OAK RIDGE National Laboratory

Inverse and Data Analytic Methods for Experimental Facilities

Rick Archibald

Second Target Station/Computer Science & Math Workshop

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

U.S. DEPARTMENT OF ENERGY

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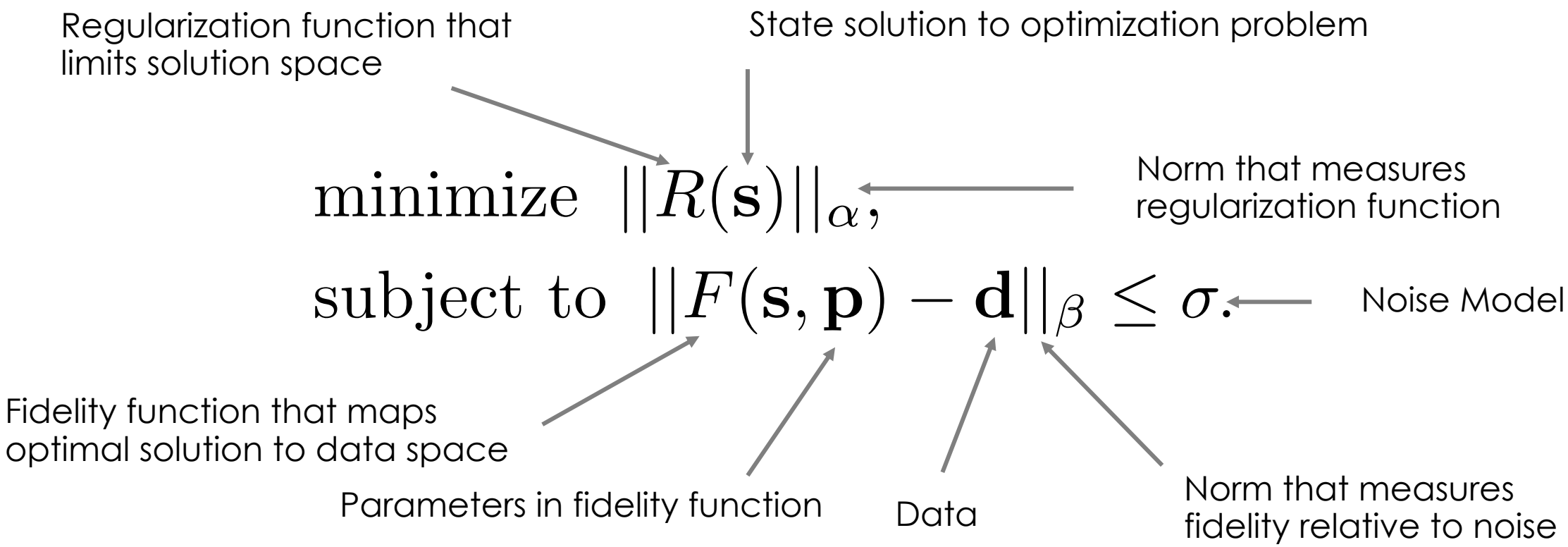
Inverse Modeling

What is measured is often not the state of interest.

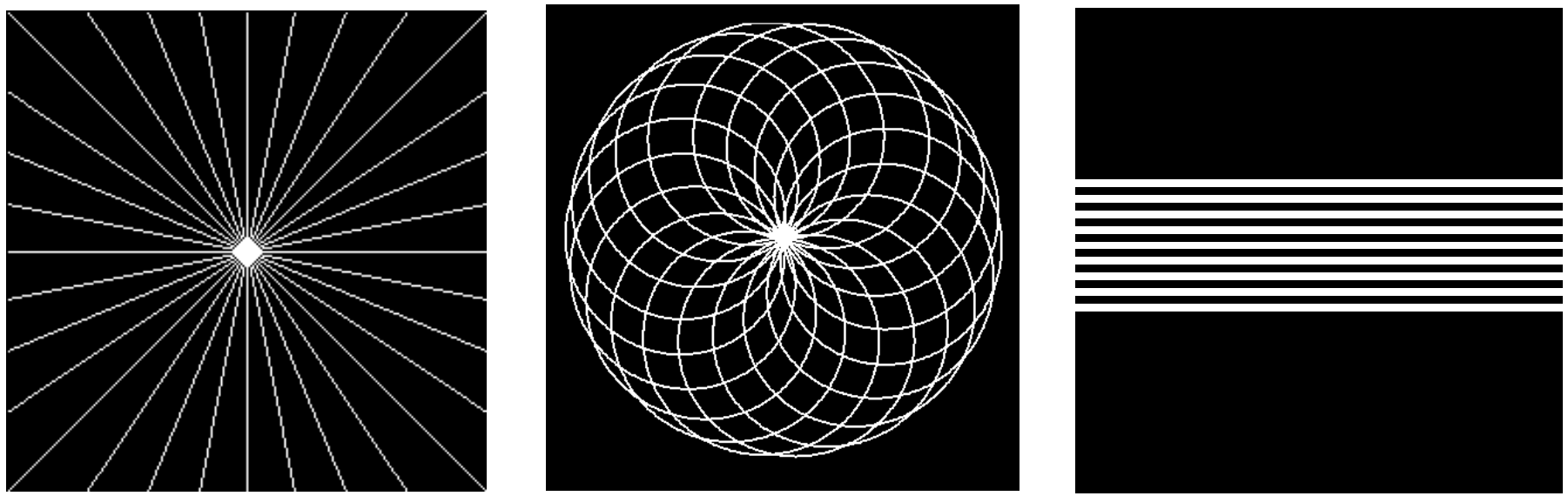


Challenge: Improve regularization, fidelity, and speed.

Inverse Modeling

Partial Fourier data problem solved with compress sensing.

$$\text{minimize } ||\nabla_x \mathbf{s}||_1 + ||\nabla_y \mathbf{s}||_1,$$
$$\text{subject to } ||\mathcal{F}(\mathbf{s}) - \mathbf{d}||_2 \leq \sigma.$$

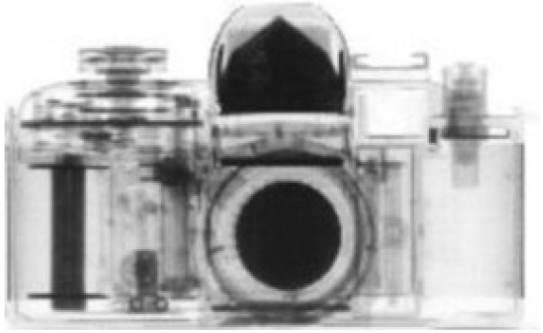


Tomography MRI Ultrasound

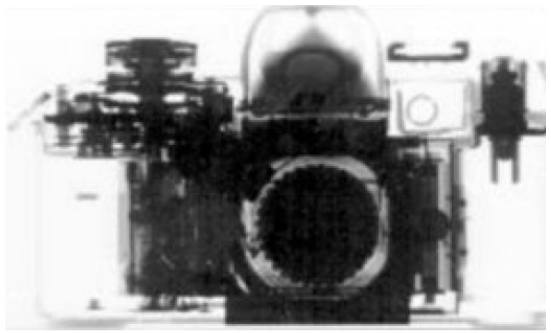
Experimental Science: SNS

$$\mathbf{d} = F(S, R) = S_{\{\Phi\}}(\mathbf{Q}, \omega) * R(\mathbf{Q}, \omega)$$

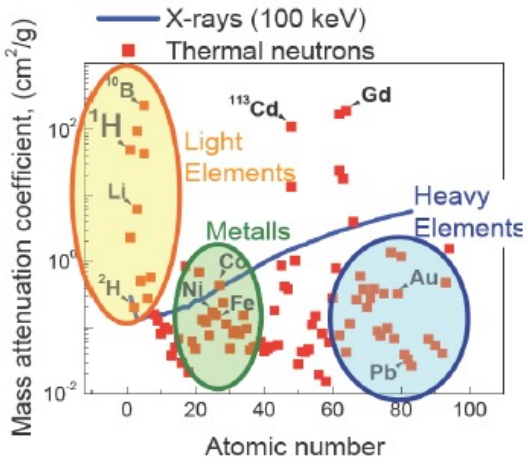
Why Neutrons?



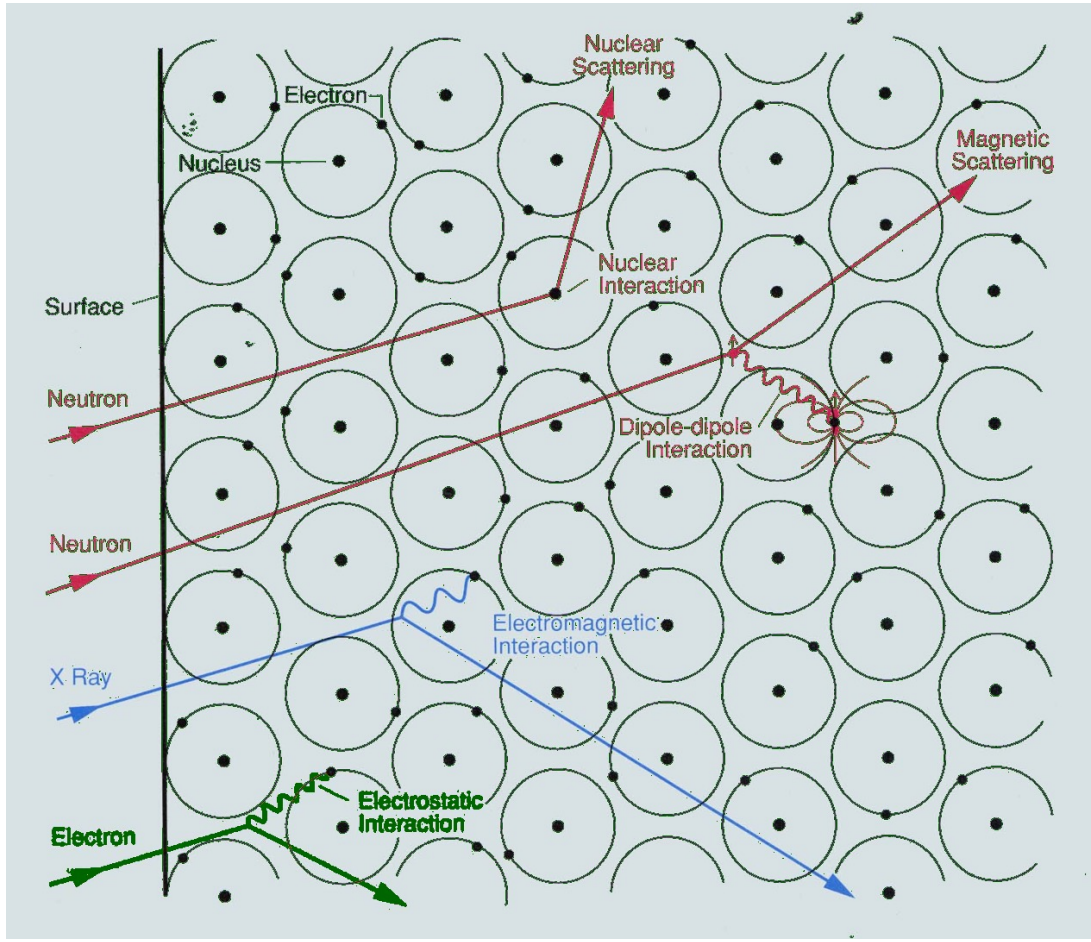
Neutrons



X-Rays

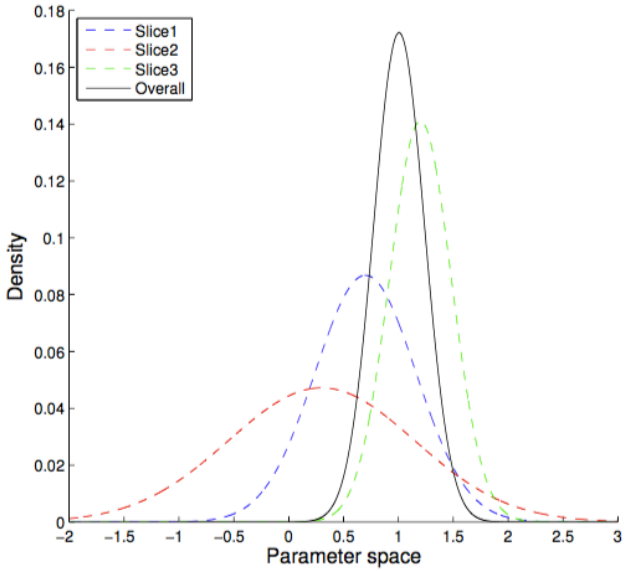


- Penetrate metals without absorbing
- Highly sensitive to water and hydrocarbons
- High contrast to light elements
- Sensitivity to magnetism
- Measure dynamics and structure



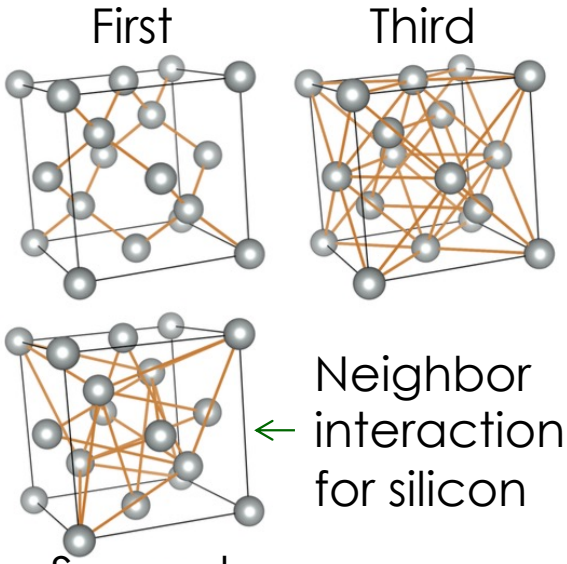
Photos: R. Pynn, 'Neutron Scattering', LANL

Inelastic Neutron Scattering Optimization



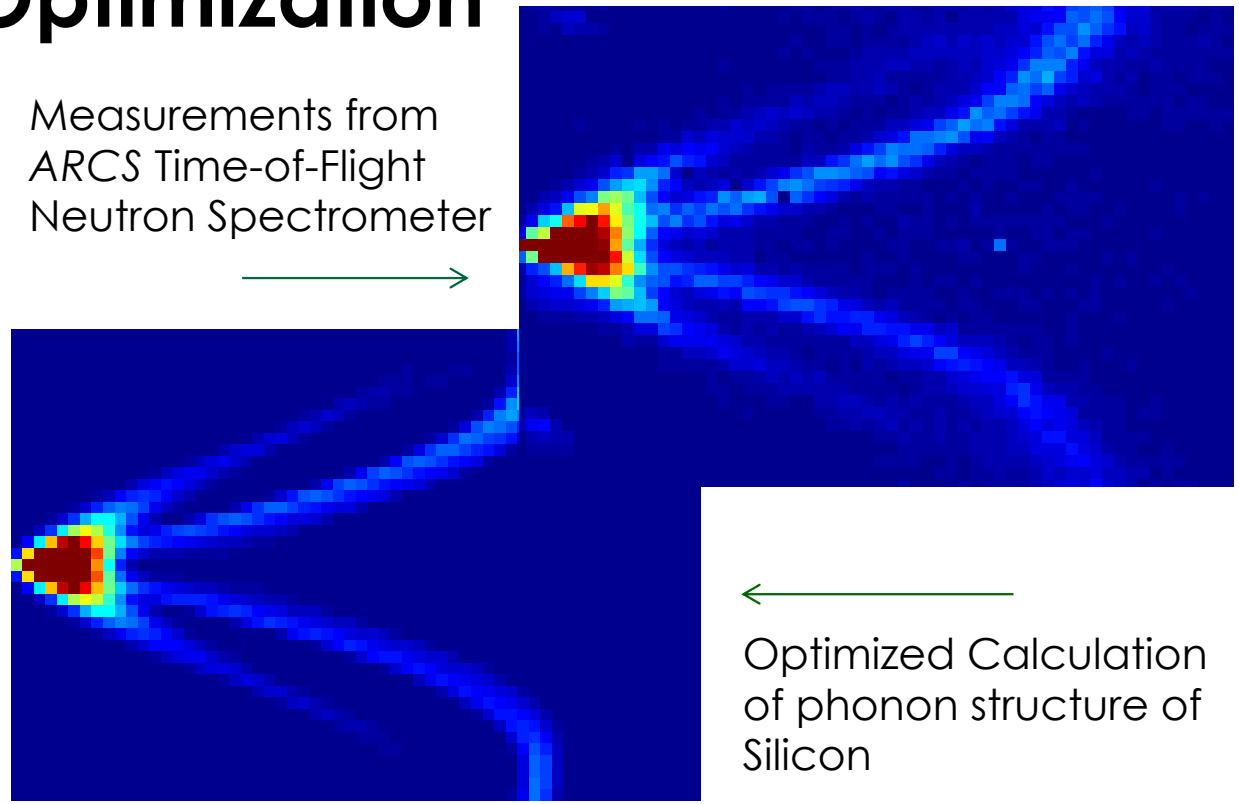
Optimization merged based UQ at each level

Exploit physics for split order modeling



Neighbor interaction for silicon

Measurements from *ARCS* Time-of-Flight Neutron Spectrometer



Optimized Calculation of phonon structure of Silicon

Bose-Einstein distribution

$$S_{\{\Phi\}}(\mathbf{Q},\omega) \propto \sum_{s,\mathbf{q}} \frac{\langle n_{s,\mathbf{q}}+1\rangle}{\omega_s^{\{\Phi\}}} \left| \sum_d (\mathbf{Q}\cdot\epsilon_{ds}^{\{\Phi\}}) \right|^2 \times \delta(\omega-\omega_s^{\{\Phi\}}(\mathbf{q}))\,\delta(\mathbf{Q}-\mathbf{q})$$

Phonon branch index in unit cell

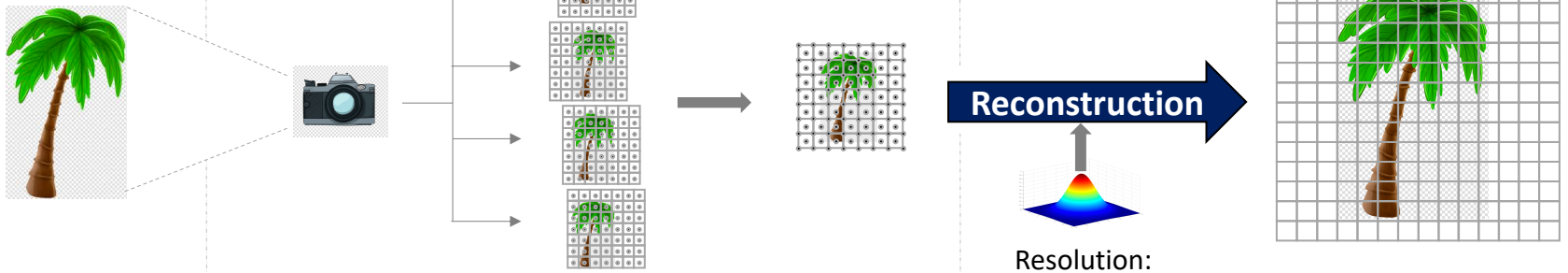
Phonon eigenvectors

Phonon frequency eigenvalues

Scalable, physics based, hierarchical, with UQ.

Super-resolution inelastic neutron spectroscopy

Super resolution multi-frame optical imagery

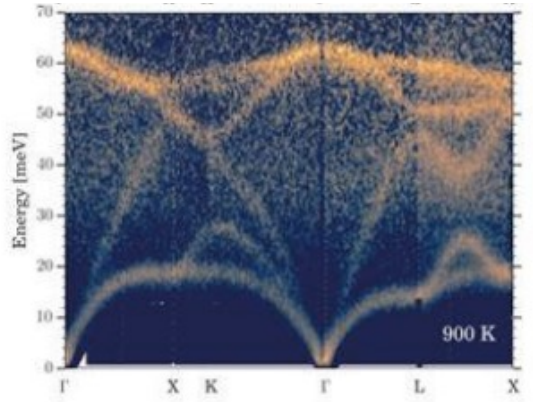


Scene

Frames with **sub-pixel displacements**

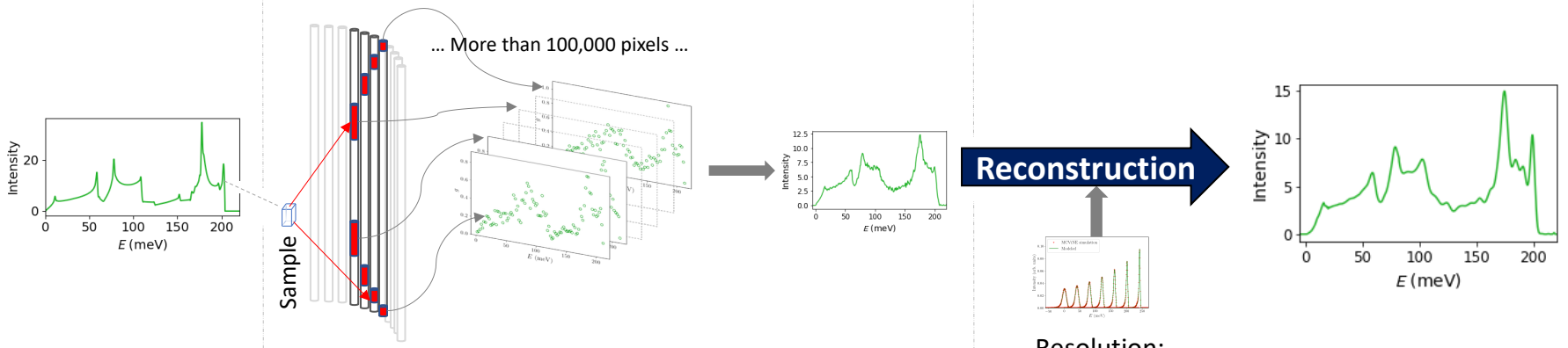
Combined image

Reconstructed image



INS snapshot displaying unit cell for La2−x(Sr,Ba)xCuO4

Super resolution phonon DOS by neutron DGS

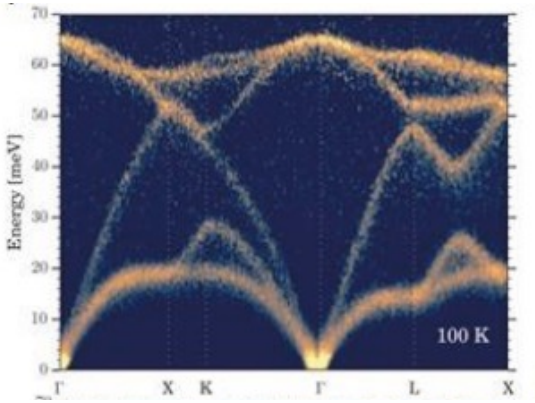


DOS

Time of flight bins converted to energy bins with **sub-*E*-bin shifts**

Combined DOS

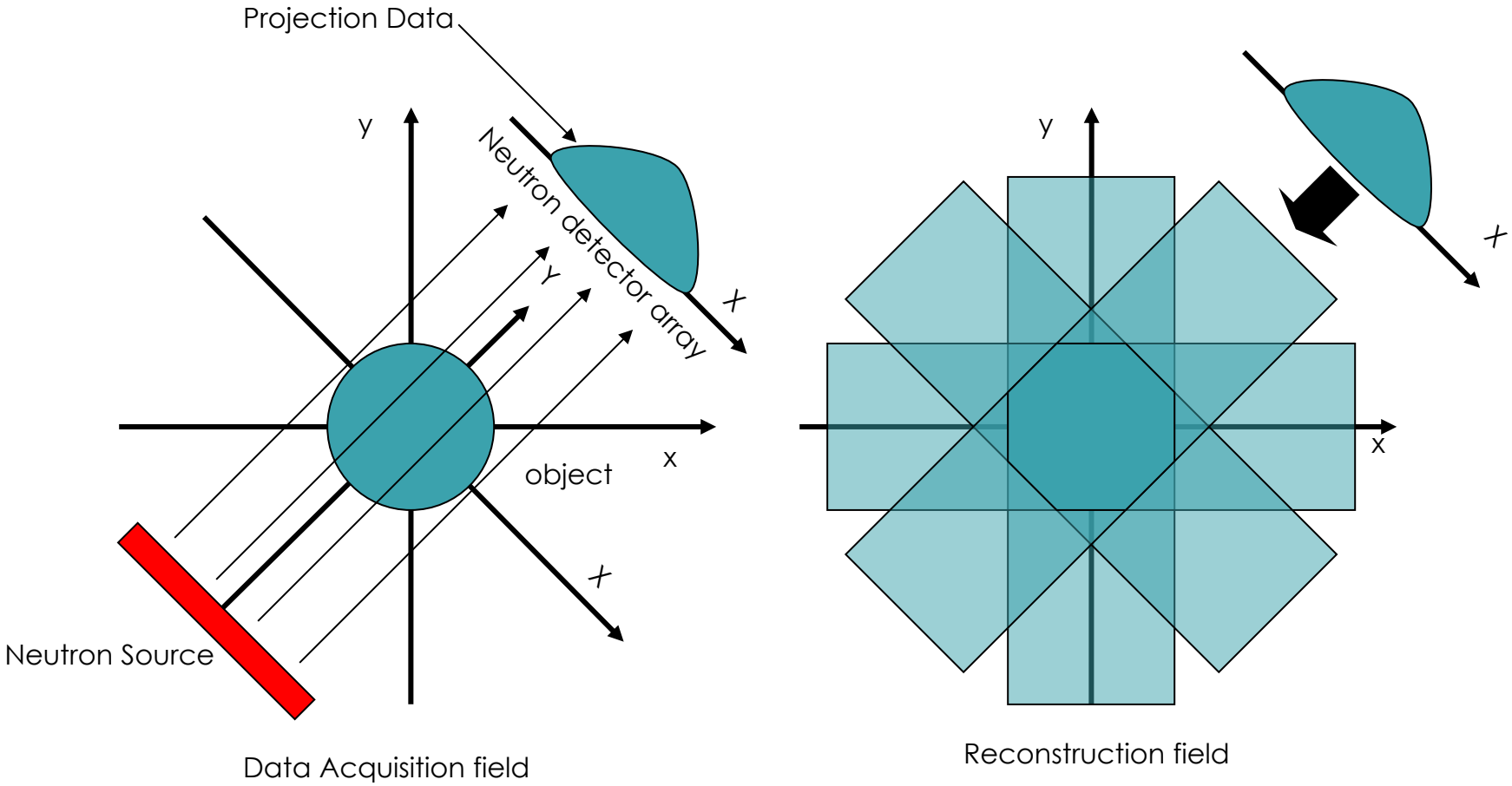
Reconstructed DOS



Super resolved phonon structure for ARCS instrument

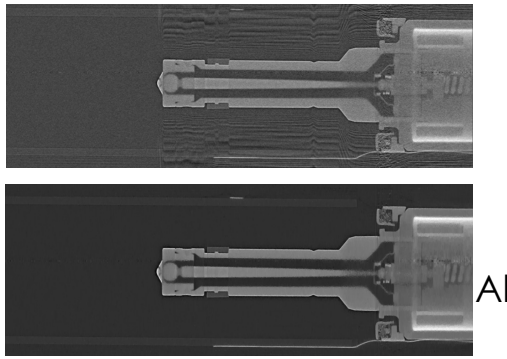
Experiment was performed at ORNL's SNS ARCS instrument.

Advanced Neutron Tomography

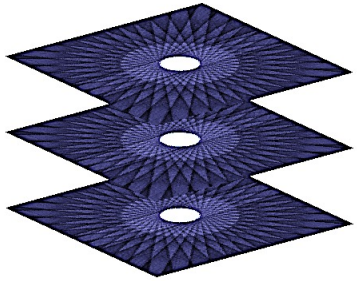


Advanced Neutron Tomography

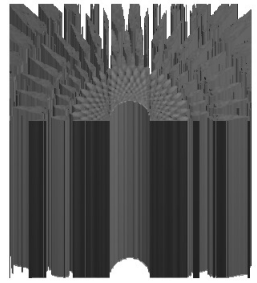
Resolving structure in fuel injector operation. (**Top**) FBP and (**Bottom**) HOTV



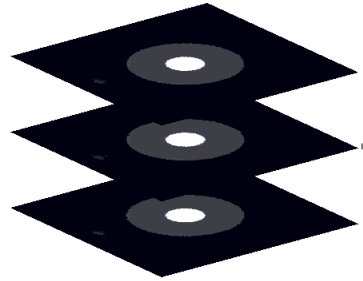
Aluminum-Steel Phantom



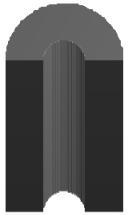
FPB



Segmentation

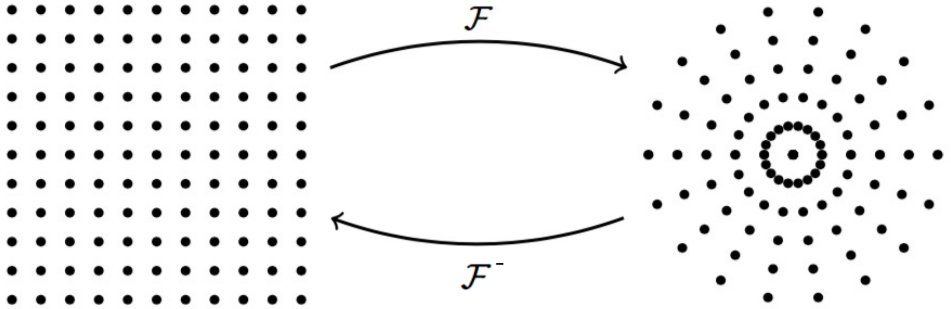


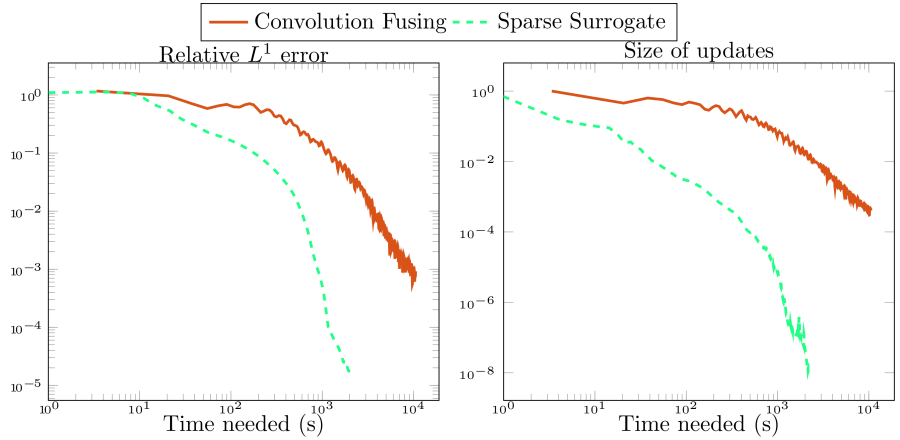
HOATV



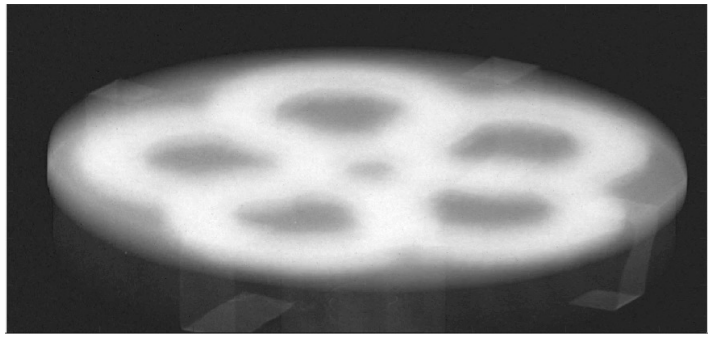
Segmentation

Using NUFFT, doubled performance over Radon Transform HOATV. Generated Surrogates for convolution step to provide orders of magnitude improvement

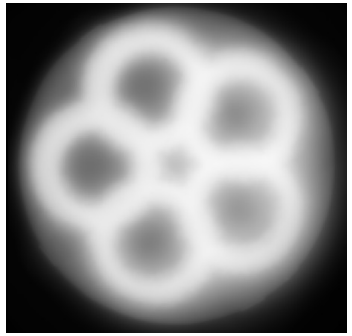




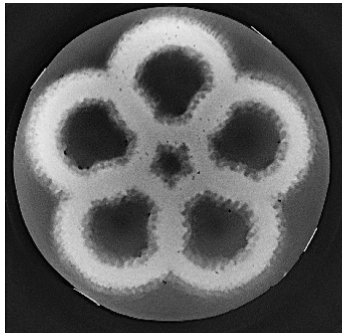
Thin slice Neutron tomography projection data



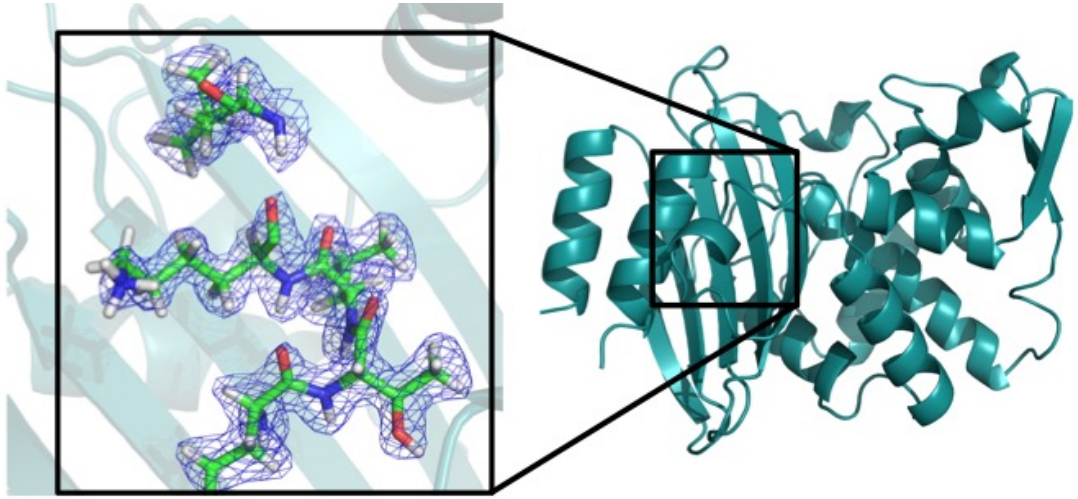
FBP



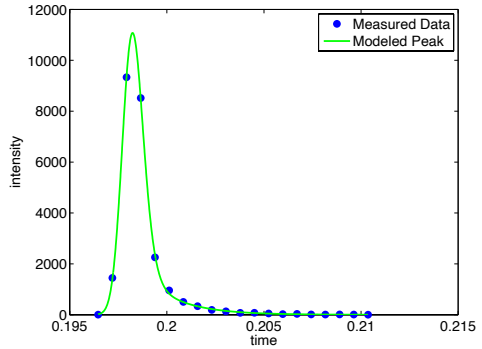
HOATV



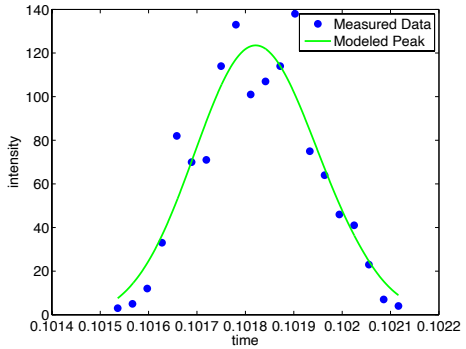
Machine learning for Neutron Science



Better characterization of Bragg Peaks by Machine Learning improves inference of nuclear density maps (blue) which improves structure calculations(teal).

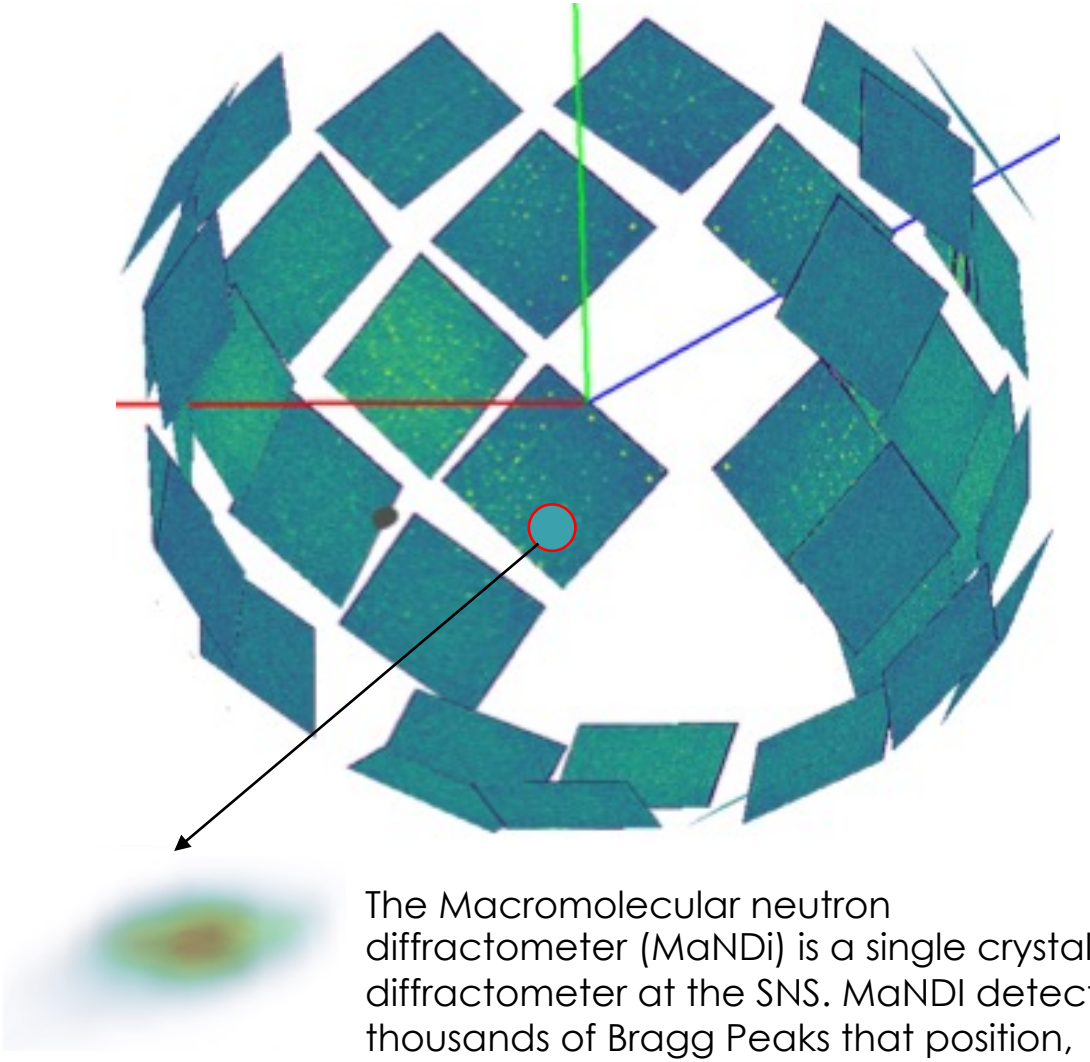


Strong peak



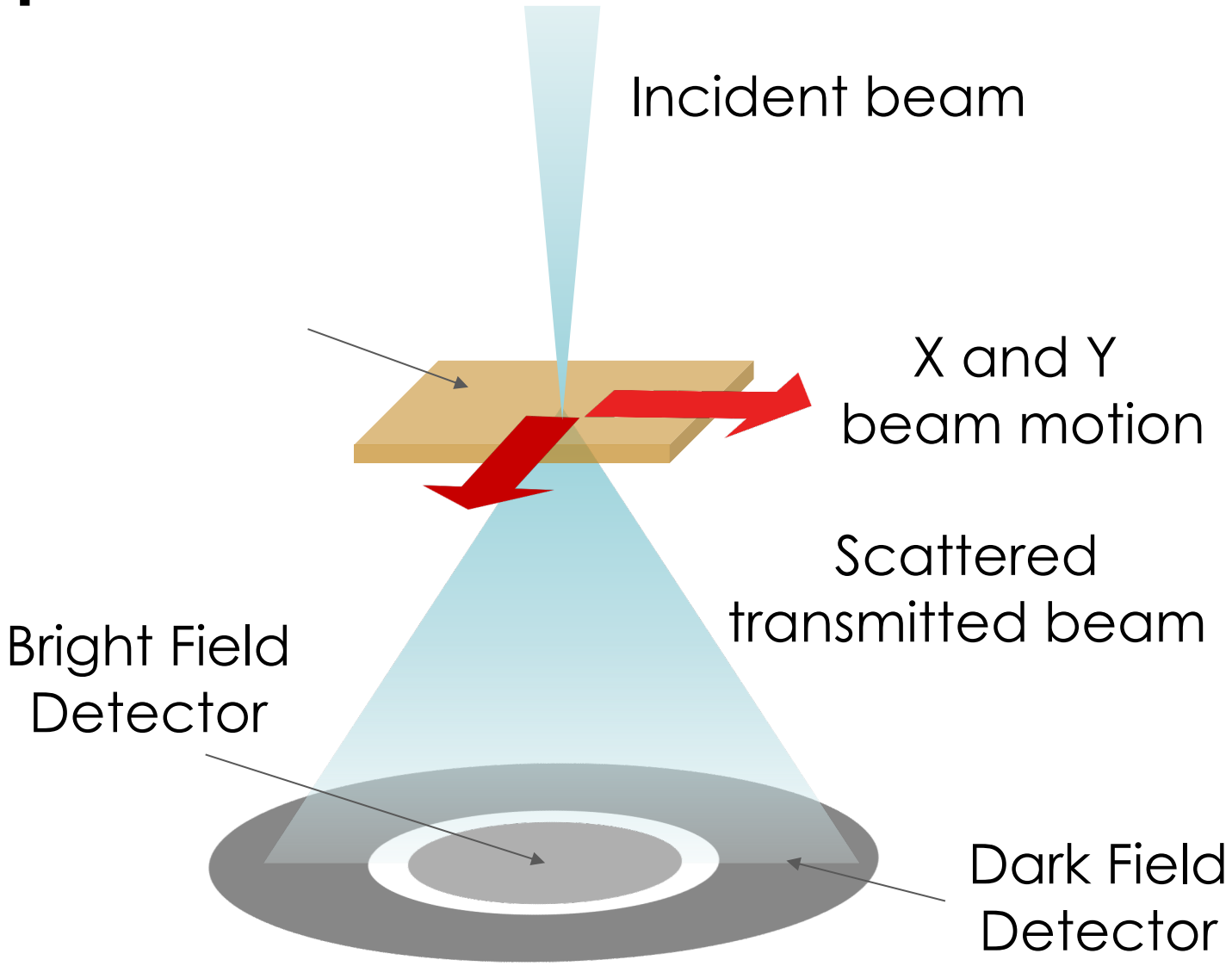
Weak peak

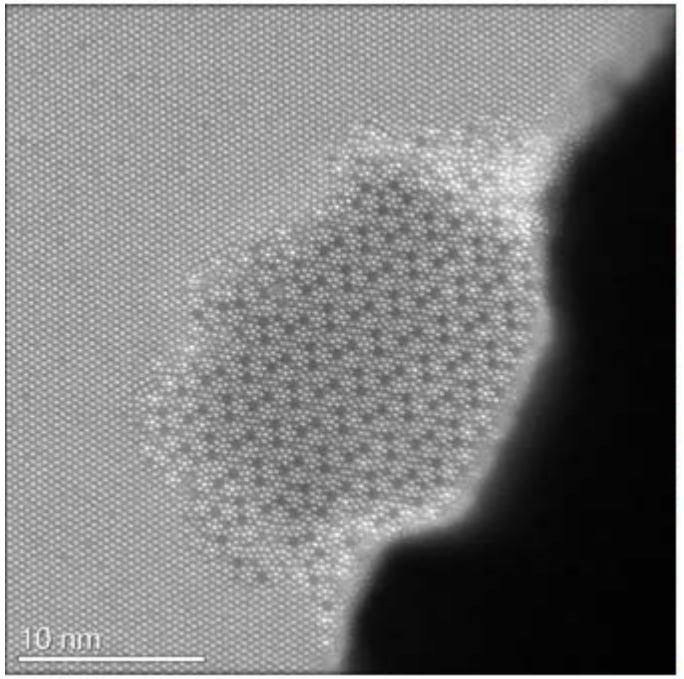
Each peak minimized to $f_{sp}(E,t') * \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{t'}{2\sigma}}$



The Macromolecular neutron diffractometer (MaNDi) is a single crystal diffractometer at the SNS. MaNDI detects thousands of Bragg Peaks that position, shape and orientation measure material properties

Experimental Science: CNMS

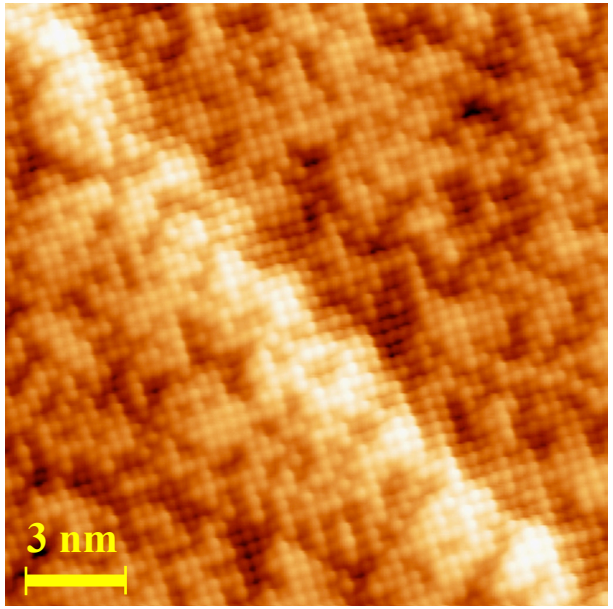




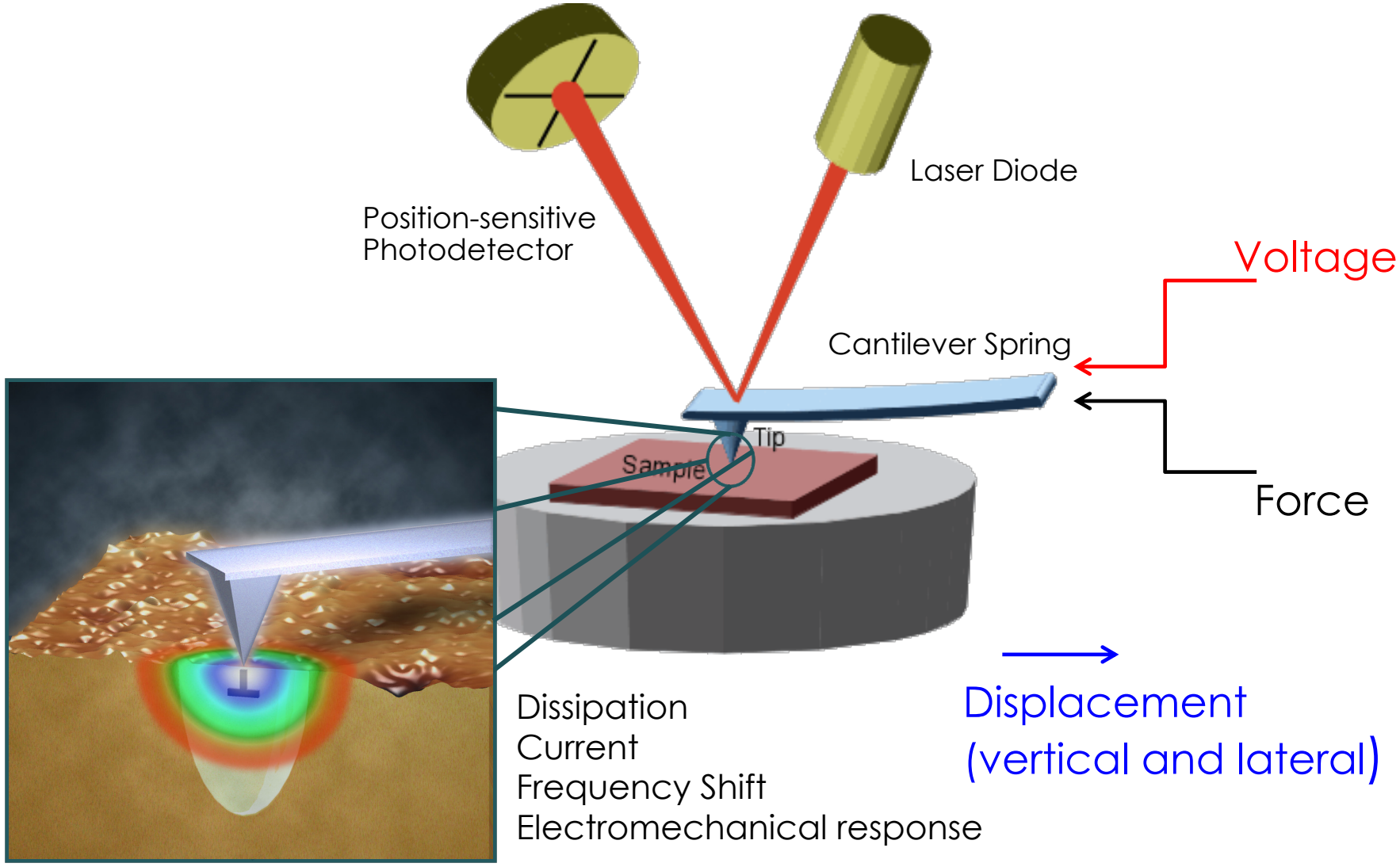
Texture analysis shows Molybdenum–Vanadium based complex oxide catalysts for propane ammoxidation

Scanning Transmission Electron Microscopy

Experimental Science: CNMS



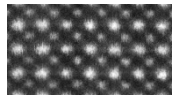
FeSeTe at the defect creating local superconductivity



Scanning Probe Microscopy

Federated Experimental Science

ORNL: STEM/EELS



CADES Compute & Data Environment for Science

Data de-noising and regularization

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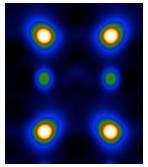
ANL: APS Focused X-Ray

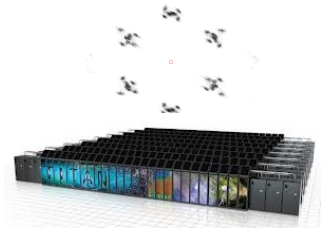
Argonne NATIONAL LABORATORY

Approximate structural models



Data Analytics

Image based Substrate and unit cell identification extraction of atomic structure and trajectories



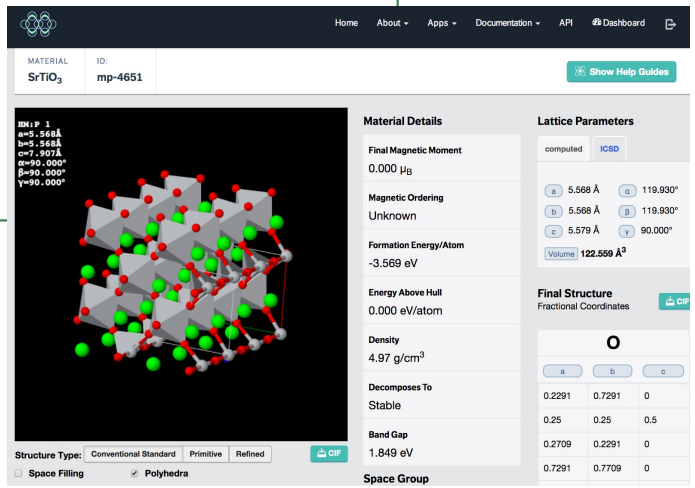
OLCF Oak Ridge Leadership Computing Facility

High throughput calculation of electronic structure of these configurations

NERSC

MATERIALS PROJECT

BERKELEY LAB

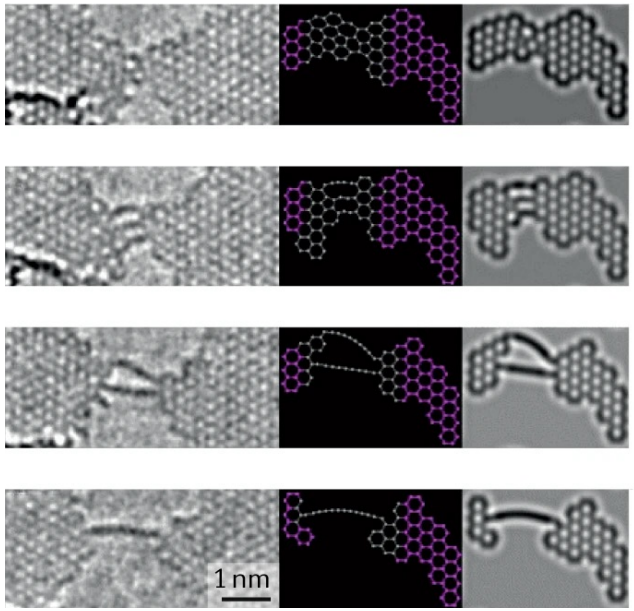


Knowledge base of experiments and simulations

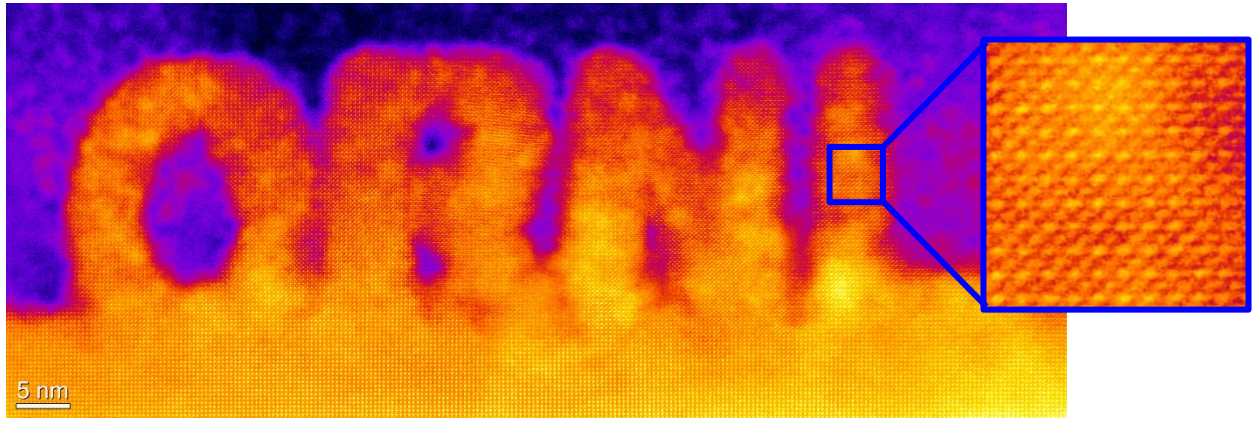
Data sharing and catalog of results

Start Up the Forge!

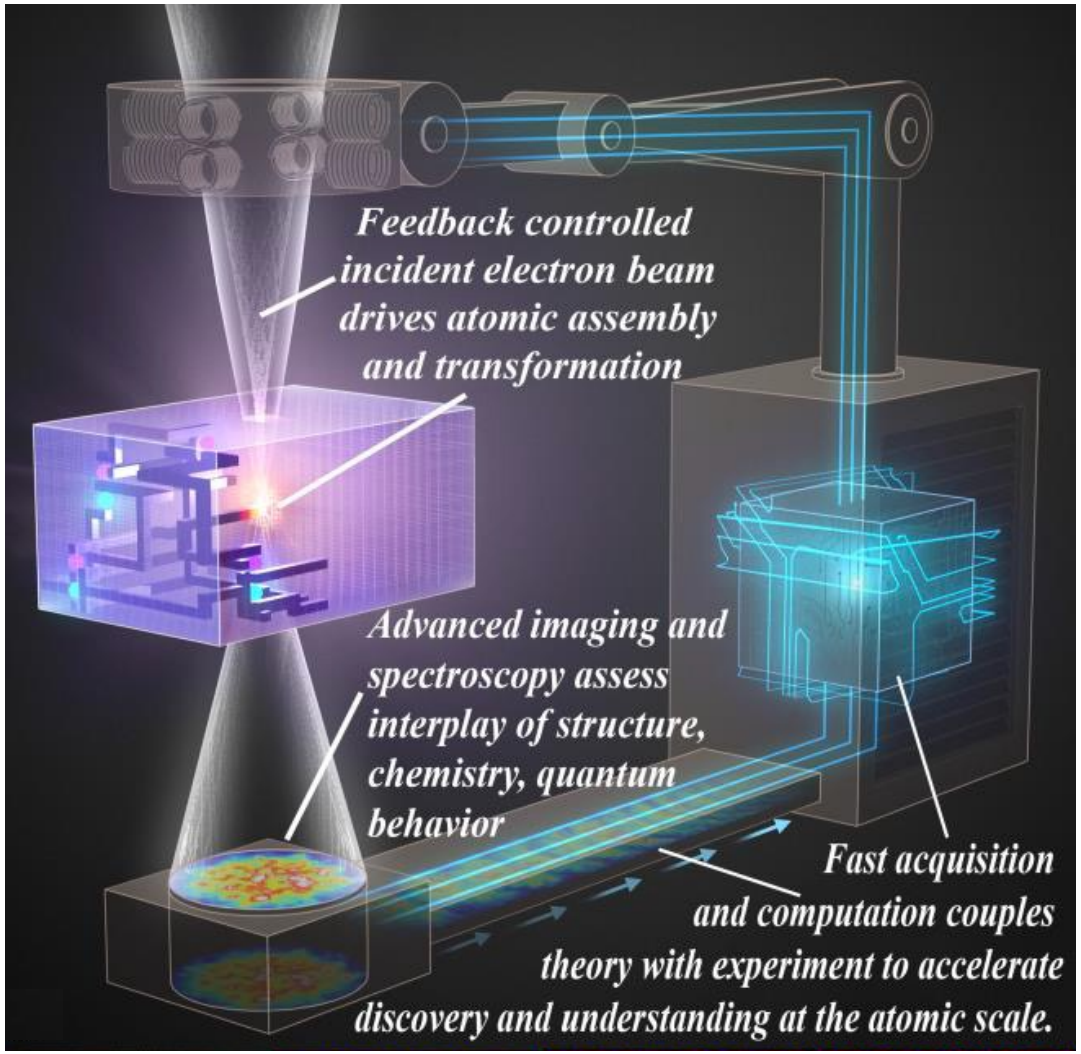
SPM writing



Carbon wires, e-beam

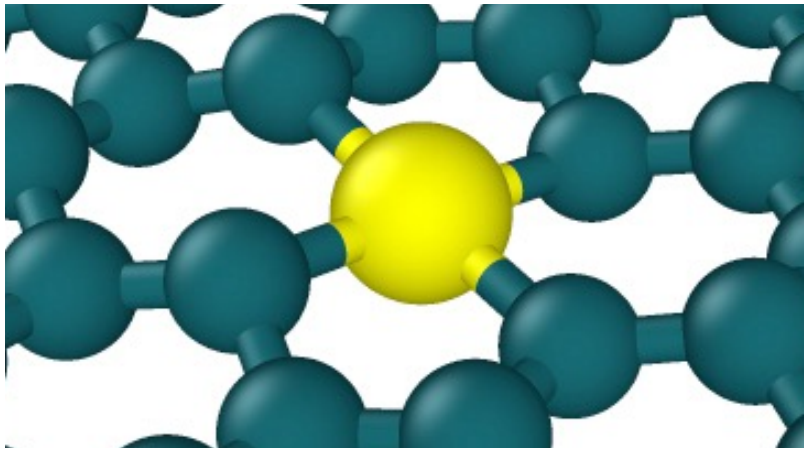


STEM e-beam induced crystallization

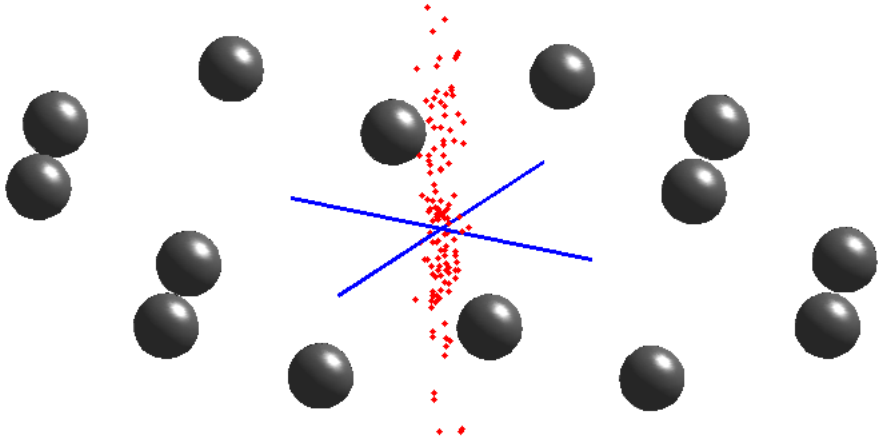


Atomic Forge concept, real-time simulation and data-controlled electron microscope to manipulate atoms.

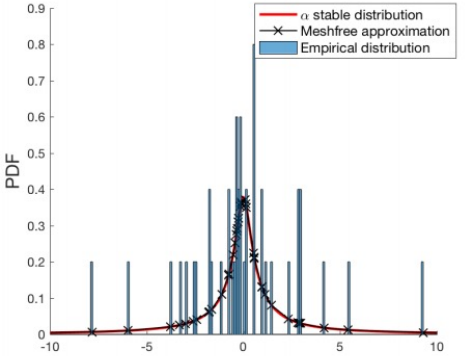
Forge Mathematics



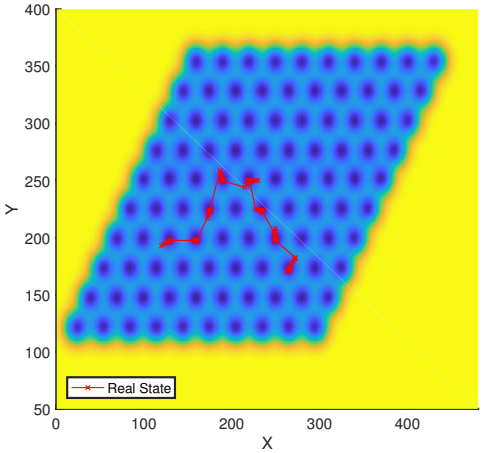
Simulation of Si in Graphene



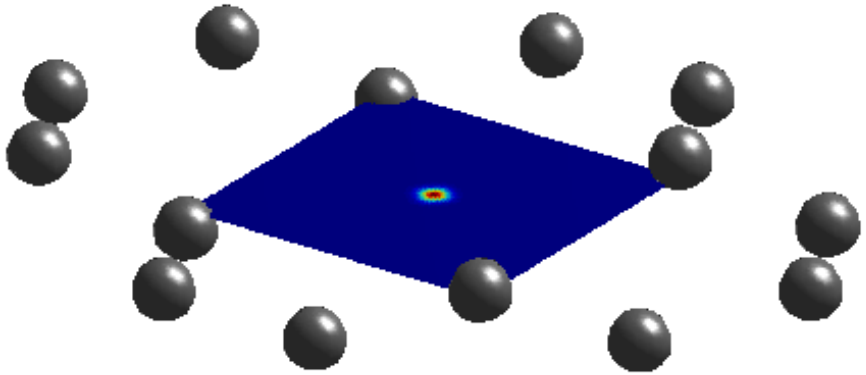
Hundred measurements of Si position referenced to average location of neighborhood carbon atoms



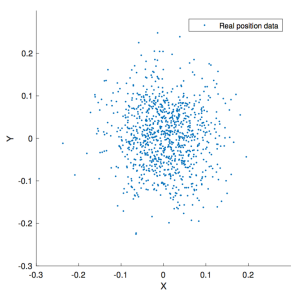
Backward SDE Meshfree approximation

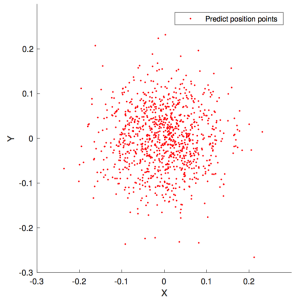


Accurate tracking of jump diffusion process of atom



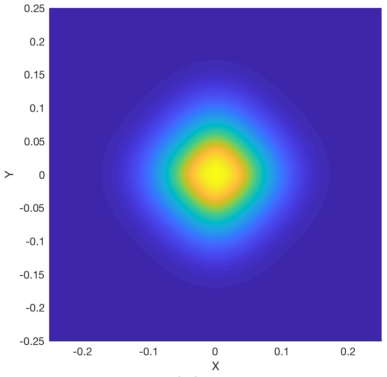
Estimated Potential





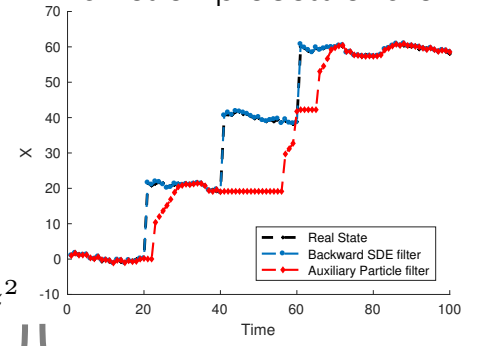
Langevin equation-based optimization of simulation data

$$dX_t = -\Delta V_t dt + \sqrt{2D} dW_t$$



Best e^{-V} in atomic coordinates

$$V = a(1 - b\cos(4\theta))e^{-\rho z^2}$$



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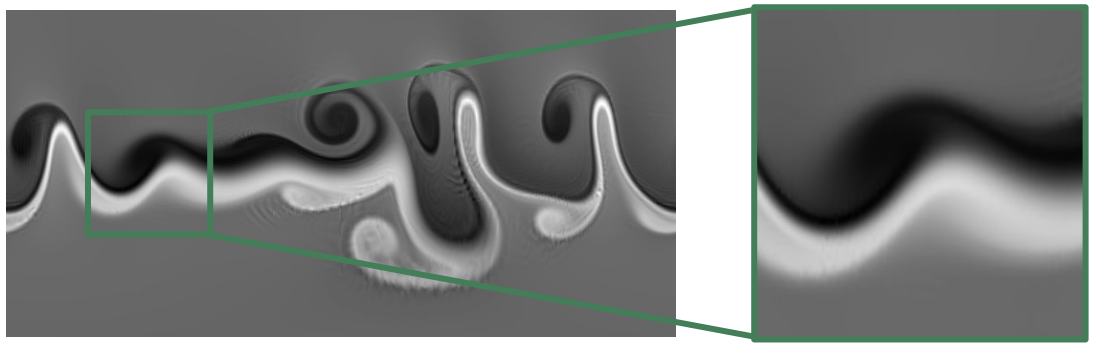
Methods to estimate forces on atoms

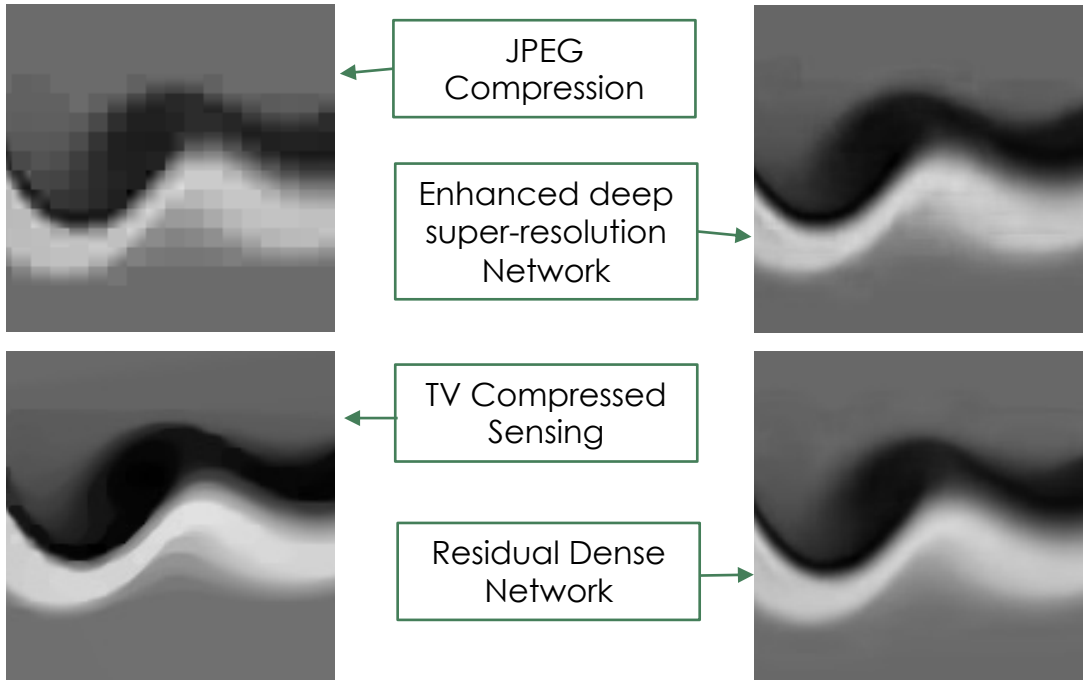
Tracking atoms

Scientific Data



Barotropic instability test

Enlarged region



- Adaptively trained NN on streaming data.
  - Training data only seen once
  - Network pre-trained
- Stored JPEG lossy compression with artifacts (ringing, blocking, etc.).
- Compressed Sensing with 400 iterations over corrects for artifacts.

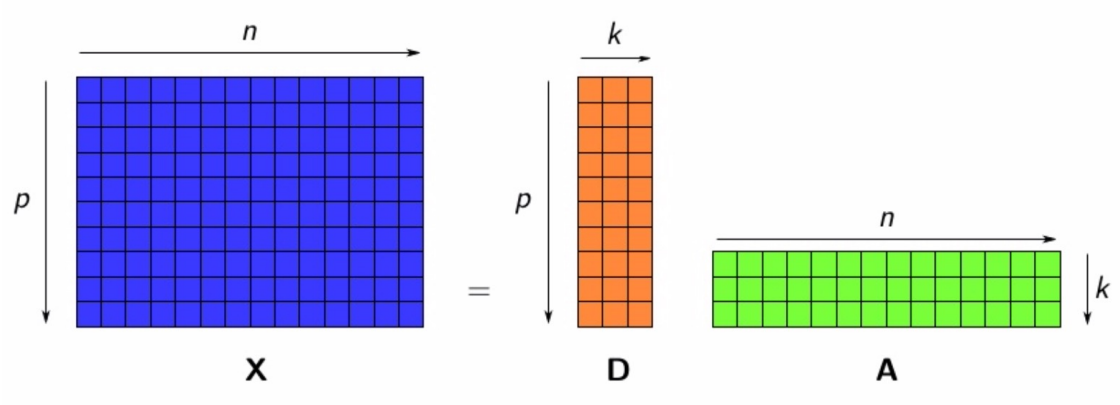
	NMSE	SSIM	PSNR
JPEG	0.038	0.971	37.245
CS w/ 400 iterations	0.045	0.973	34.534
EDSR	0.024	0.989	41.071
RDN	0.022	0.989	42.224

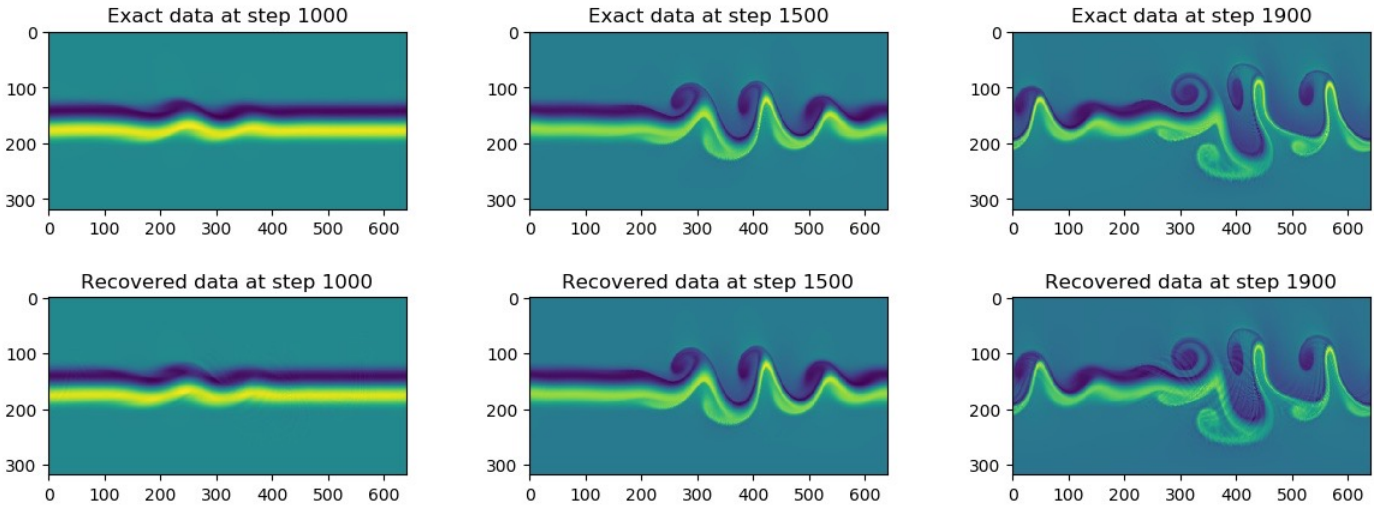
Scientific Data

We develop a matrix factorization approach based upon out of core linear algebra methods for data compression, reconstruction and interpretable decomposition:

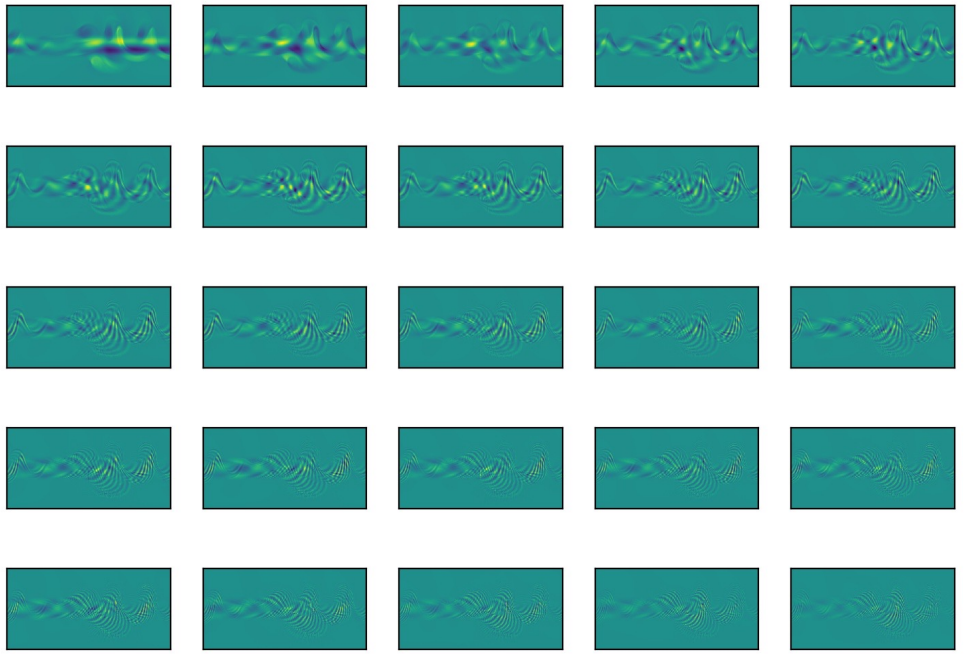
$$X \approx DA$$

- Data (signals, images) are stacked into $X \in \mathbb{R}^{p \times n}$.
- D: dictionary; A: sparse code.





Original and reconstructed data from online dictionary learning



Complete Dictionary

Question?