

Inverse Modeling for Experimental Science and Data Analytic

Rick Archibald

ICL Virtual Lunch Talk

July 24th, 2020

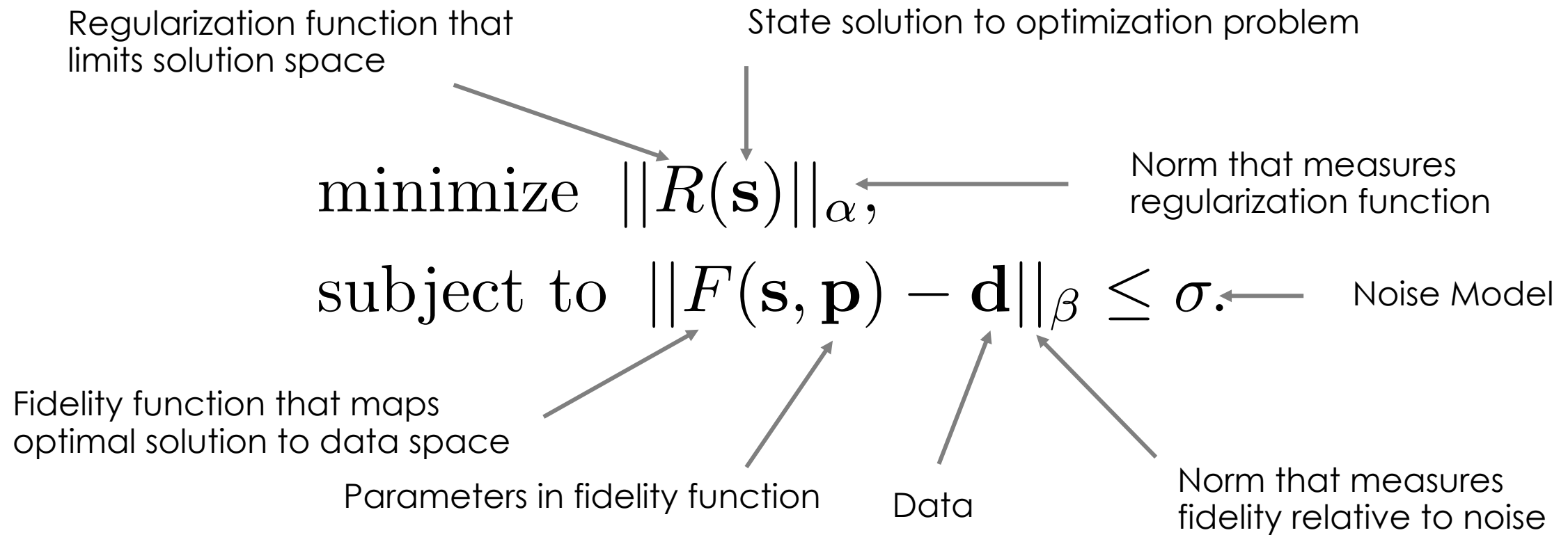
ORNL is managed by UT-Battelle, LLC for the US Department of Energy



U.S. DEPARTMENT OF
ENERGY

Inverse Modeling

What is measured is often not the state of interest.

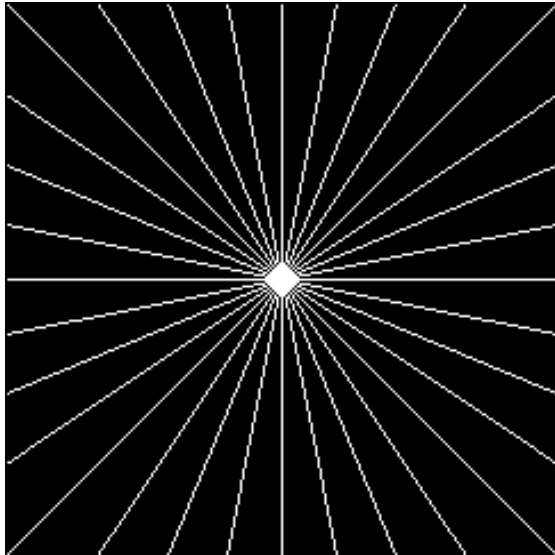


Challenge: Improve regularization, fidelity, and speed.

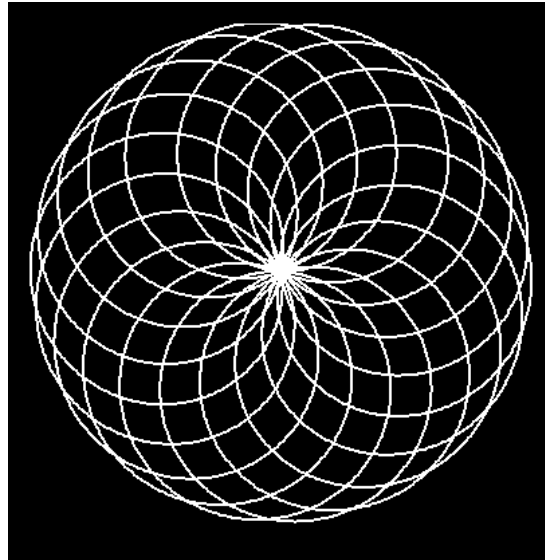
Inverse Modeling

Partial Fourier data problem solved with compress sensing.

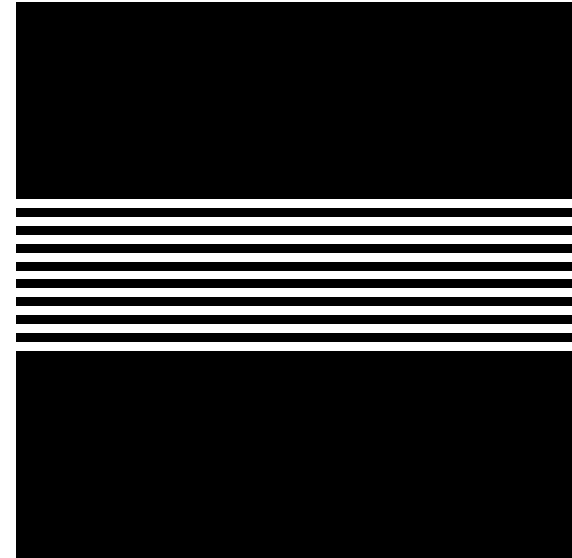
$$\begin{aligned} &\text{minimize } ||\nabla_x \mathbf{s}||_1 + ||\nabla_y \mathbf{s}||_1, \\ &\text{subject to } ||\mathcal{F}(\mathbf{s}) - \mathbf{d}||_2 \leq \sigma. \end{aligned}$$



Tomography



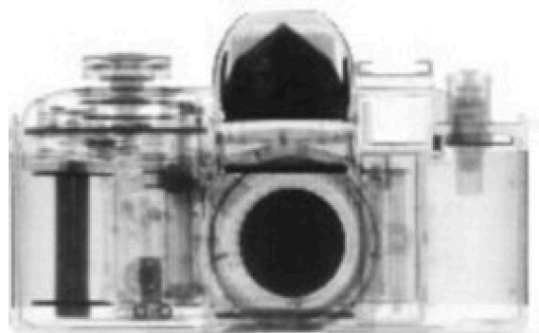
MRI



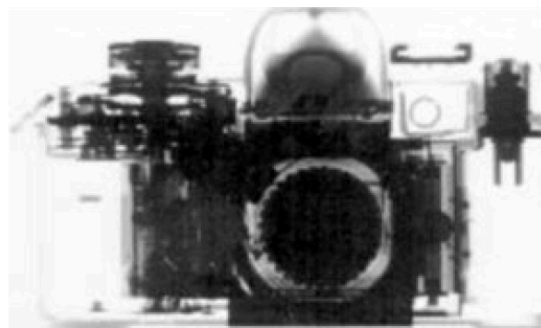
Ultrasound

Experimental Science: SNS

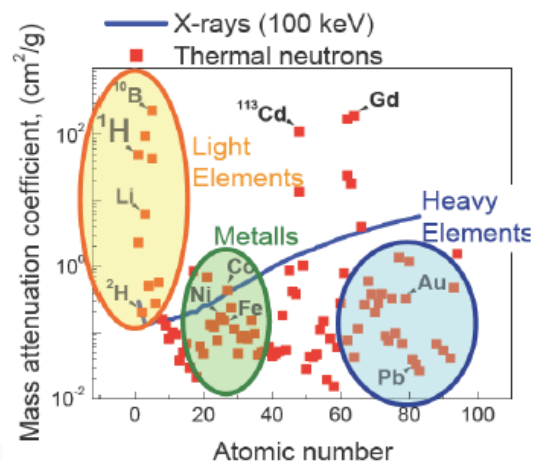
Why Neutrons?



Neutrons

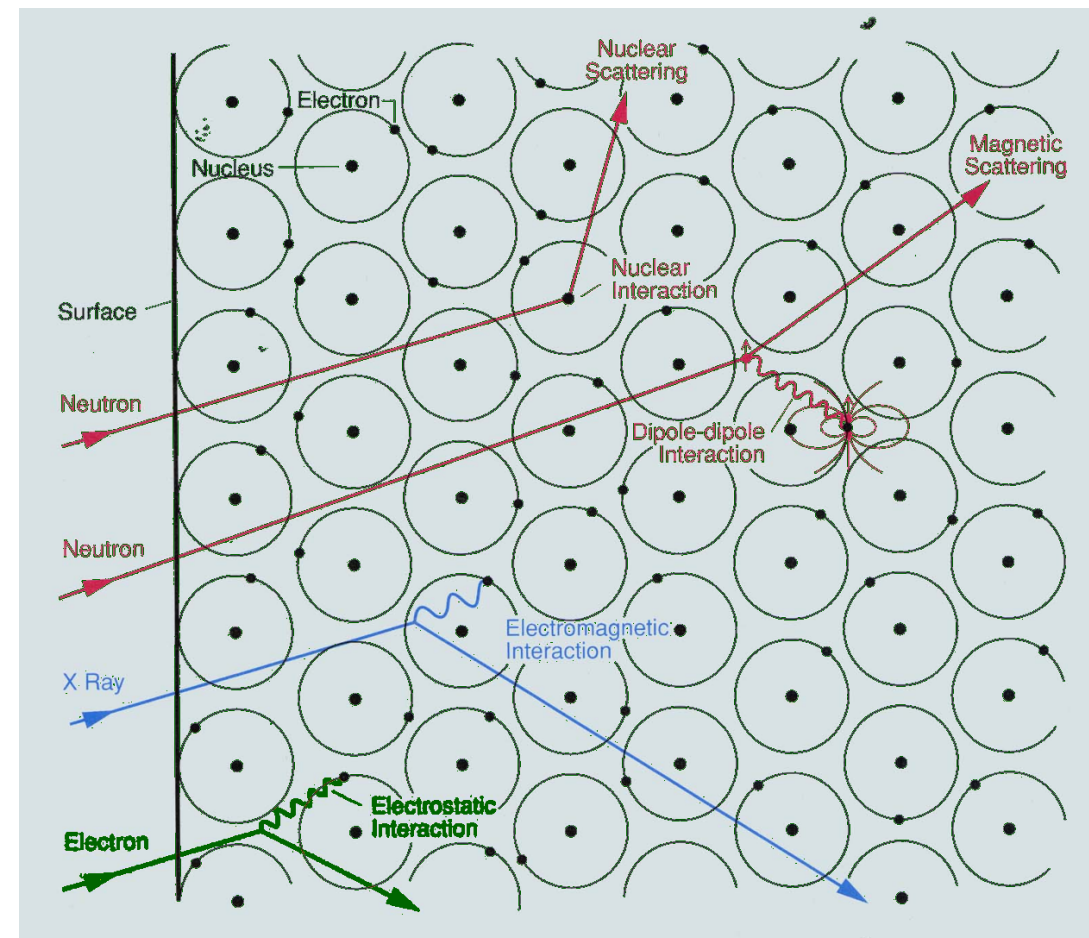


X-Rays



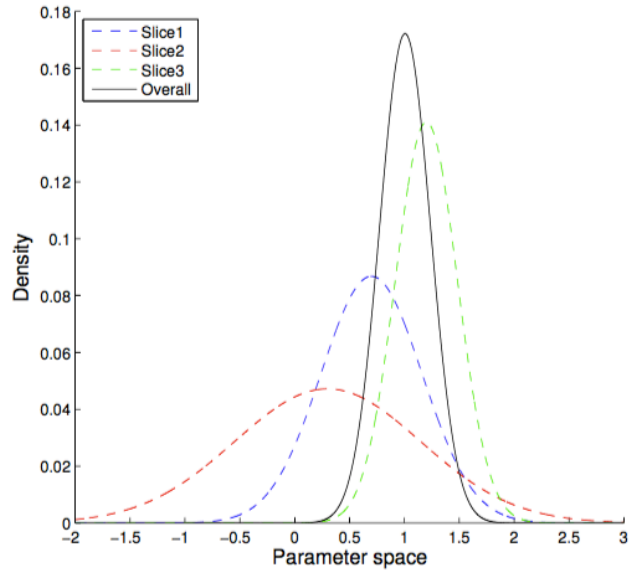
- Penetrate metals without absorbing
- Highly sensitive to water and hydrocarbons
- High contrast to light elements
- Sensitivity to magnetism
- Measure dynamics and structure

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



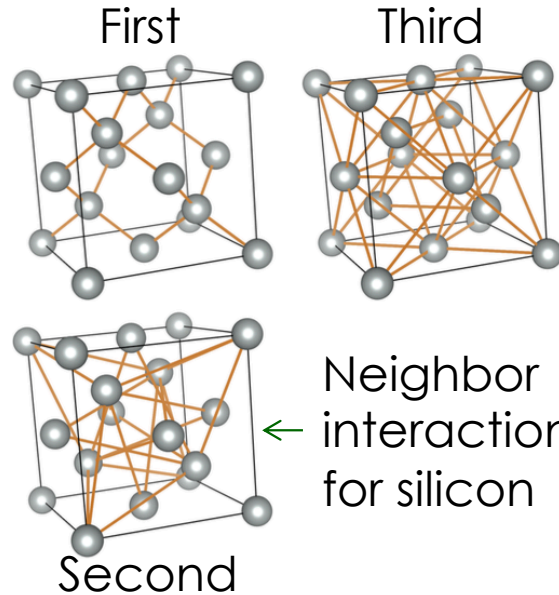
Photos: R. Pynn, 'Neutron Scattering', LANL

Inelastic Neutron Scattering Optimization

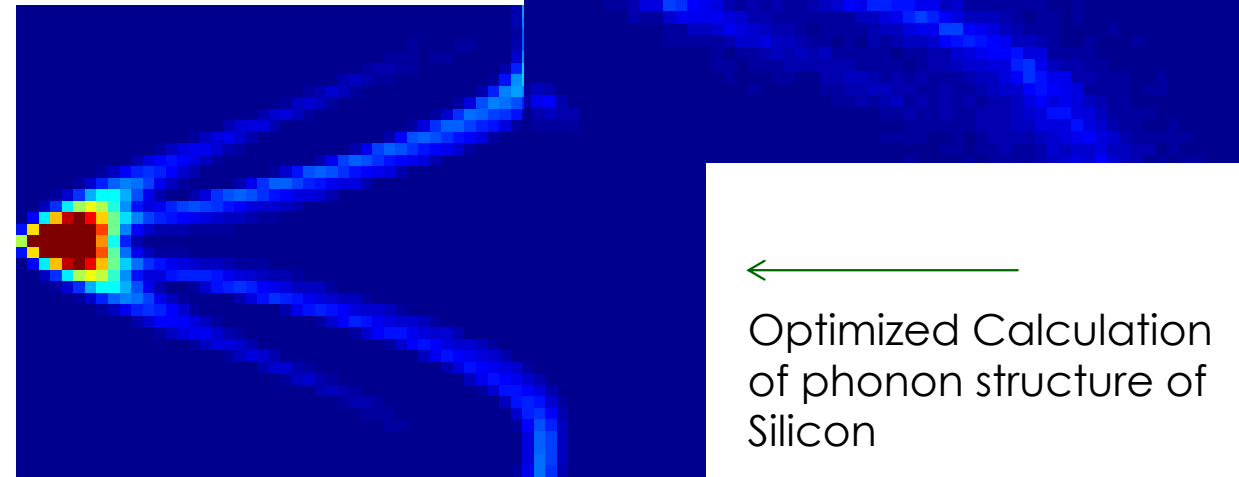


Optimization merged based UQ at each level

Exploit physics for split order modeling



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

Super-resolution inelastic neutron spectroscopy

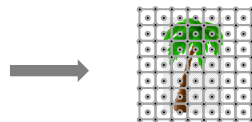
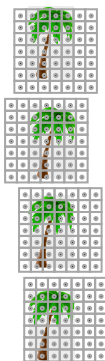
Super resolution
multi-frame optical imagery



Scene

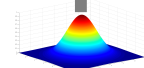


Frames with
sub-pixel displacements

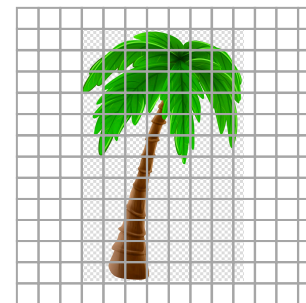


Combined
image

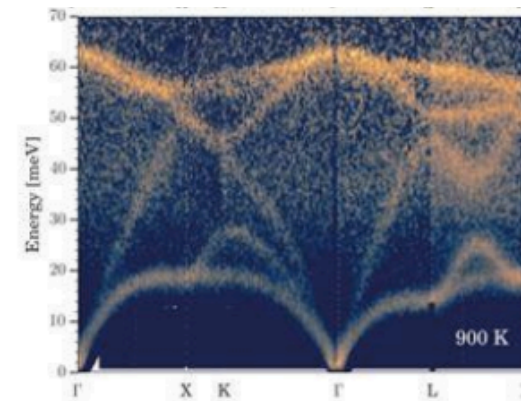
Reconstruction



Resolution:
2D gaussian

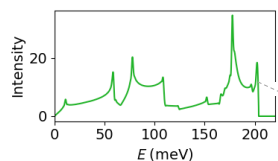


Reconstructed
image

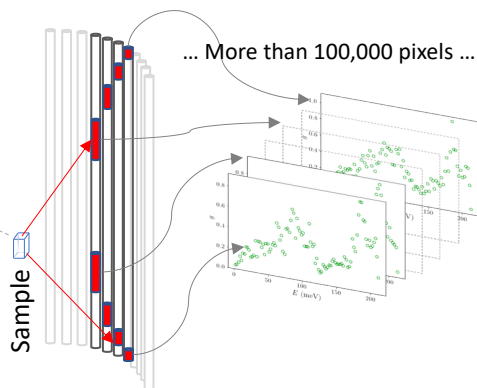


INS snapshot
displaying unit cell for
 $\text{La}_{2-x}(\text{Sr,Ba})_x\text{CuO}_4$

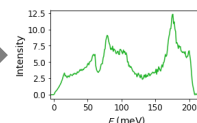
Super resolution phonon
DOS by neutron DGS



DOS

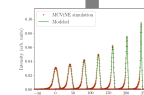


Time of flight bins converted to
energy bins with **sub-E-bin shifts**

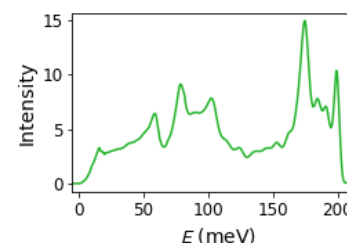


Combined
DOS

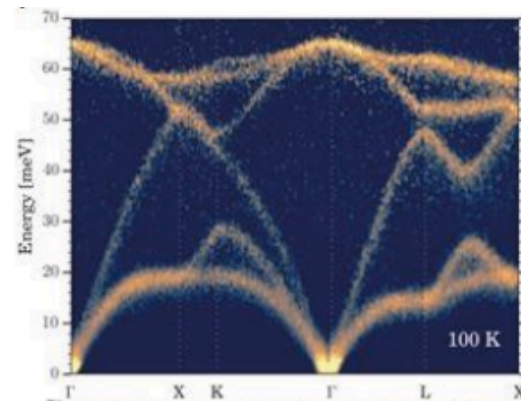
Reconstruction



Resolution:
1D, asymmetric,
energy-dependent



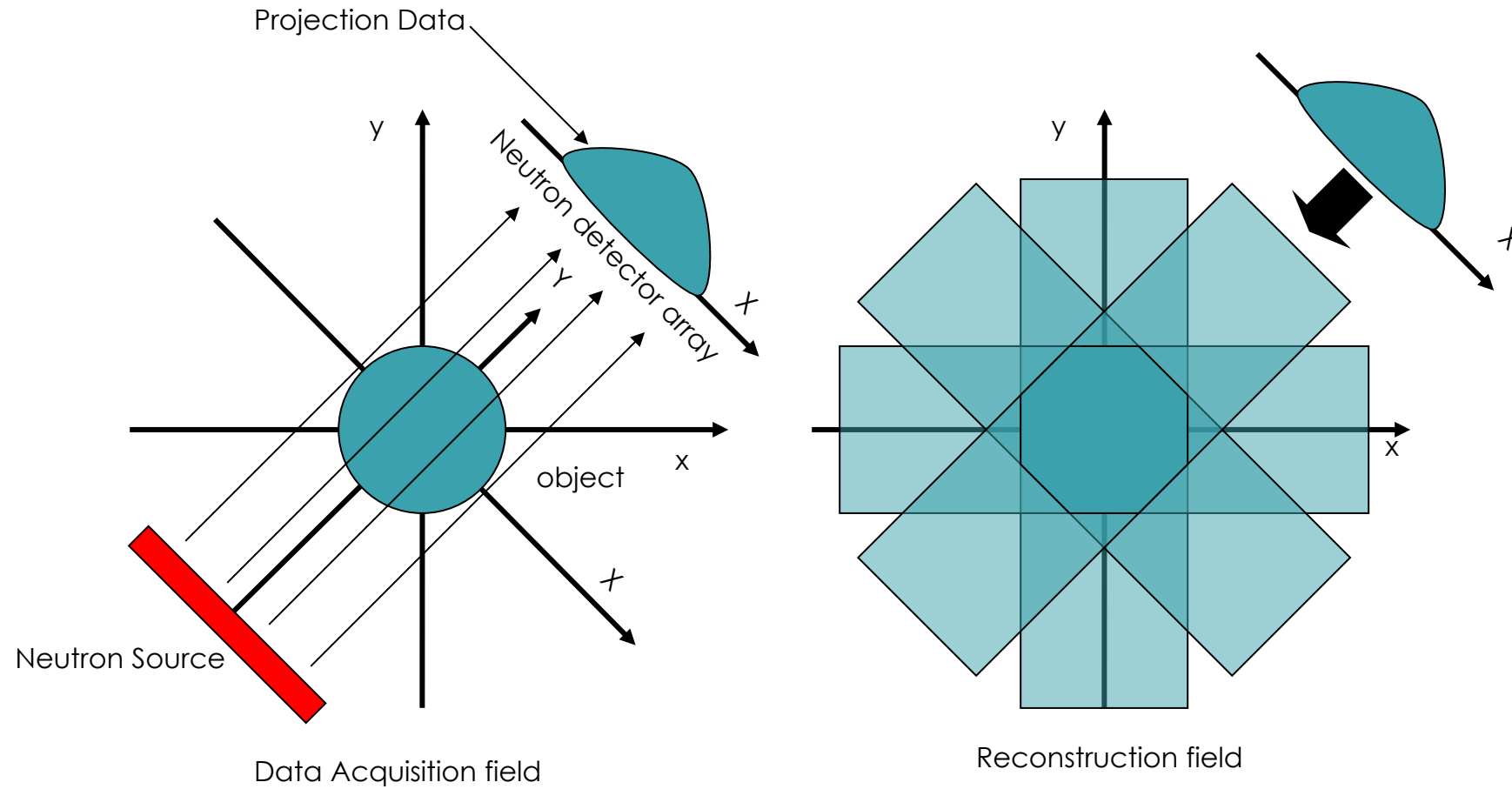
Reconstructed
DOS



Super resolved
phonon structure for
ARCS instrument

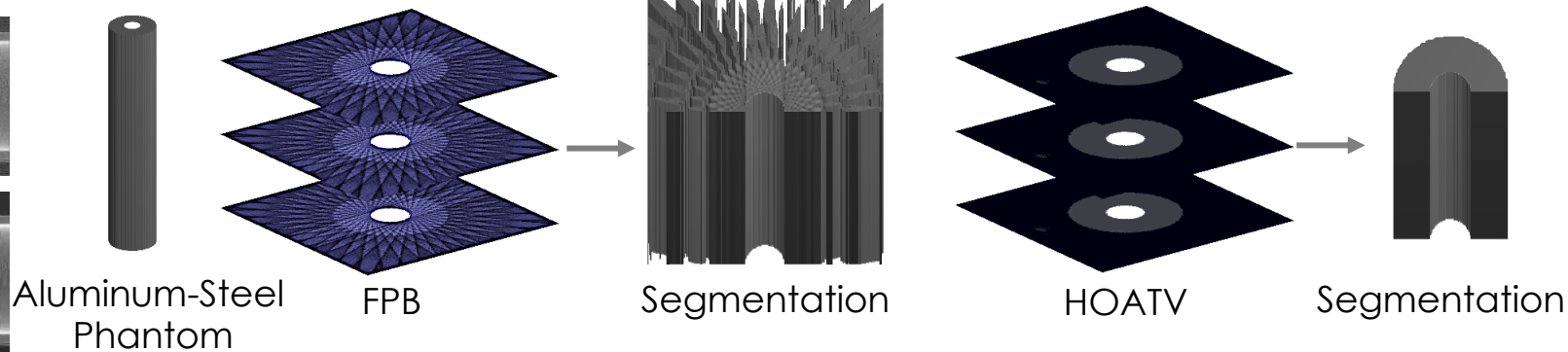
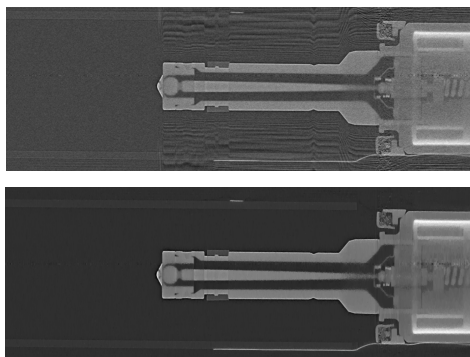
Experiment was performed at ORNL's SNS ARCS instrument.

Advanced Neutron Tomography

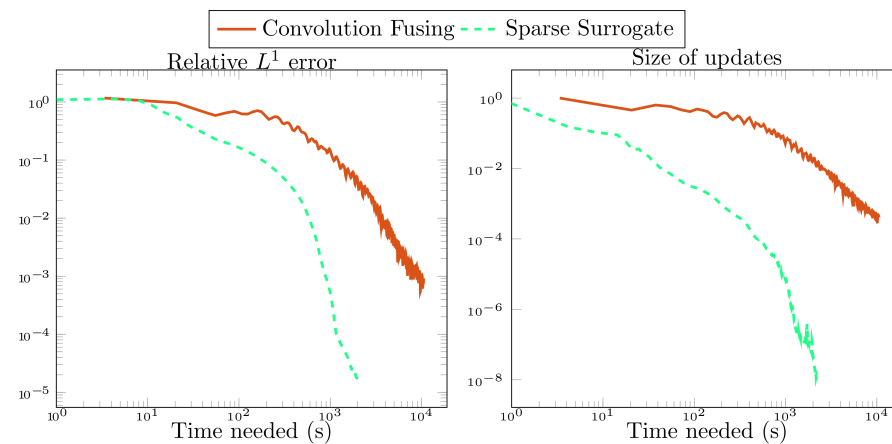
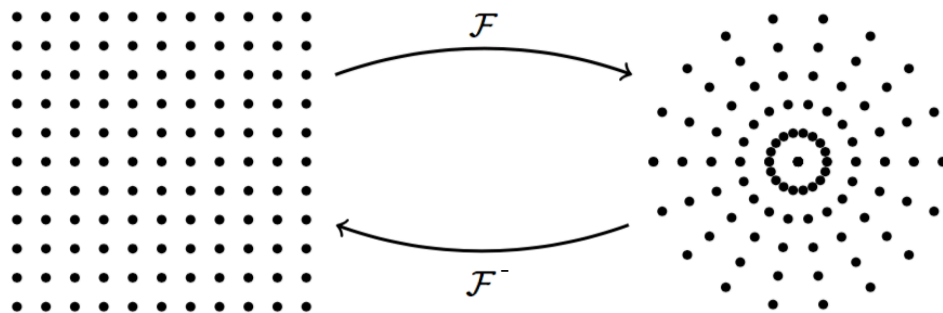


Advanced Neutron Tomography

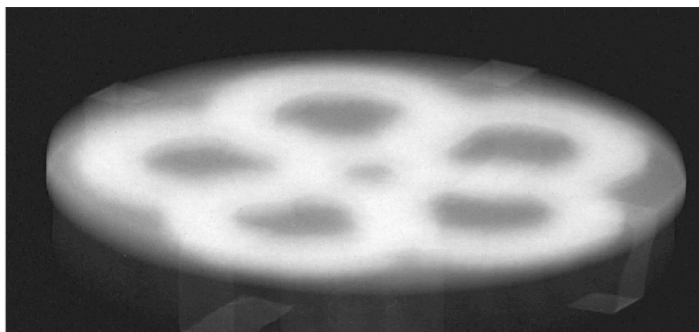
Resolving structure in fuel injector operation. **(Top)** FBP and **(Bottom)** HOTV



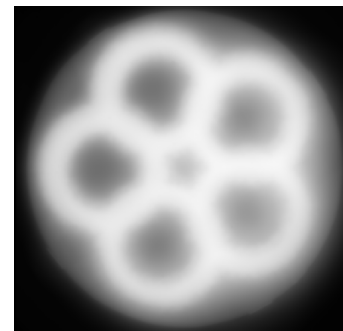
Using NUFFT, doubled performance over Radon Transform HOATV. Generated Surrogates for convolution step to provide orders of magnitude improvement



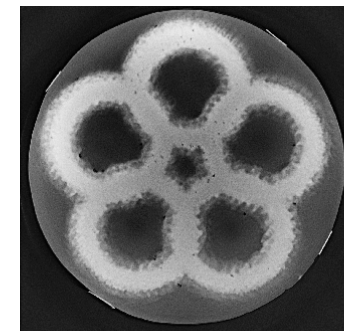
Thin slice Neutron tomography projection data



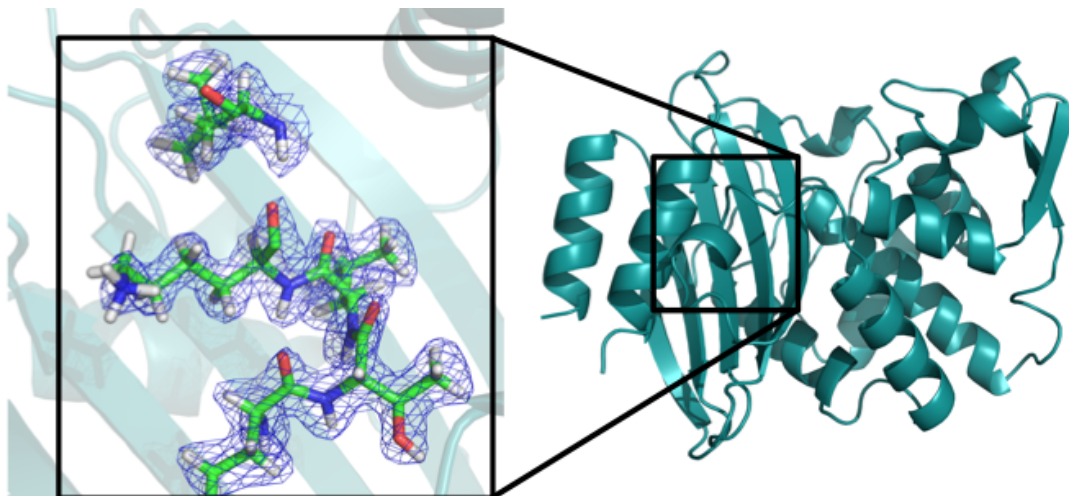
FBP



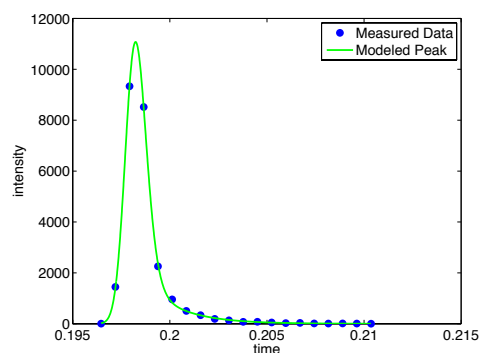
HOTV



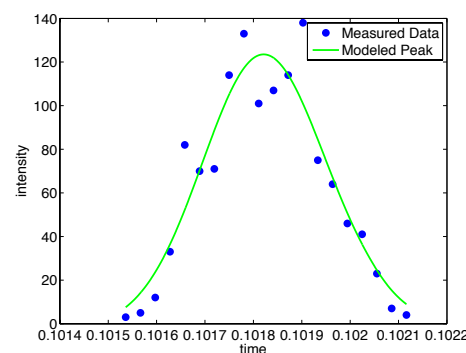
Machine learning for Neutron Science



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

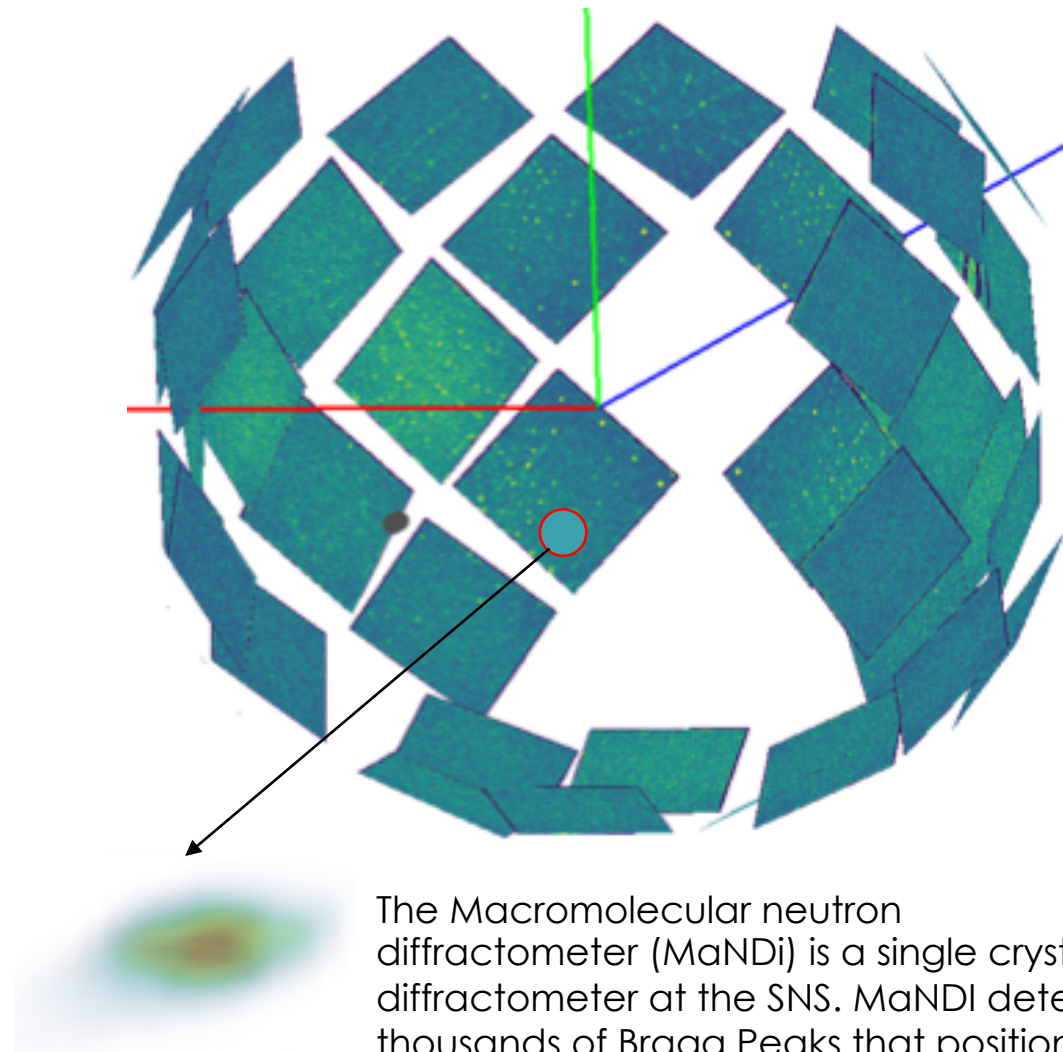


Strong peak



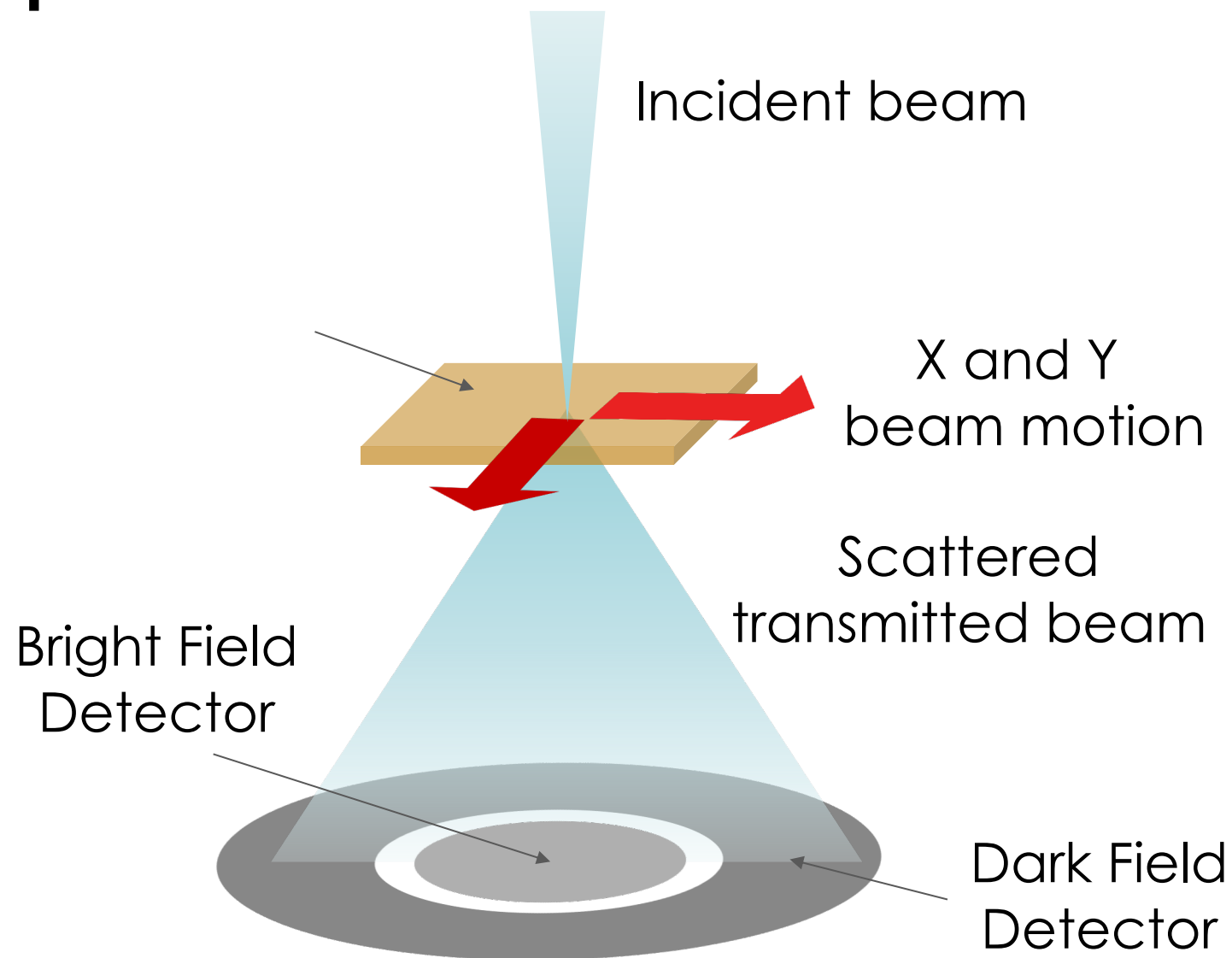
Weak peak

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

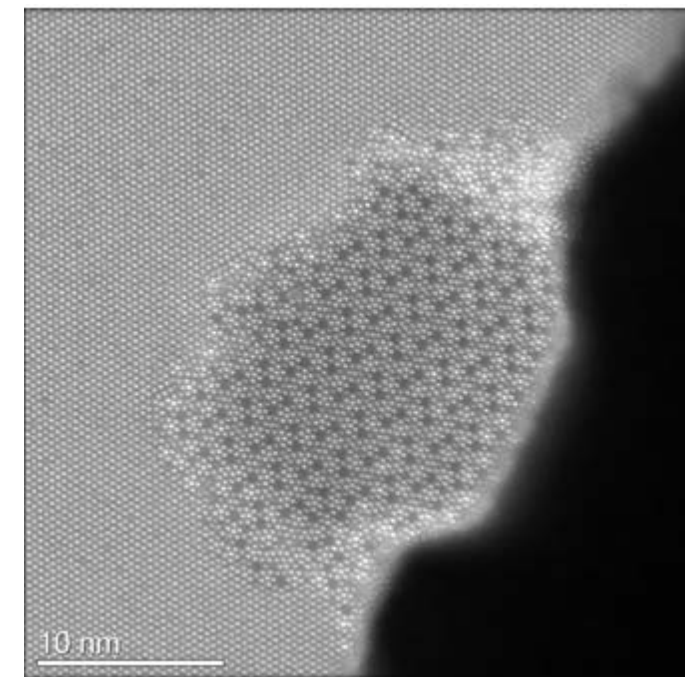


The Macromolecular neutron diffractometer (MaNDi) is a single crystal diffractometer at the SNS. MaNDi detects thousands of Bragg Peaks that position, shape and orientation measure material properties

Experimental Science: CNMS

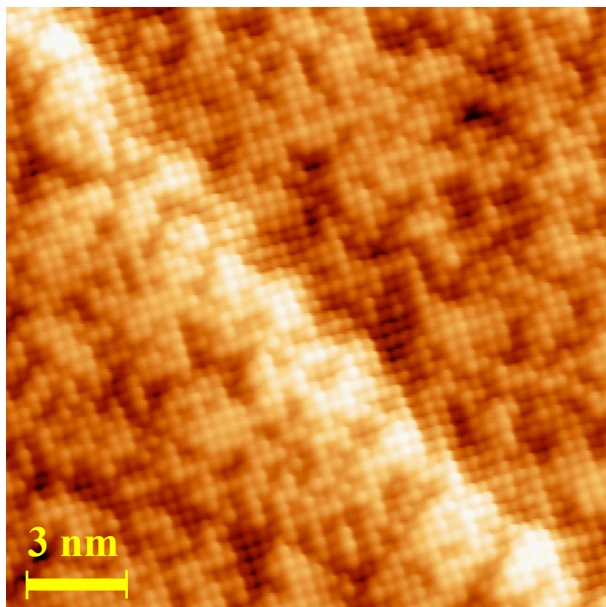


Scanning Transmission Electron Microscopy

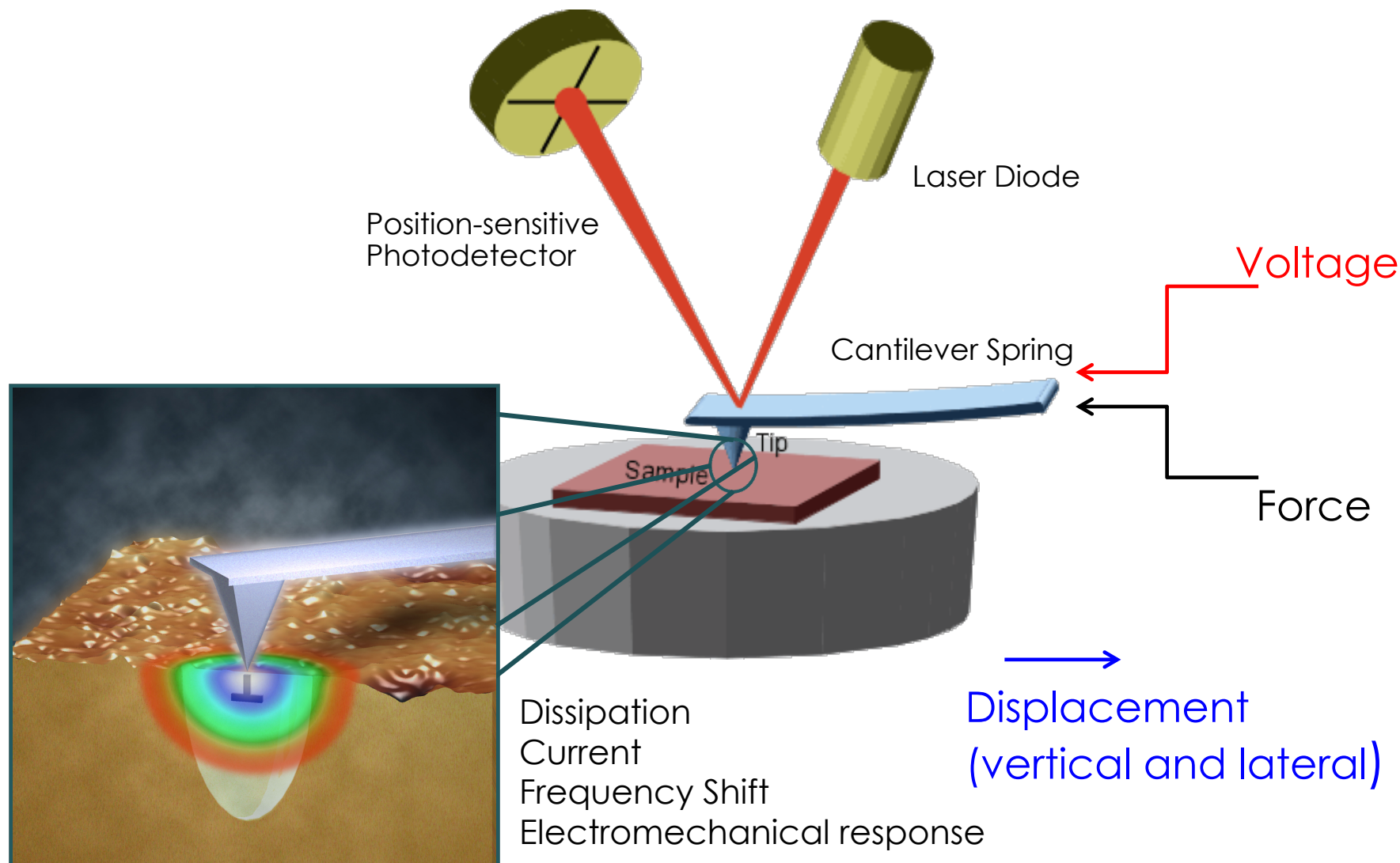


Texture analysis shows Molybdenum–Vanadium based complex oxide catalysts for propane ammoxidation

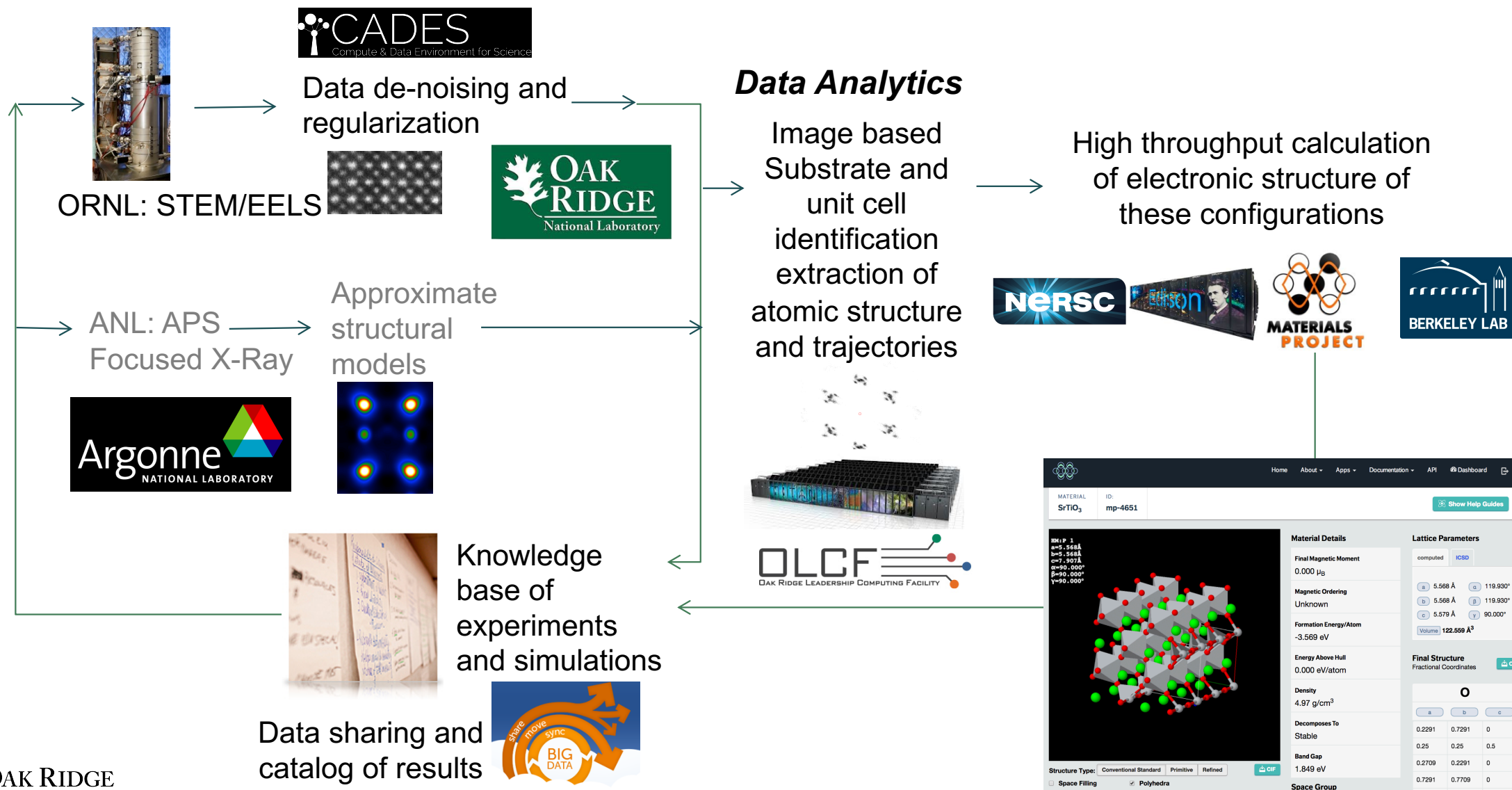
Experimental Science: CNMS



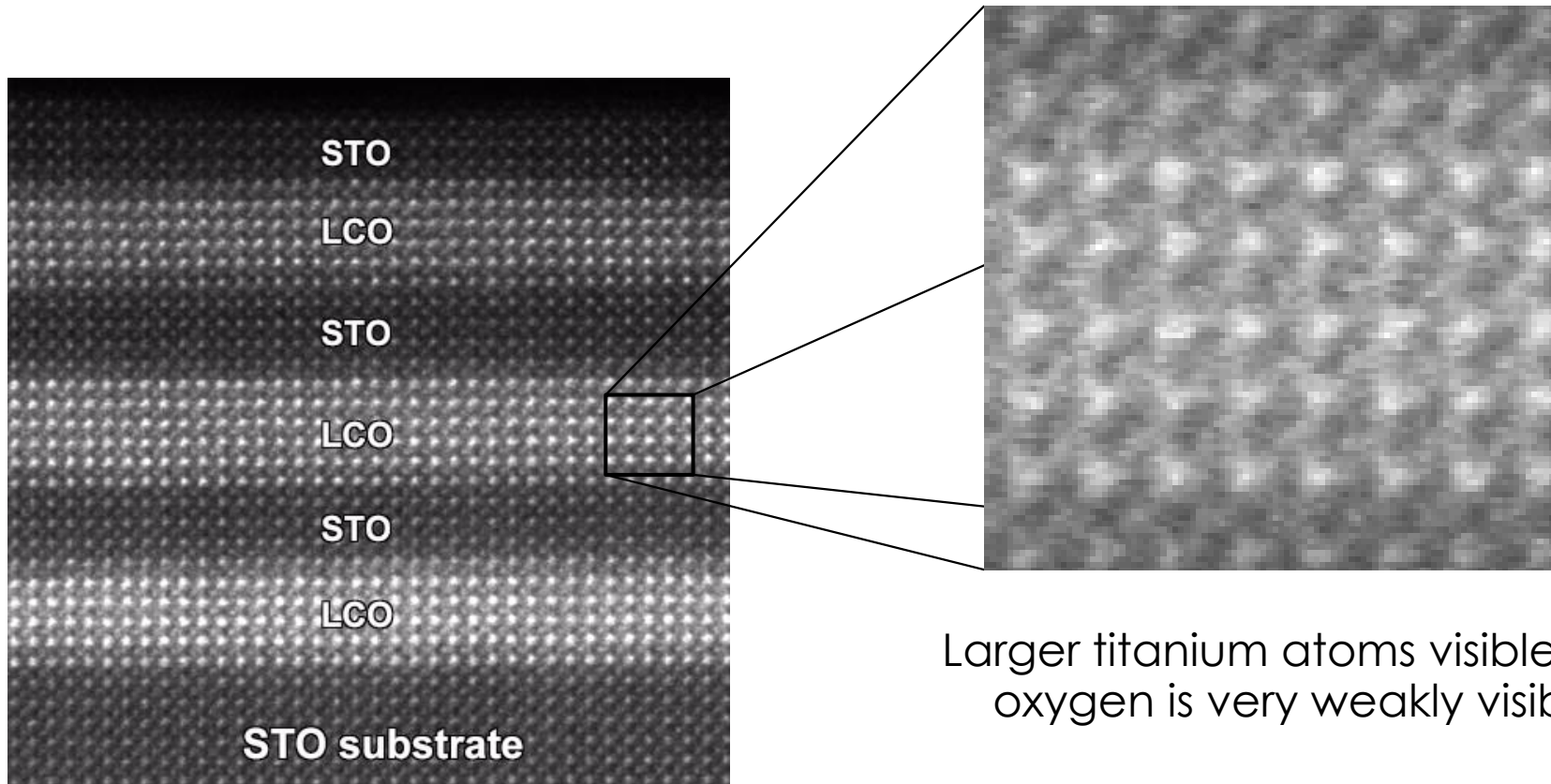
FeSeTe at the defect
creating local
superconductivity



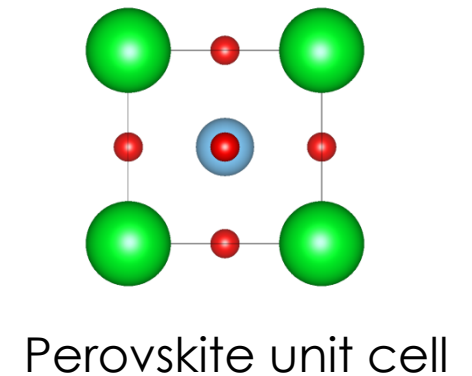
Federated Experimental Science



Federated Experimental Science

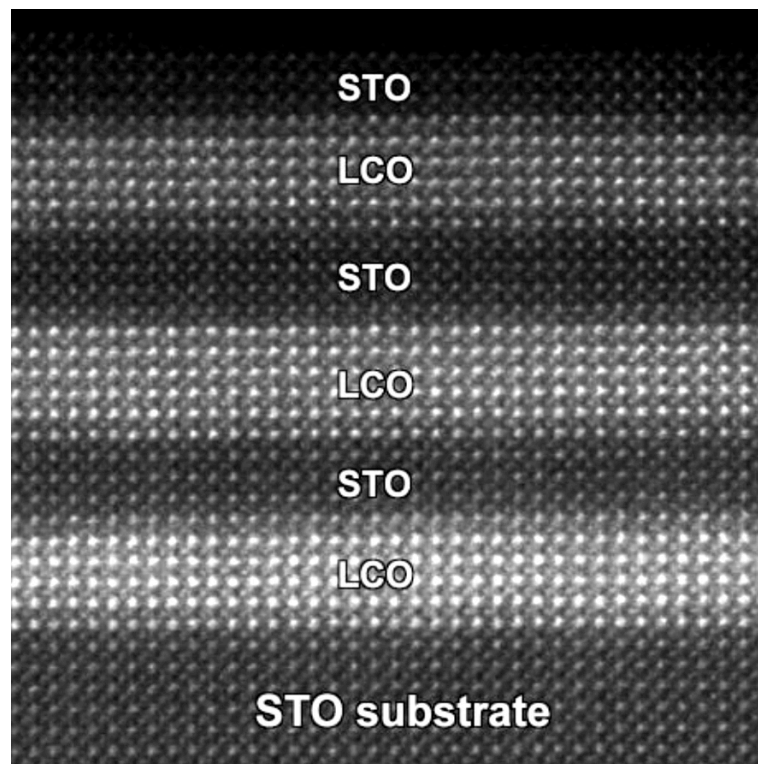


Vacancy ordering (11, 14.5, and 18 nm confinement layer)

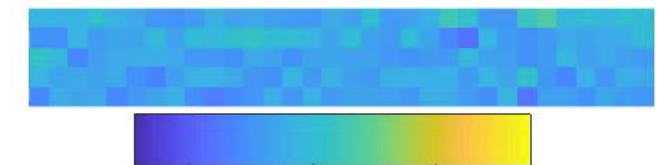


Capability: Environmental 1000 images/sec; 10 min pulse; 11-13 TB/day
Dynamic 1,000,000 images/sec; 10 sec pulse; **20 TB /burst**

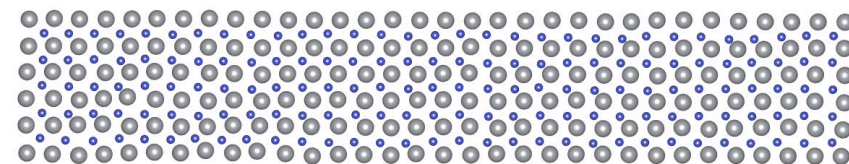
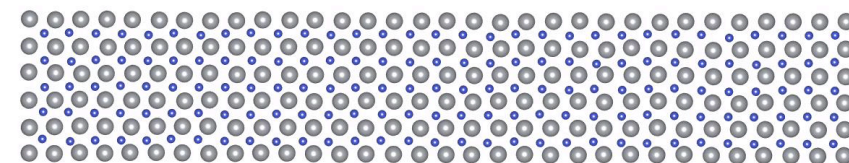
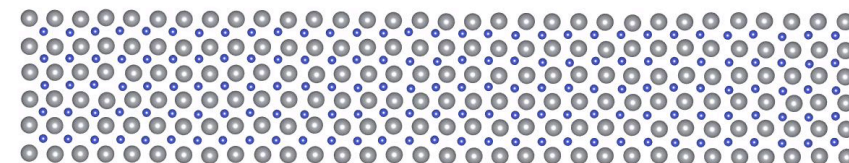
Federated Experimental Science



Vacancy ordering (11, 14.5, and 18 nm confinement layer)



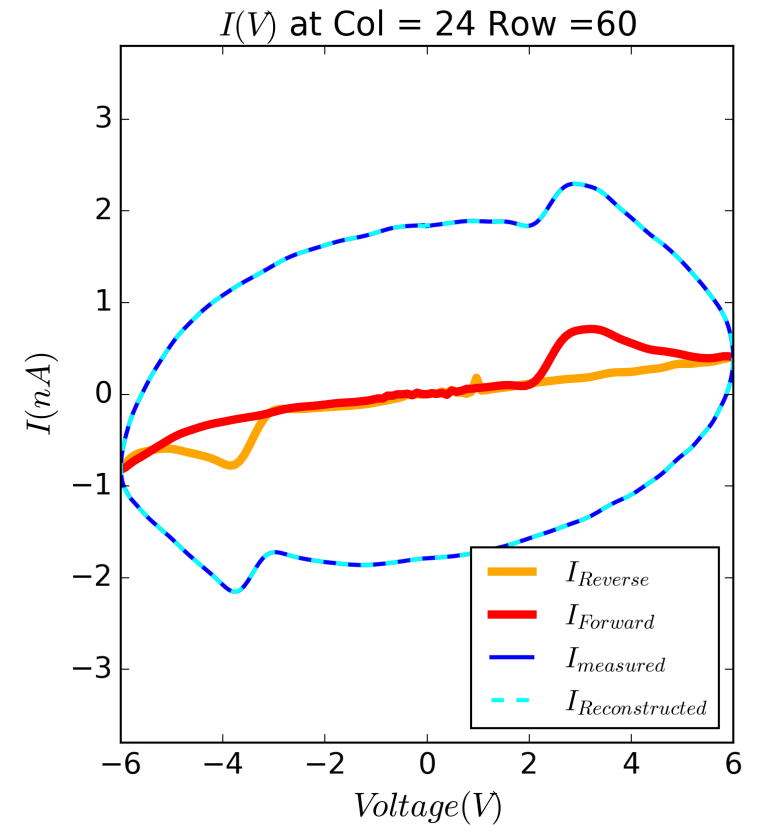
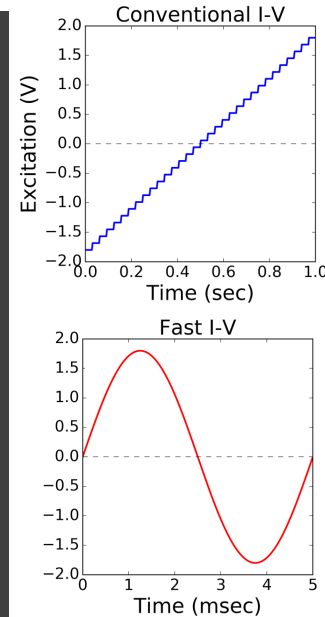
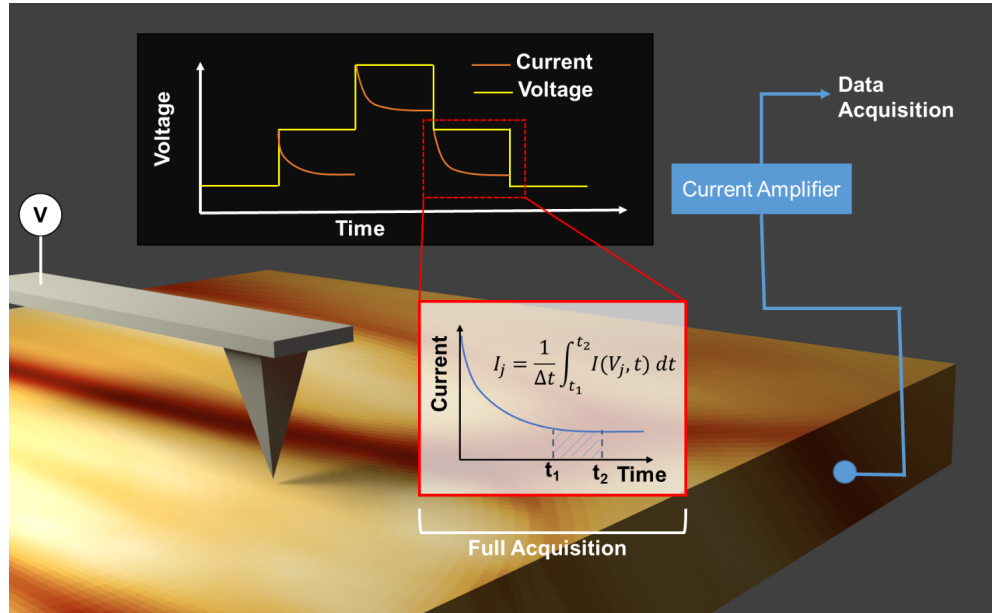
Moving average max separation between middle LCO layers.



Each titanium and oxygen atom found using HPC.

Capability: Environmental 1000 images/sec; 10 min pulse; 11-13 TB/day
Dynamic 1,000,000 images/sec; 10 sec pulse; **20 TB /burst**

Accelerating Data Acquisition



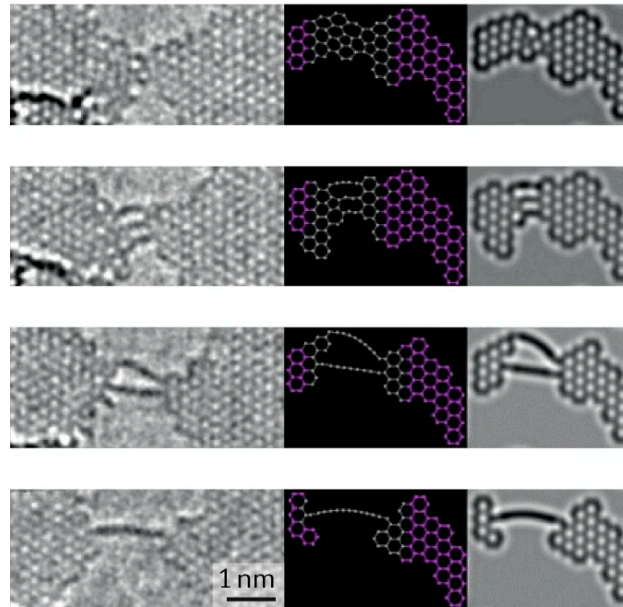
- Acquisition of current-voltage curves for electronic materials characterization at the nanoscale dates back decades
- We increase speed of acquisition by 1000x through full information capture + Bayesian inference methods

Bayesian reconstruction shows that I-V curves can be accurately modeled demonstrating the potential of full information capture of the underlying physics of the materials.

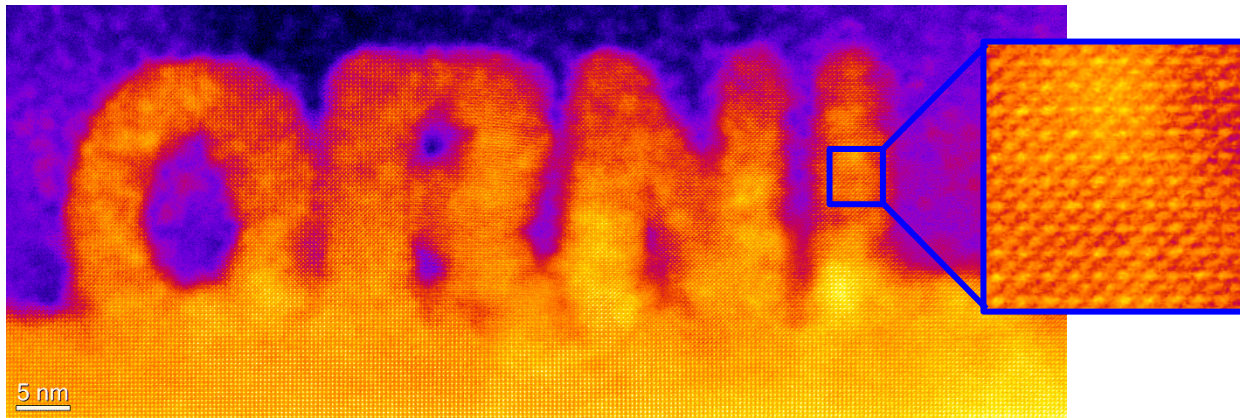
Start Up the Forge!



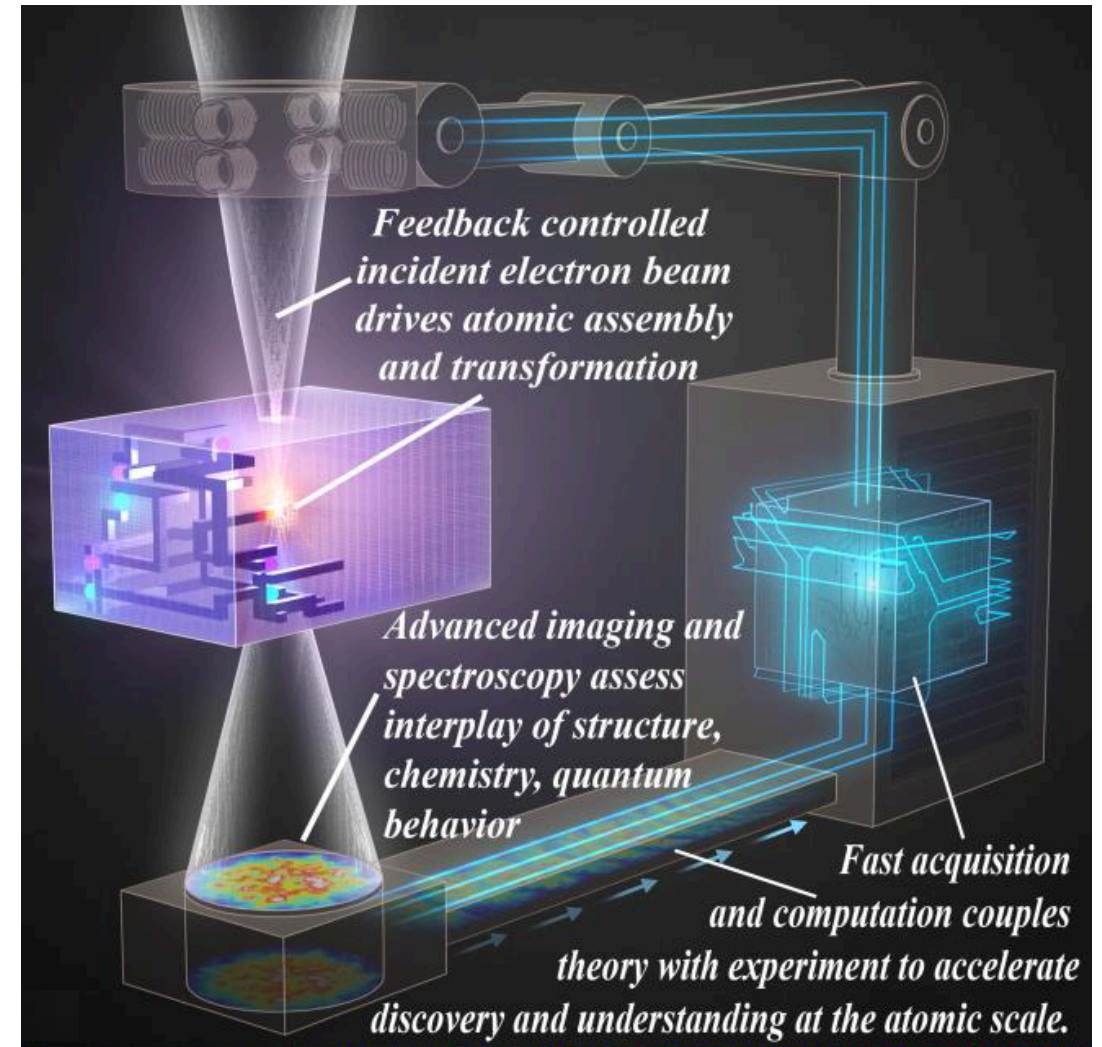
SPM writing



Carbon wires, e-beam

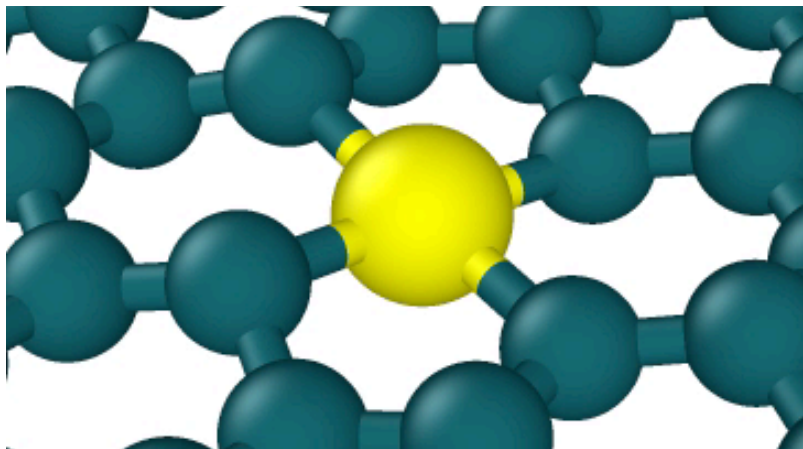


STEM e-beam induced crystallization

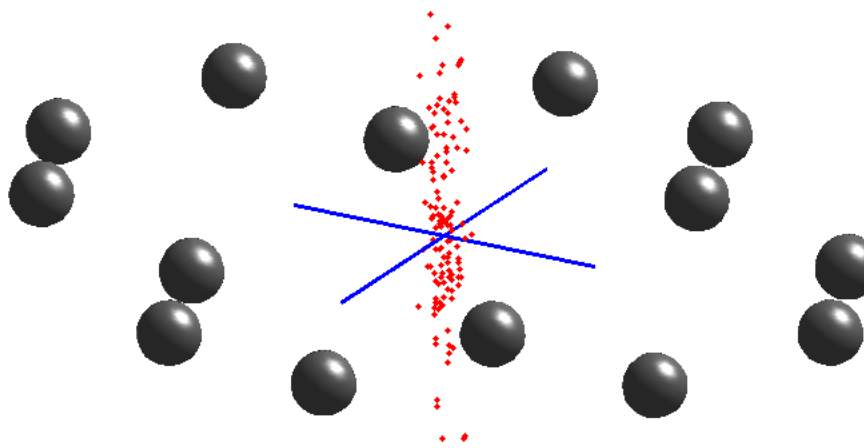


Atomic Forge concept, real-time simulation and data-controlled electron microscope to manipulate atoms.

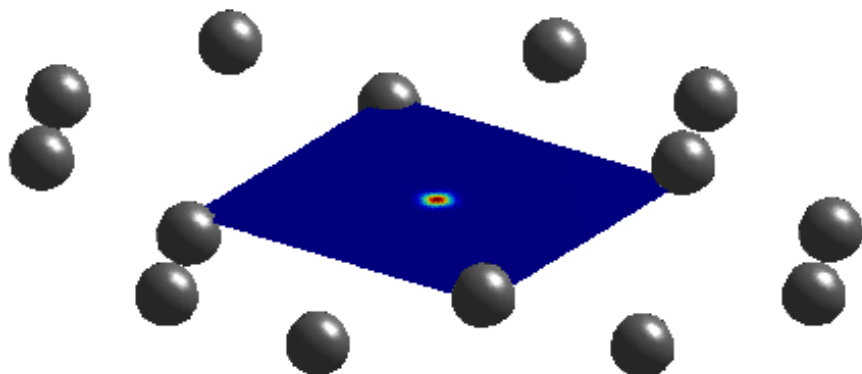
Forge Mathematics



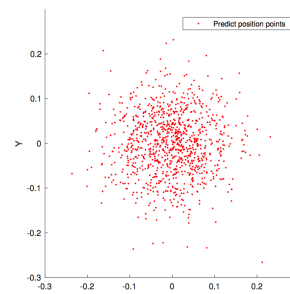
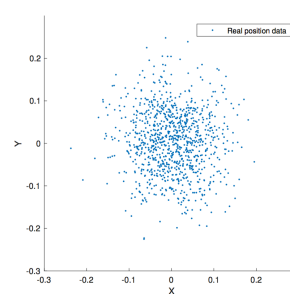
Simulation of Si in Graphene



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

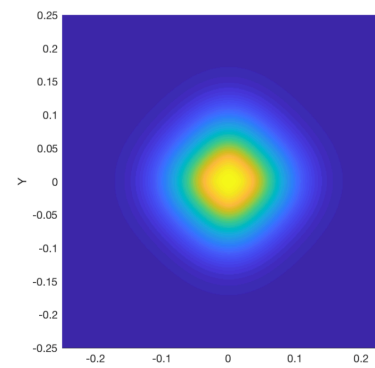


Estimated Potential

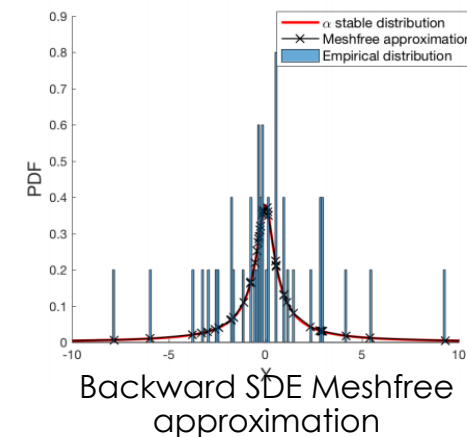


Langevin equation-based optimization of simulation data

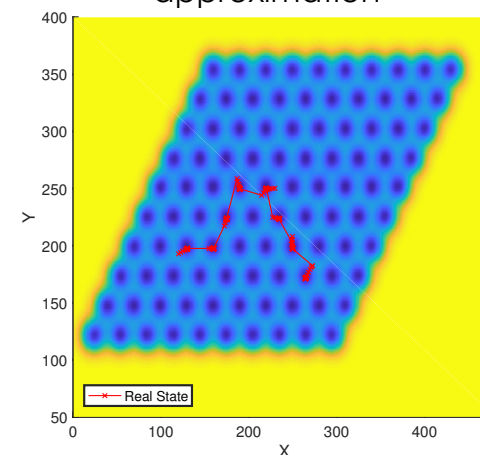
$$dX_t = -\Delta V_t dt + \sqrt{2D} dW_t \quad V = a(1 - b \cos(4\theta))e^{-\rho z^2}$$



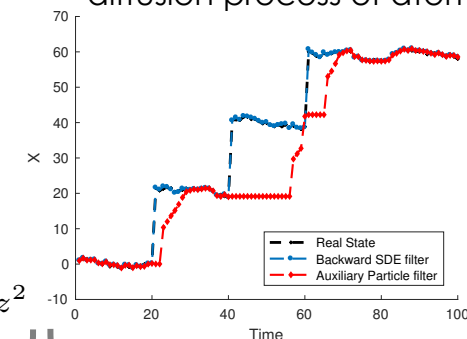
Best e^{-V} in atomic coordinates



Backward SDE Meshfree approximation

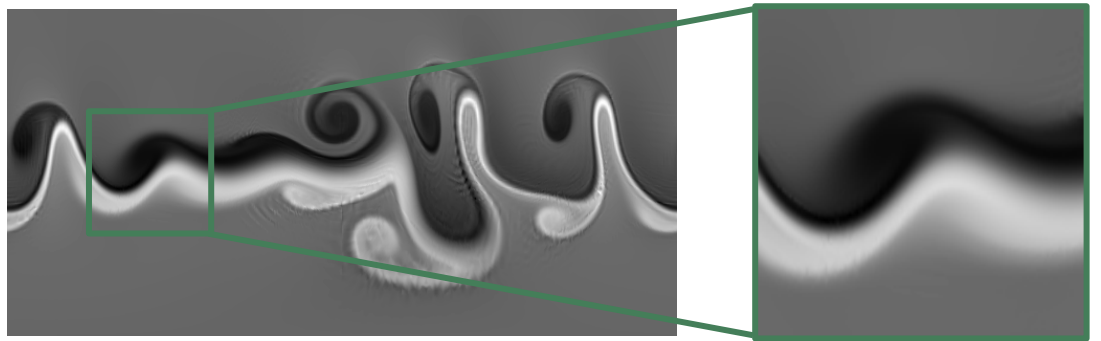


Accurate tracking of jump diffusion process of atom



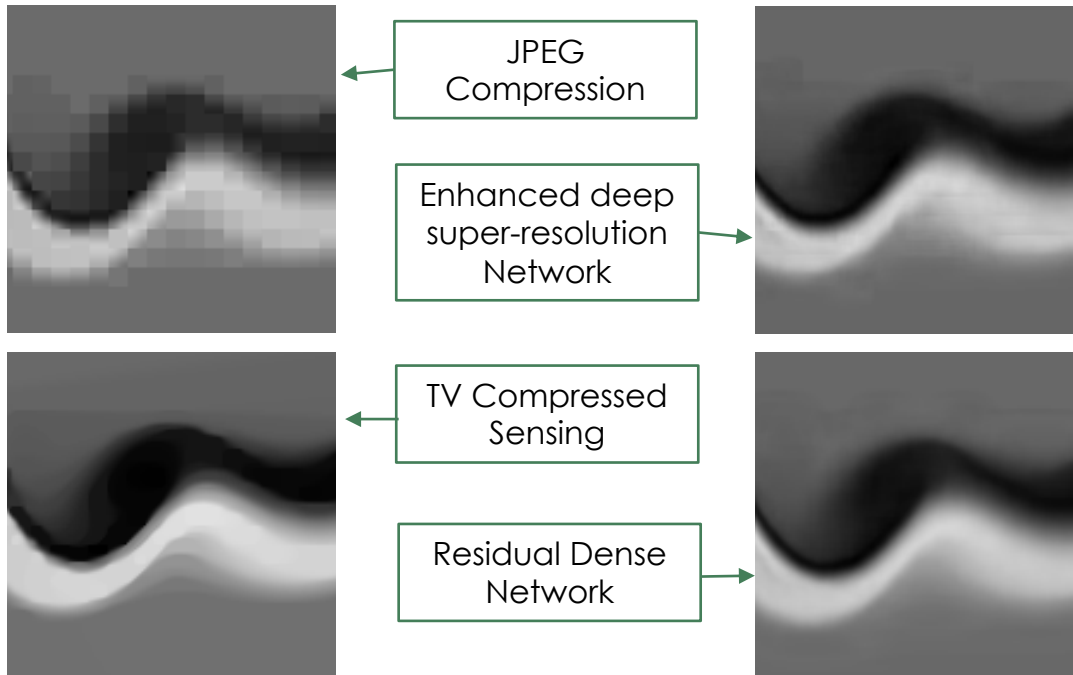
Tracking atoms

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.

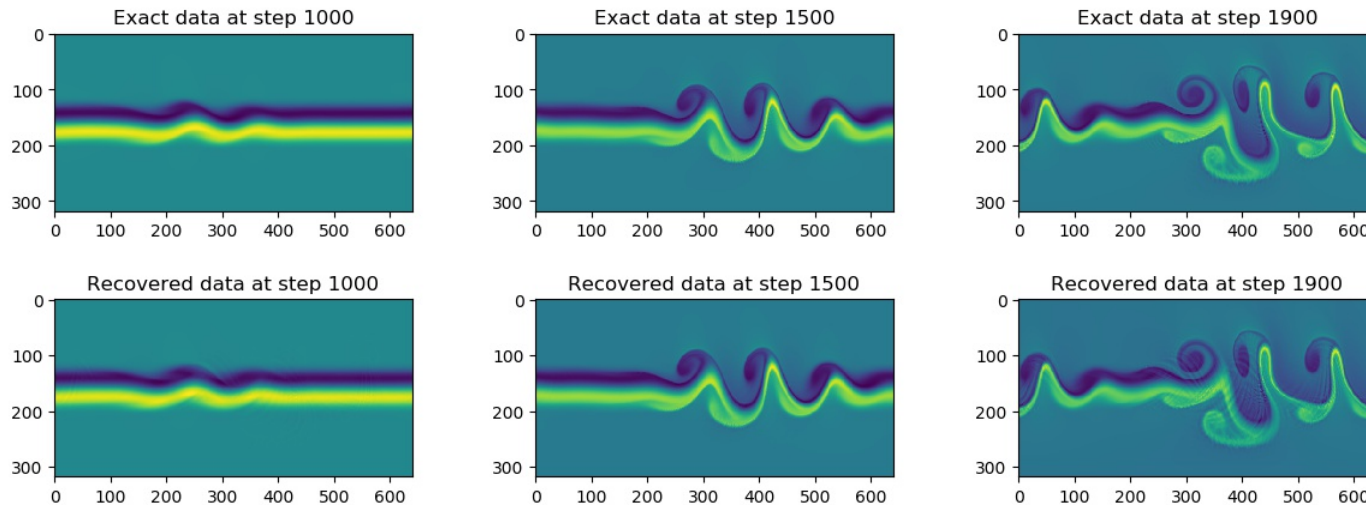
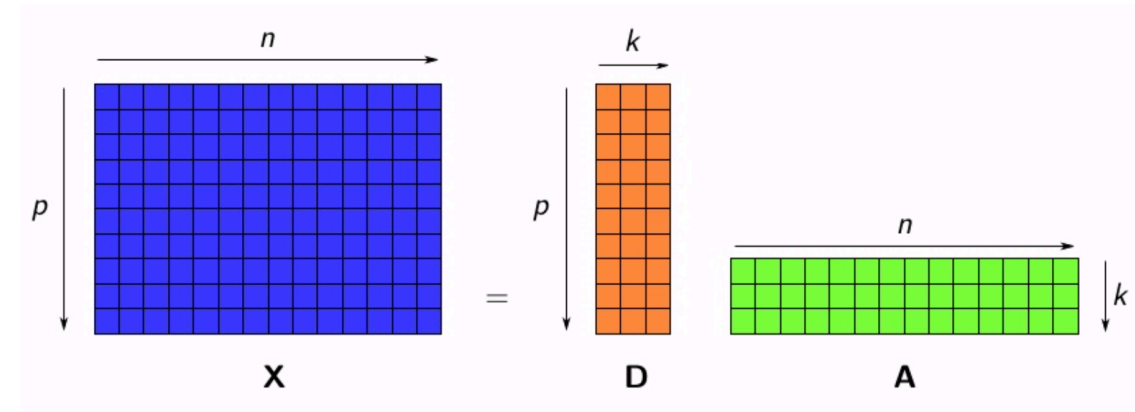
	NMSE	SSIM	PSNR
JPEG	0.038	0.971	37.245
CS w/ 400 iterations	0.045	0.973	34.534
EDSR	0.024	0.989	41.071
RDN	0.022	0.989	42.224

Scientific Data

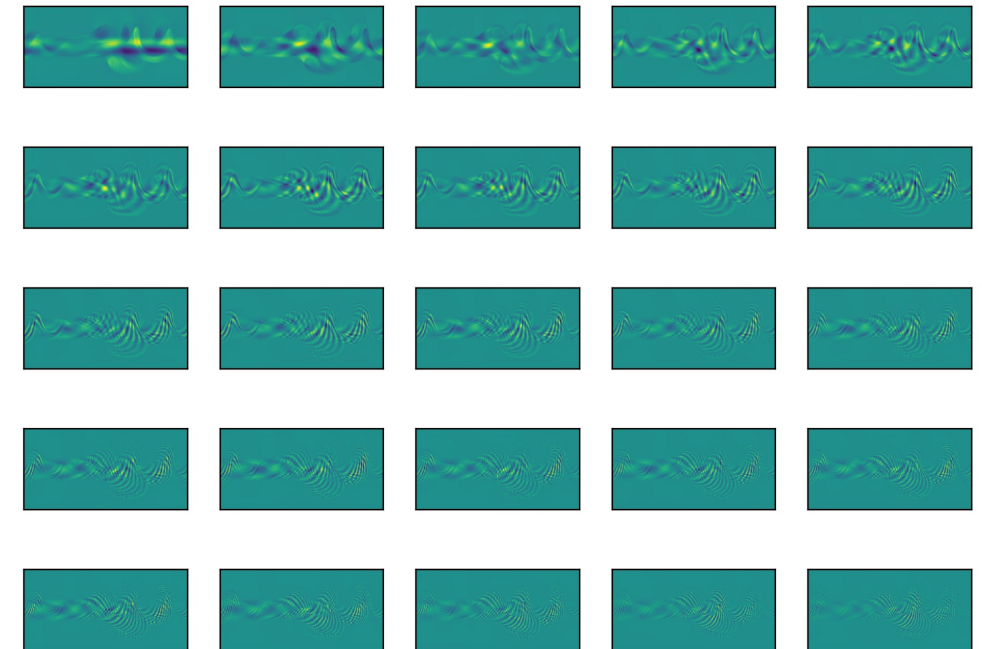
We develop a matrix factorization approach based upon out of core linear algebra methods for data compression, reconstruction and interpretable decomposition:

$$X \approx DA$$

- 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