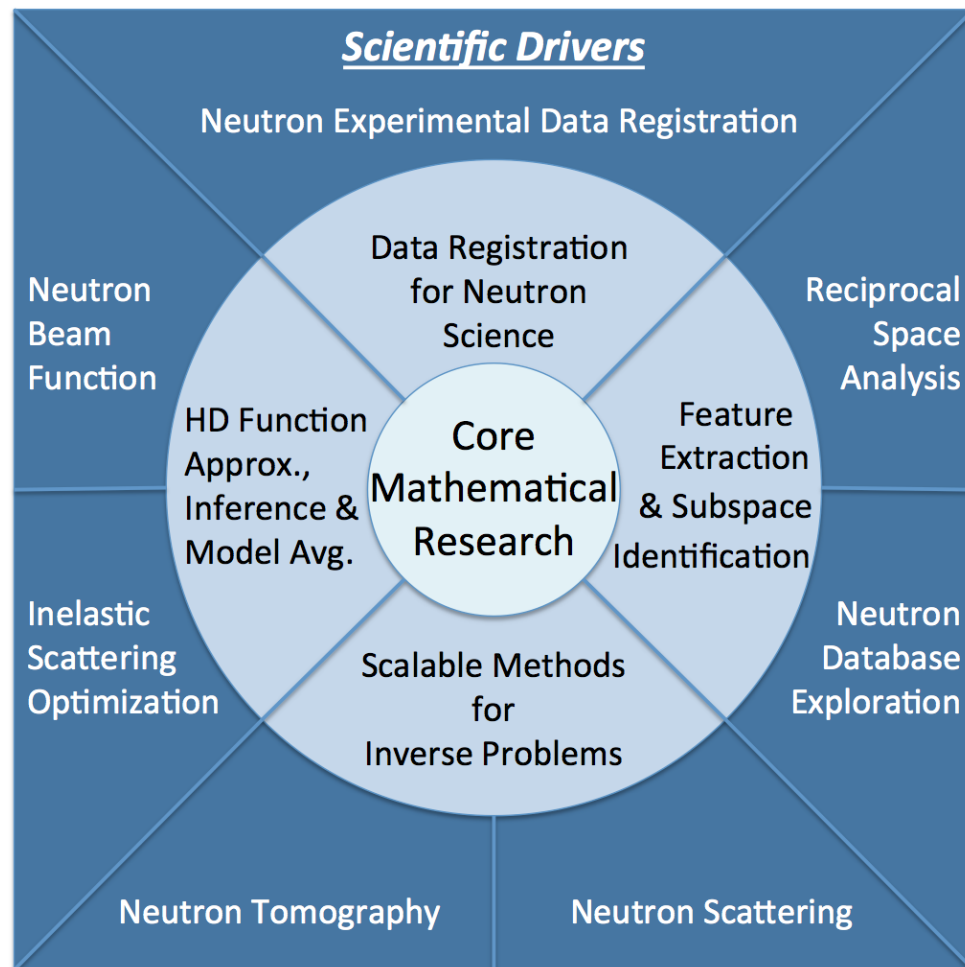
*State-of-the-art nanoscience experimental
equipment including STEM-TITAN, Atomic
Probe, & SPM*



OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY


UT-BATTELLE

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



ACUMEN will develop scalable mathematical research that will impact neutron science.

ASCR Funded Project under Dr. Steve Lee.

ACUMEN integrates Mathematics with Instruments Scientists

ORNL Facility

Instrument Scientist



Dr. Sergei Kalinin

*Burton Medal, Microscopy Soc. of America
Dir. of Inst. Funct. Imaging of Materials*

Dr. Greg Smith

*NSSA Fellow
Structure and Dynamics of Soft Matter GL*

Dr. Mark Lumsden

*Time-of-Flight Spectroscopy GL
Mantid Scientific Committee Member*

Dr. Anibal Ramirez-Cuesta

*Spectroscopy GL
Instrument Lead for VISION*

Dr. Olivier Delaire, 2008-2011

*Clifford G. Shull Fellow,
DOE Early Career Research Award 2014*

Dr. Garrett Granroth

*Scientific Data Analysis GL
Instrument Lead for SEQUOIA*



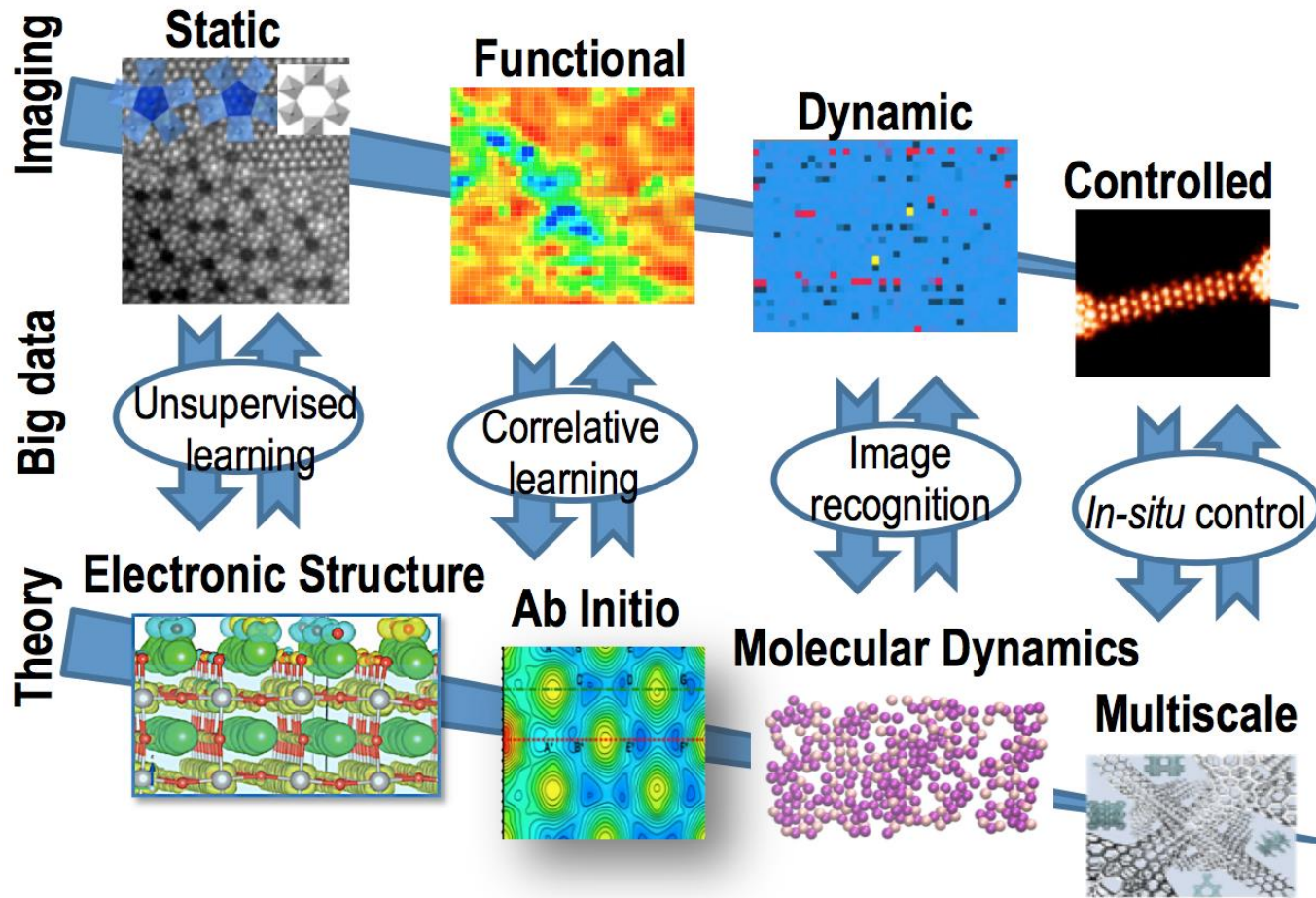
The logo for the High Flux Isotope Reactor (HFIR), featuring a green shield with the letters "HFIR" in white, and a stylized neutron beam or particle path extending from the shield.

Dr. Hassina Bilheux

*Lead for HFIR Beam line CG-1D
Instrument Lead for future SNS VENUS*

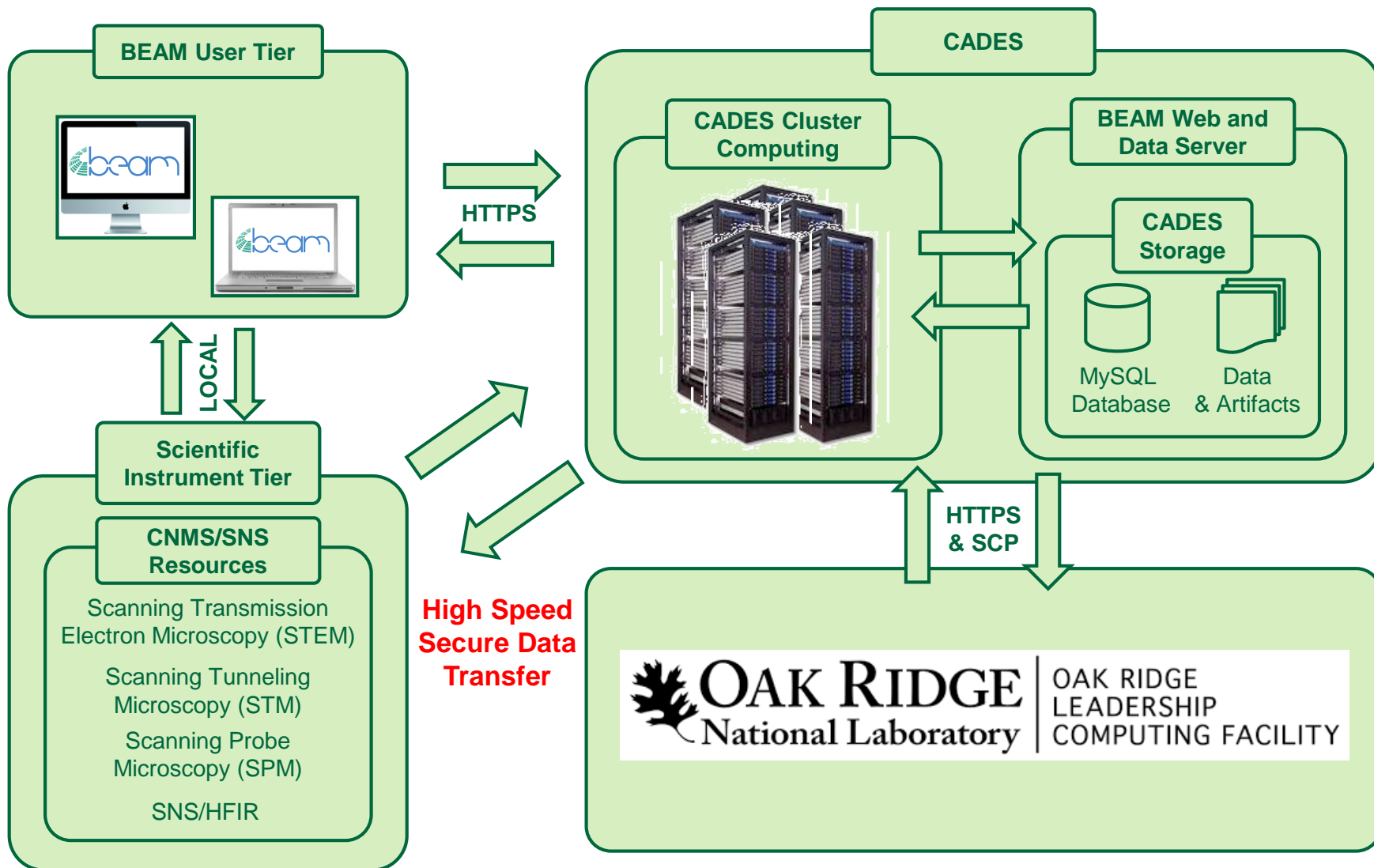
Connecting with ORNL Institutes and Infrastructure

Collaboration - Institute for Functional Imaging of Materials



Institute will bridge imaging and theory using HPC data analytics to reveal local physical, chemical and structure-properties in materials, and use this knowledge to enable the design of new materials with tailored functionalities.

Big Data and High Performance Computing



Mathematical Challenges at ORNL Facilities

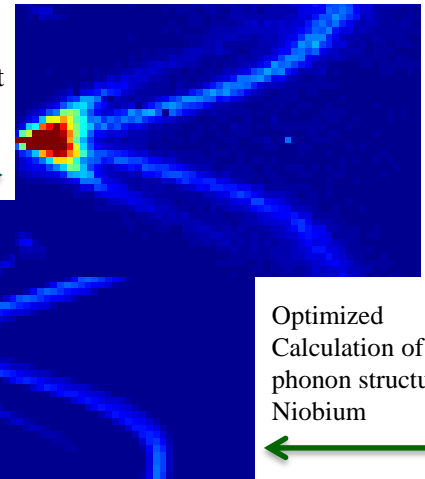
ASCR – R. Archibald, C. Webster, F. Bao, R. Barnard, E. D’Azvedo, E. Endeve, M. Stoyanov, & G. Zhang

BES – H. Bilheux, O. Delaire, G. Granroth, S. Kalinin, M. Lumsden, A. Ramirez-Cuesta, & G. Smith



Building fast HPC algorithms that can be used for near-real time computational feedback for experimentalist.

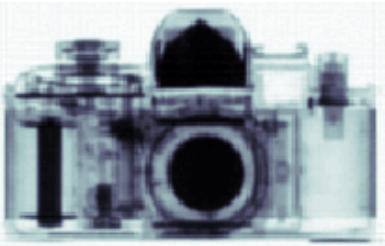
Measurements from ARCS Time-of-Flight Neutron Spectrometer



Optimized Calculation of phonon structure of Niobium

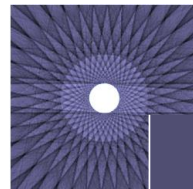
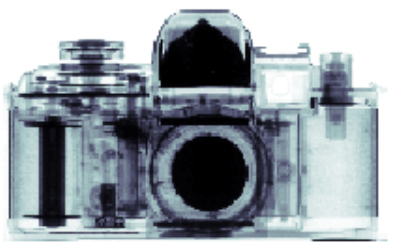


* courtesy of D. Abernathy

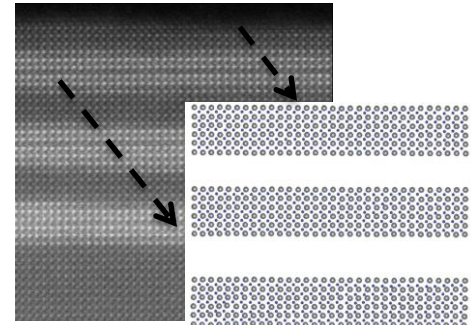


AGUMEN Accurate Quantified Mathematical Methods for Neutron Science

Advanced reconstruction methods improve accuracy and speed in Neutron tomography.



* Perovskite Superlattice measured by STEM, courtesy of A. Borisevich



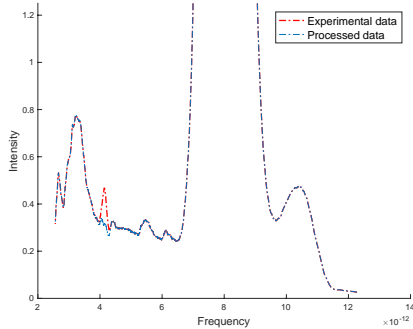
* HFIR data courtesy of H. Bilheux



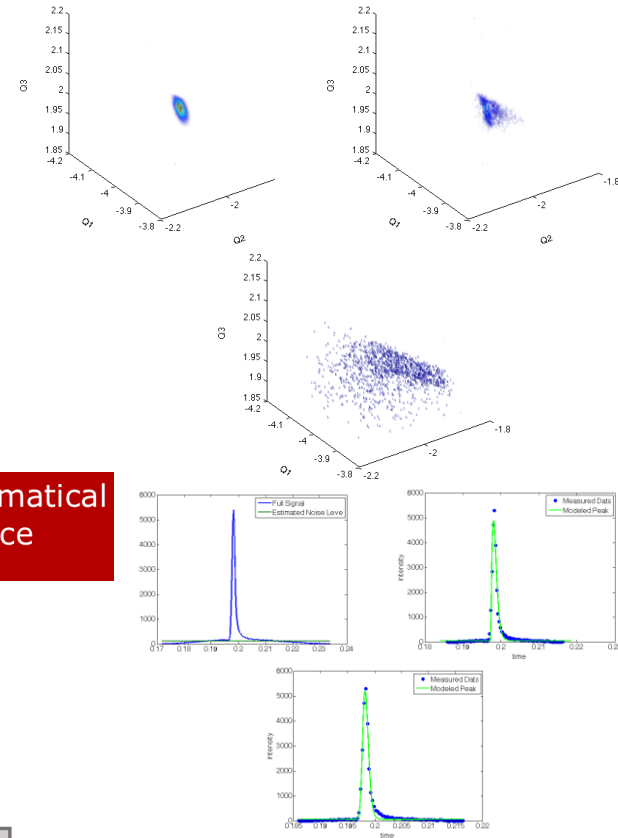
Providing algorithms to connect experimentalists with HPC to provide complete analysis of the big data being produced

Mathematical Challenges at ORNL Facilities

ASCR – R. Archibald, F. Bao, R. French, T. Johnston, R. Patton, & G. Zhang
 BES Y. Cheng, M. Doucet, G. Granroth, W. Heller, A. Ramirez-Cuesta

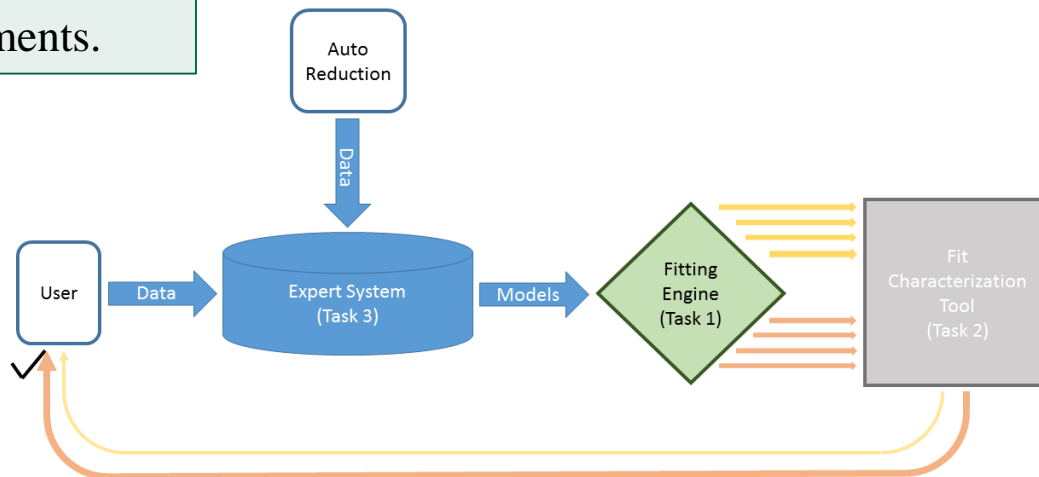


Post process VISION signals to remove neutrons with half wavelength that are not completely removed by physical filter.



Using Machine learning to accelerate scientific discovery for SANS experiments.

AGUMEN Accurate Quantified Mathematical Methods for Neutron Science



Providing algorithms to robustly optimize the IC curve to experimental data, estimating peak location, volume, and background noise level.

Thank You.

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