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Towards Autonomous (Hyperspectral) Computed Tomography (CT) Instruments

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HyperCT

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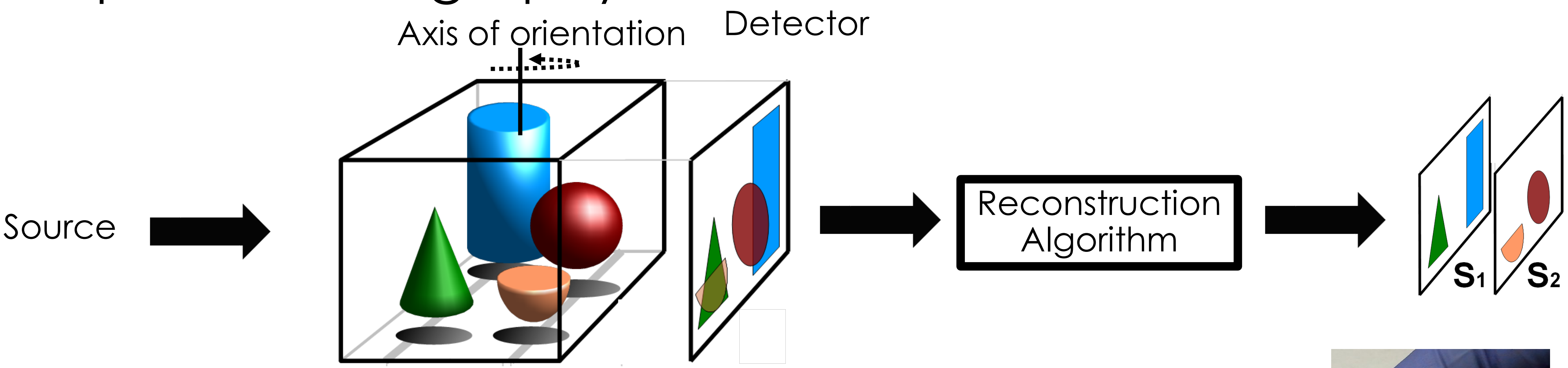
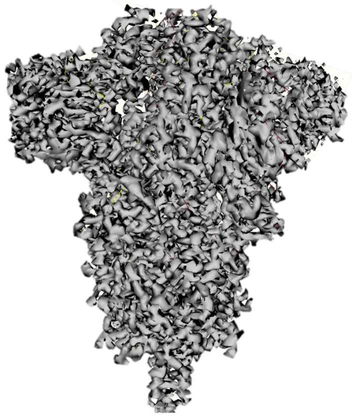
Computed Tomography for Science



Virus Structures

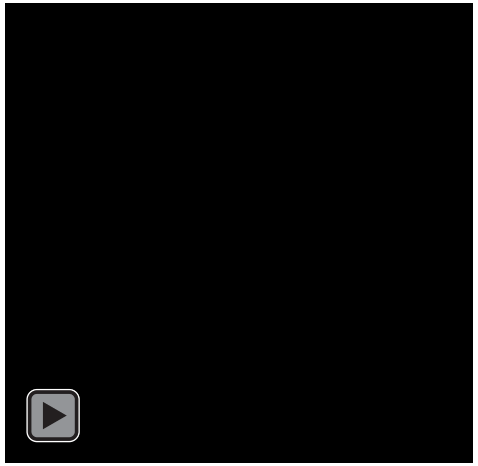


Walls AC, Park YJ, Tortorici MA, Wall A, McGuire AT, Veesler D Cell (2020)

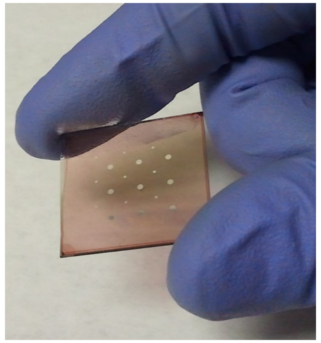
Lithium iron phosphate nano-particles

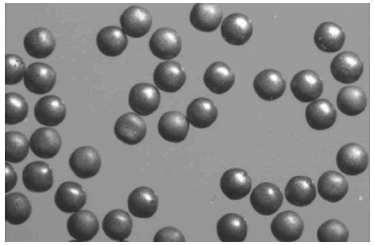
Young-Sang Yu et al., Nat. Comm. Vol. 9, No. 921, 2018

TRISO fuel element



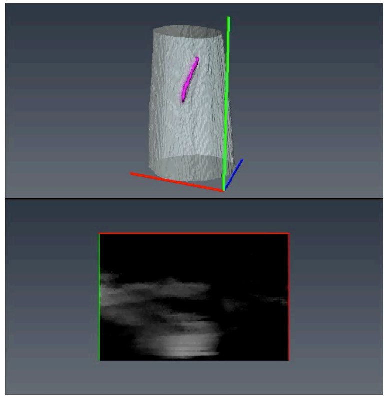
Grant Helmreich, ORNL

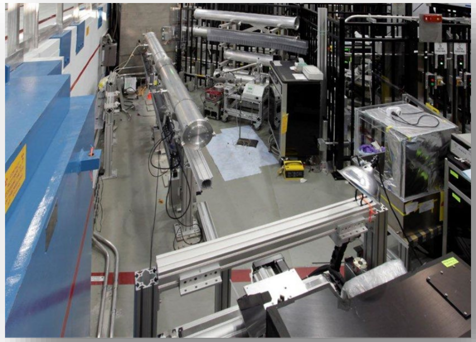


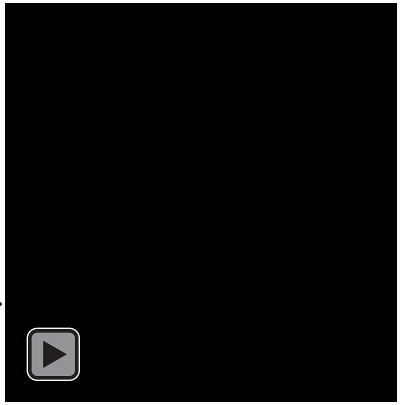


Accurate characterization is critical to determine structure-function relationships

Jose David Arregui-Mena et al. Journal of Nuclear Materials 2020

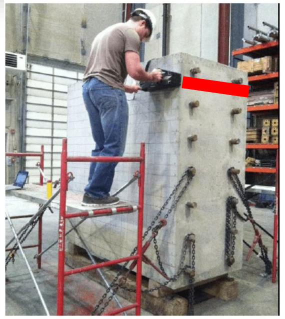


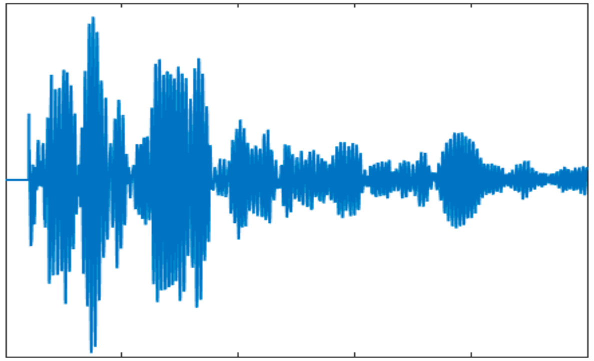




A. Ziabari et al., IMECE 2020

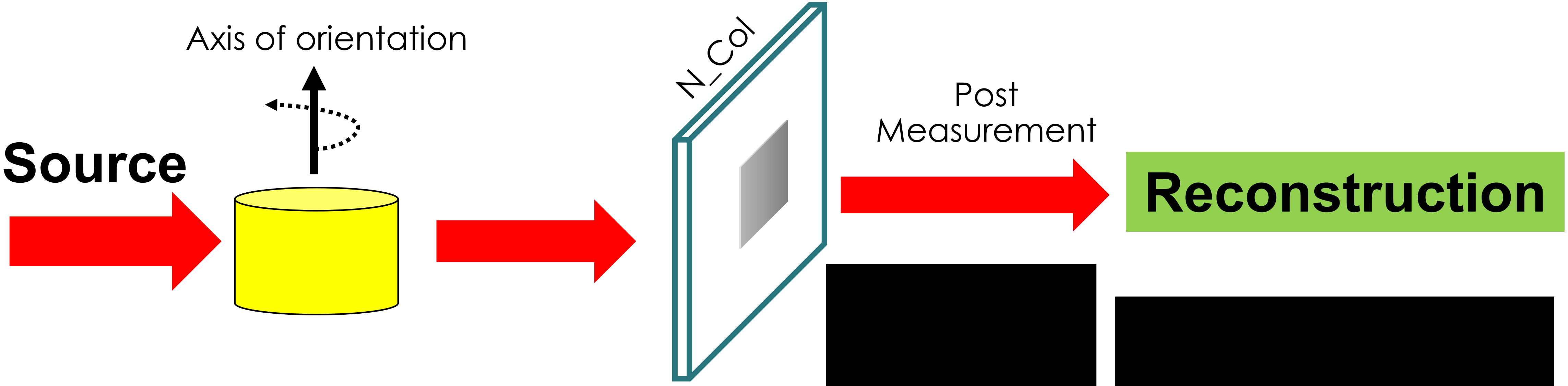
J. Warren et al. (BSD, ORNL)

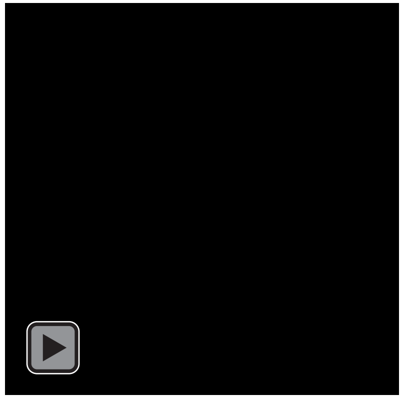


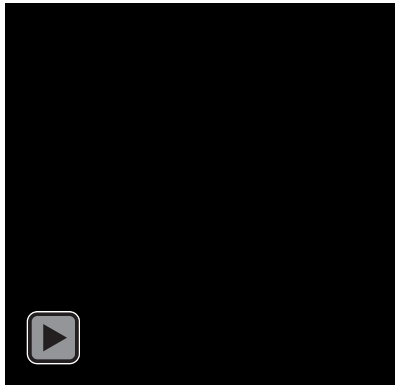


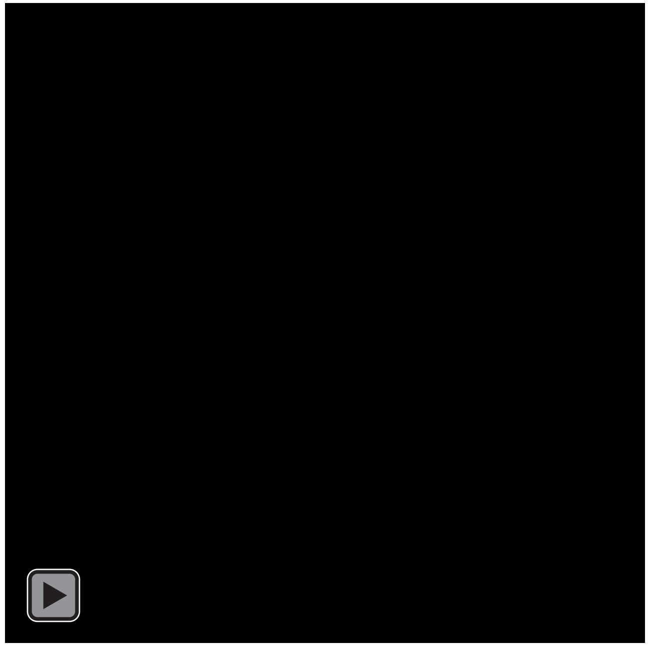
** Hani AlMansouri et al, IEEE TCI 2019*

Current Open-Loop Approach







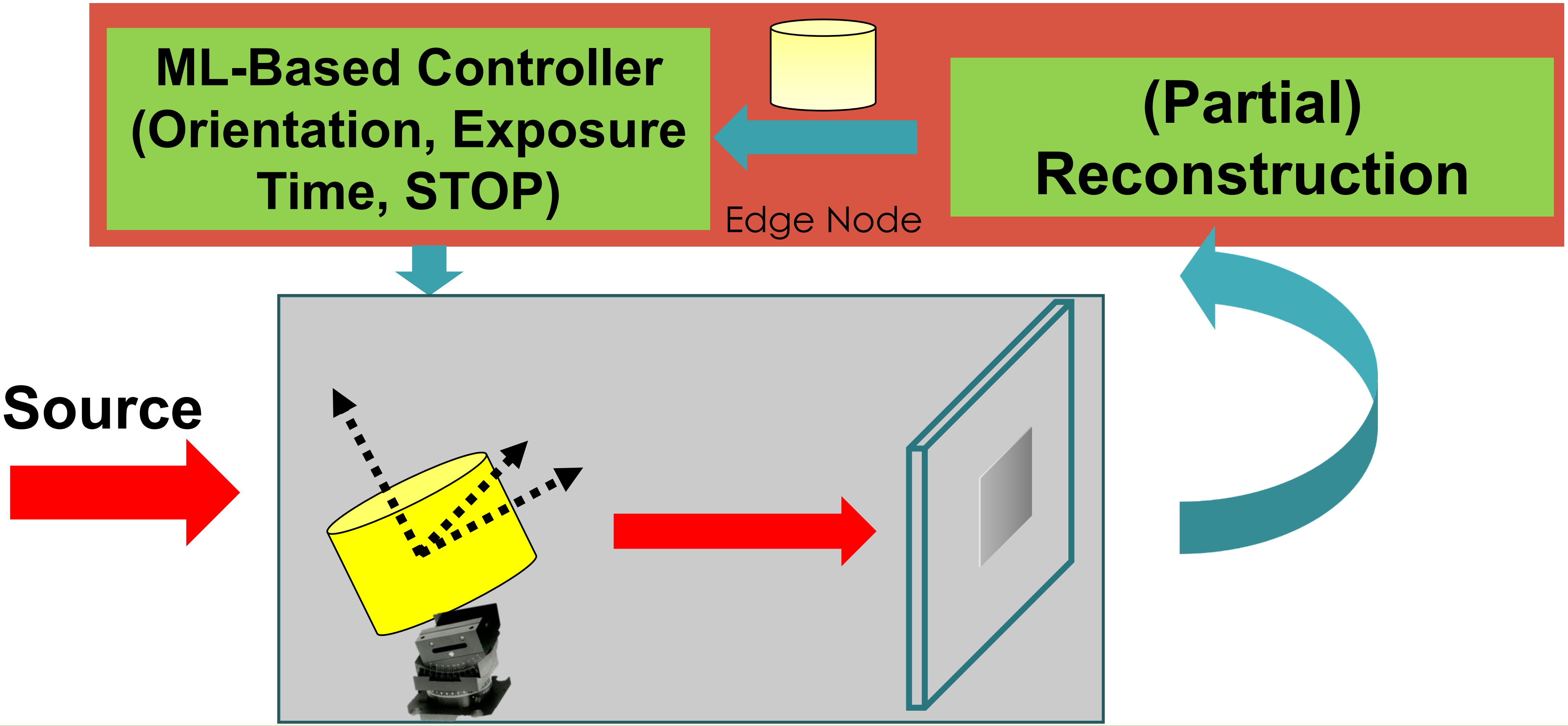


Idea Sampling Rate :
Number of Images = N_col

Total Measurement Time
Number of Images* Time/image

Example:
512 * 2h ~ 1024 hours
In practice
50 * 2h ~ 100 hours

Autonomous Streaming Neutron-CT Systems



- *Fast + high-fidelity reconstruction from partial, sparse, low SNR, and different orientations measurements*
- *Sample adaptive acquisition strategies*
- *Algorithms for dynamic control (stopping, re-orientation etc.)*

Outline

- Advanced algorithms for neutron CT
  - Model-based Image Reconstruction (**MBIR**)
  - Deep-Learning based Reconstruction
- Machine Learning Methods for Automated CT Experiments
- Conclusions

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Model-based Reconstruction Algorithms for Neutron CT

- Low SNR Hyper-Spectral Data
- Sparse Set of Measurements
- Arbitrary Orientations

Model-Based Image Reconstruction (MBIR)

$$\hat{f} = \boxed{\text{argmin}_f} \{ \boxed{l(g; f)} + \boxed{s(f)} \}$$

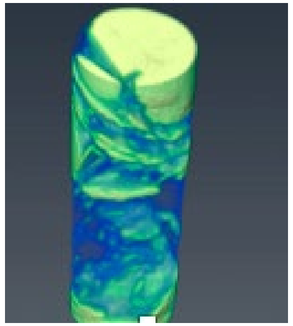
Data-fidelity (Physics, noise)

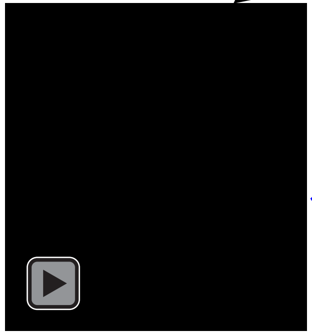
Regularizer

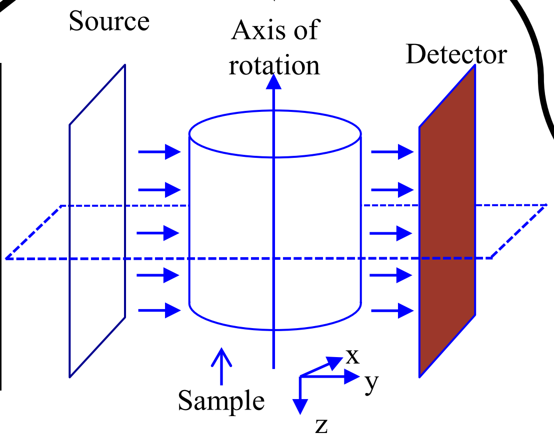
Fitting term that encodes **physics and noise statistics**

Encourages **similarity between neighboring voxels**

$$\hat{f} \leftarrow \arg\min_f \left\{ \frac{1}{2} ||g - Af||_W^2 + \sum_{i,j \in \chi} \rho(f_i - f_j) \right\}$$







Inv. ***Noise variance***

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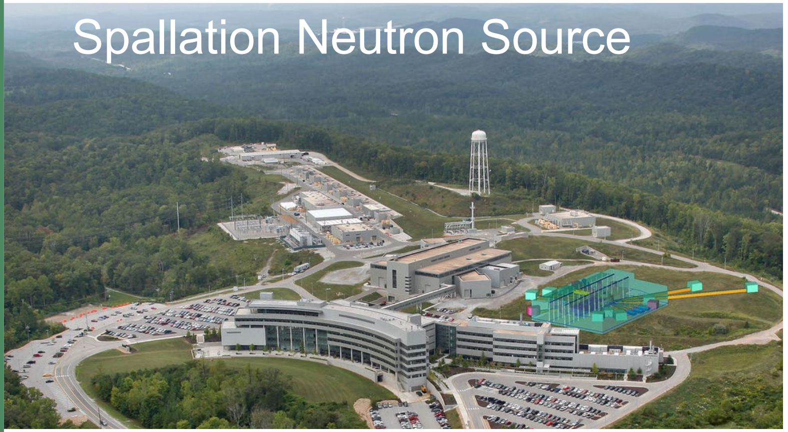
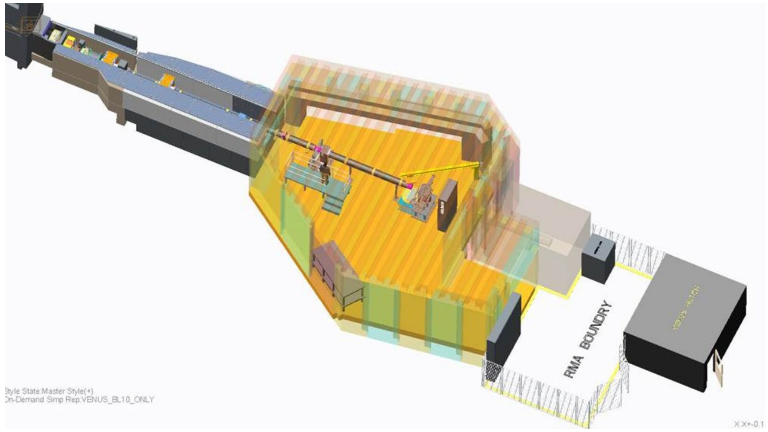
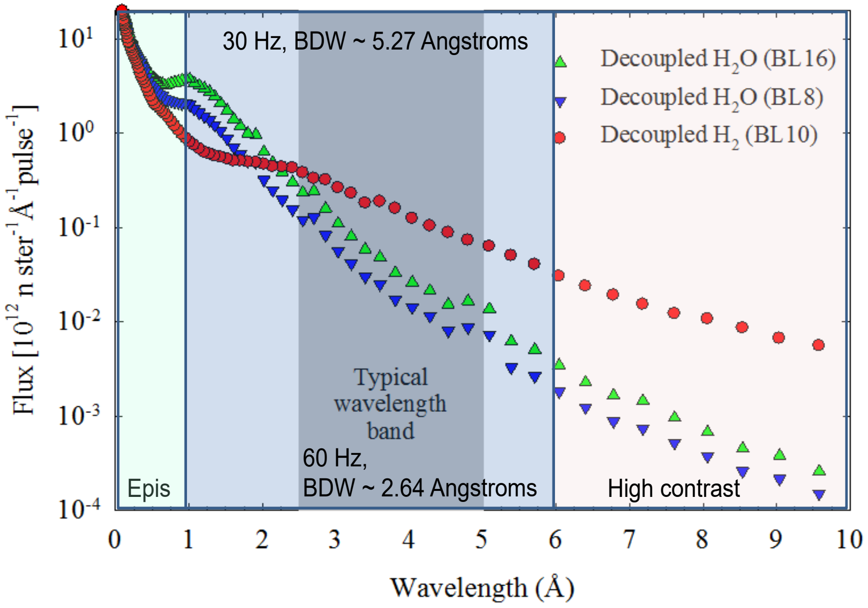
Iteratively update the variables to minimize cost function

Spallation Neutron Source: (Future) Imaging Beamline - VENUS



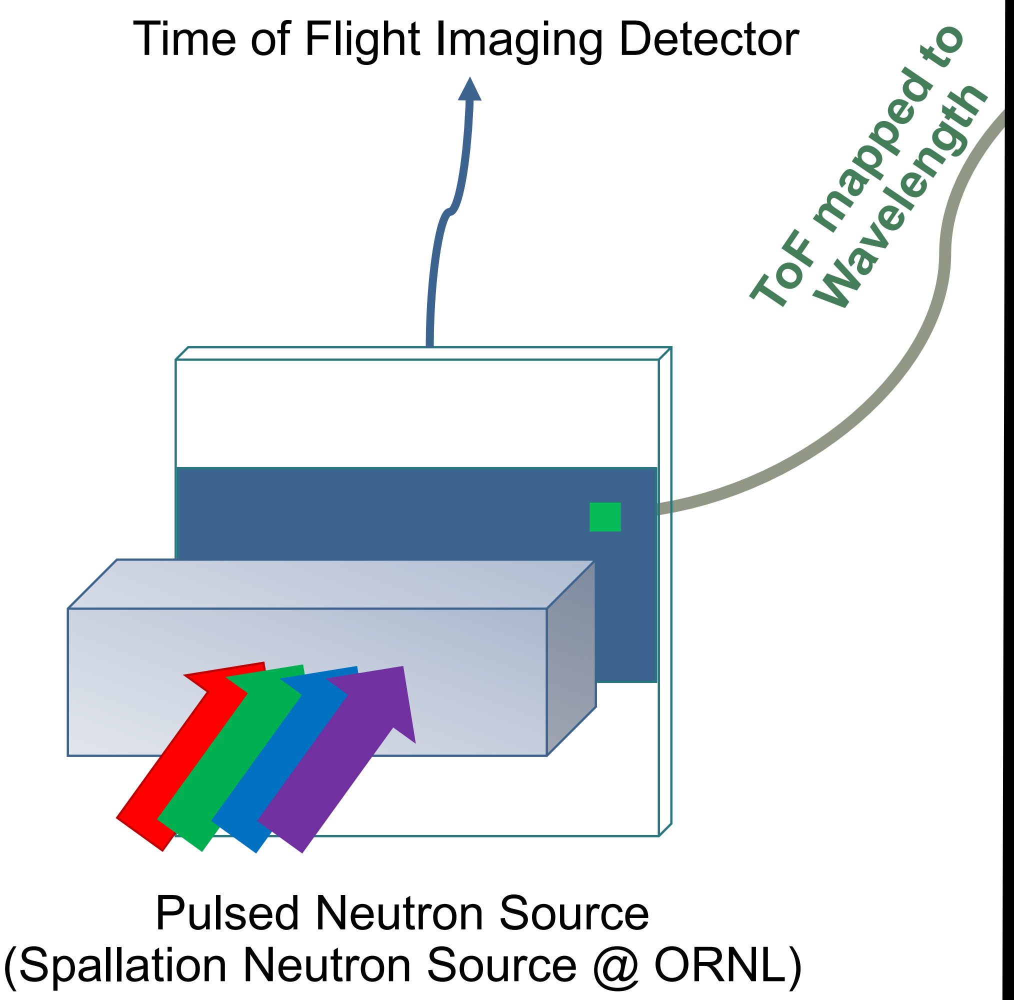


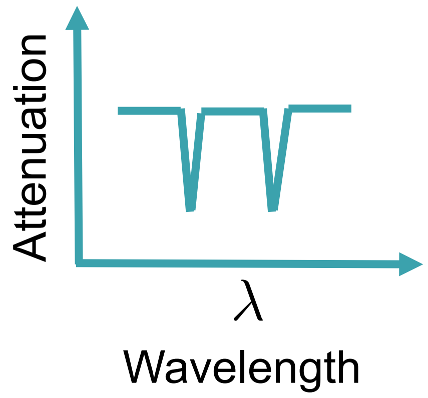


Beamline	Optimized for	Completion date	L/D	Max FOV (cm2)	Maximum Wavelength or BDW (Å)	Time resolution	Spatial resolution	Flux (n/cm2/s)
VENUS, ORNL (20 to 60 Hz, 1.4 MW) (20 and 25 m)	Imaging	TBD (**3.5 years from start date)**	Up to 2000	28 x 28	Up to 20 2.4 BDW (25 m)	Δλ/λ=0.15% (at 1 Å)	< 15 microns	1 x 10^8 (L/D = 400)

Slide Courtesy: Hassina Billheux

ToF Neutron Imaging Applications





- Materials mapping – using hyper-spectral signature

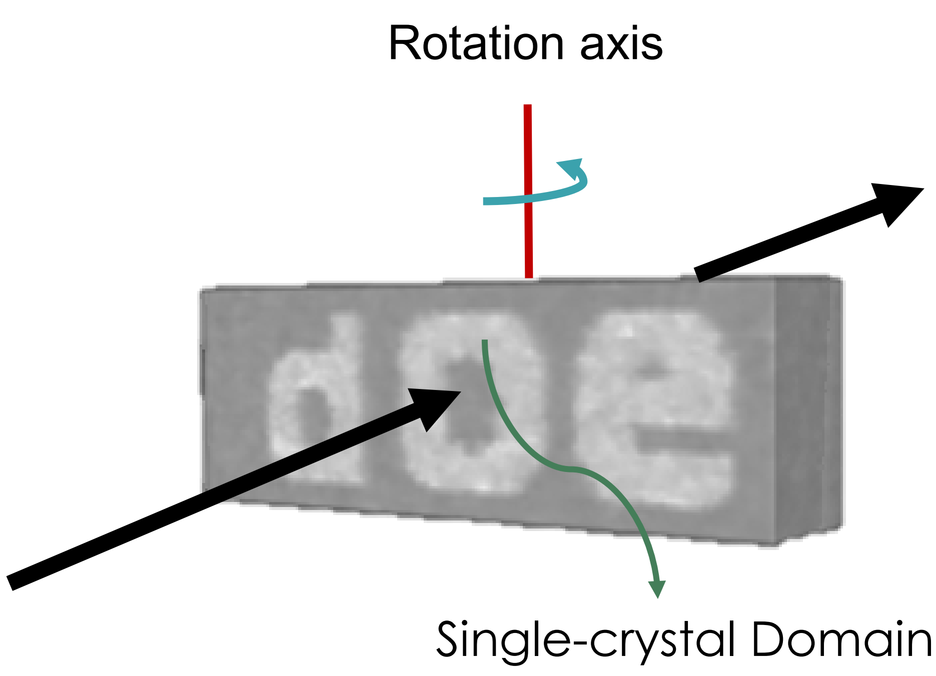
- *Engineering* materials (crystalline) - using Bragg scatter

$$n\lambda = 2d\sin(\theta)$$

d Distance between crystallographic planes

θ Angle between incident beam and cryst. plane

Challenges in ToF Neutron Tomography



Simulated ToF Radiograph

Data - very noisy (low-flux)

Time–consuming scans (~hour per “image”)

Imperfections in source beam

Single-crystal i.e. going beyond standard CT

MBIR for Basic ToF CT (For Each Wavelength)

$$(\hat{f}, \hat{B}) \leftarrow \text{R-MBIR}(g; T)$$

Reconstruction

Binary map of anomalies

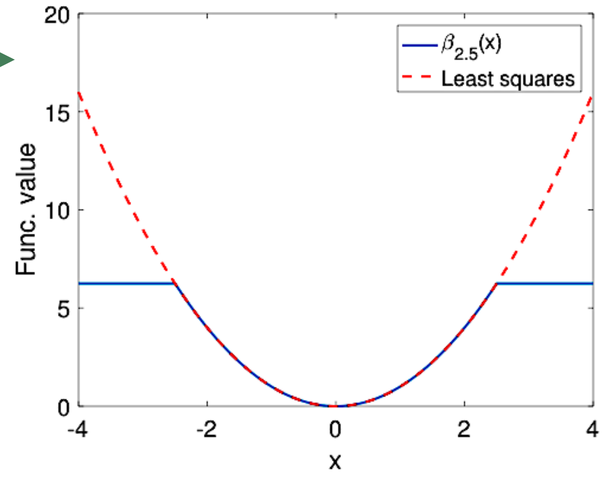
Normalized data

Outlier Threshold

- Effectively find a minimum of

$$c(f) = \frac{1}{2}\sum_{i=1}^{M} \beta_T \left((g_i - [Af]_i)\sqrt{W_{ii}} \right) + s(f)$$

$$c(f) = \frac{1}{2}\sum_{i=1}^{M} \beta_T \left(e_i(f)\sqrt{W_{ii}} \right) + s(f)$$



Edge-preserving regularizer

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Optimization Algorithm

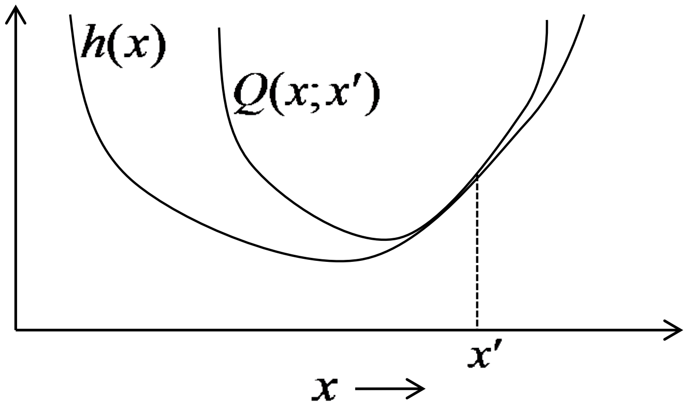
- **Problem** : Minimizing the cost – computationally complex

Solution : Construct a surrogate to the original cost

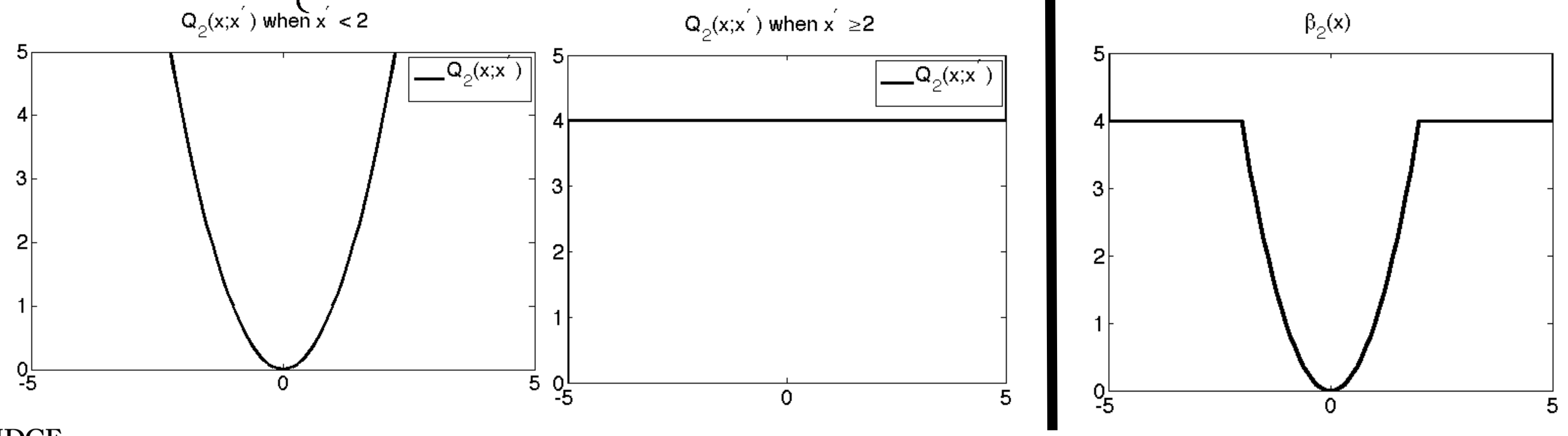
$Q(x;x')$ is a surrogate to $h(x)$ if

$$Q(x;x') \geq h(x) \ \forall x$$

$$Q(x';x') = h(x')$$

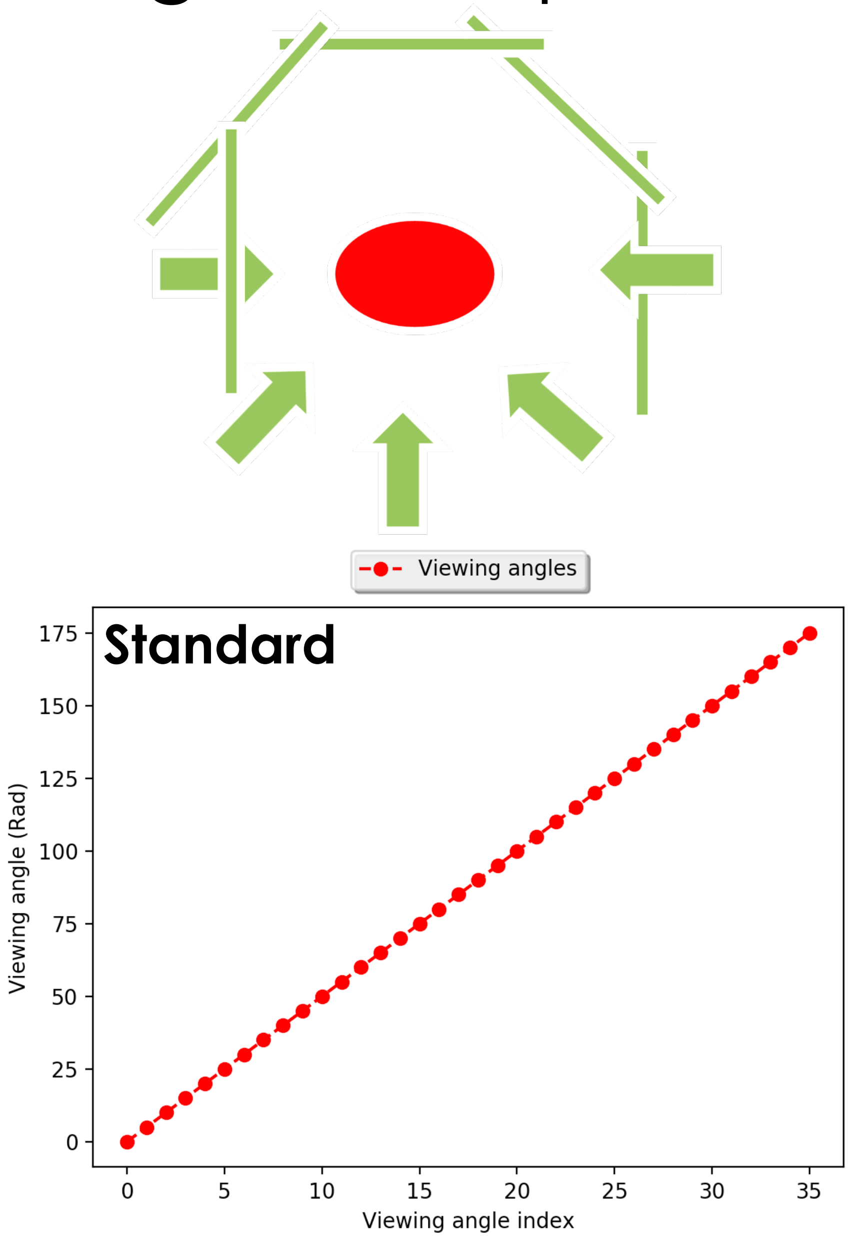


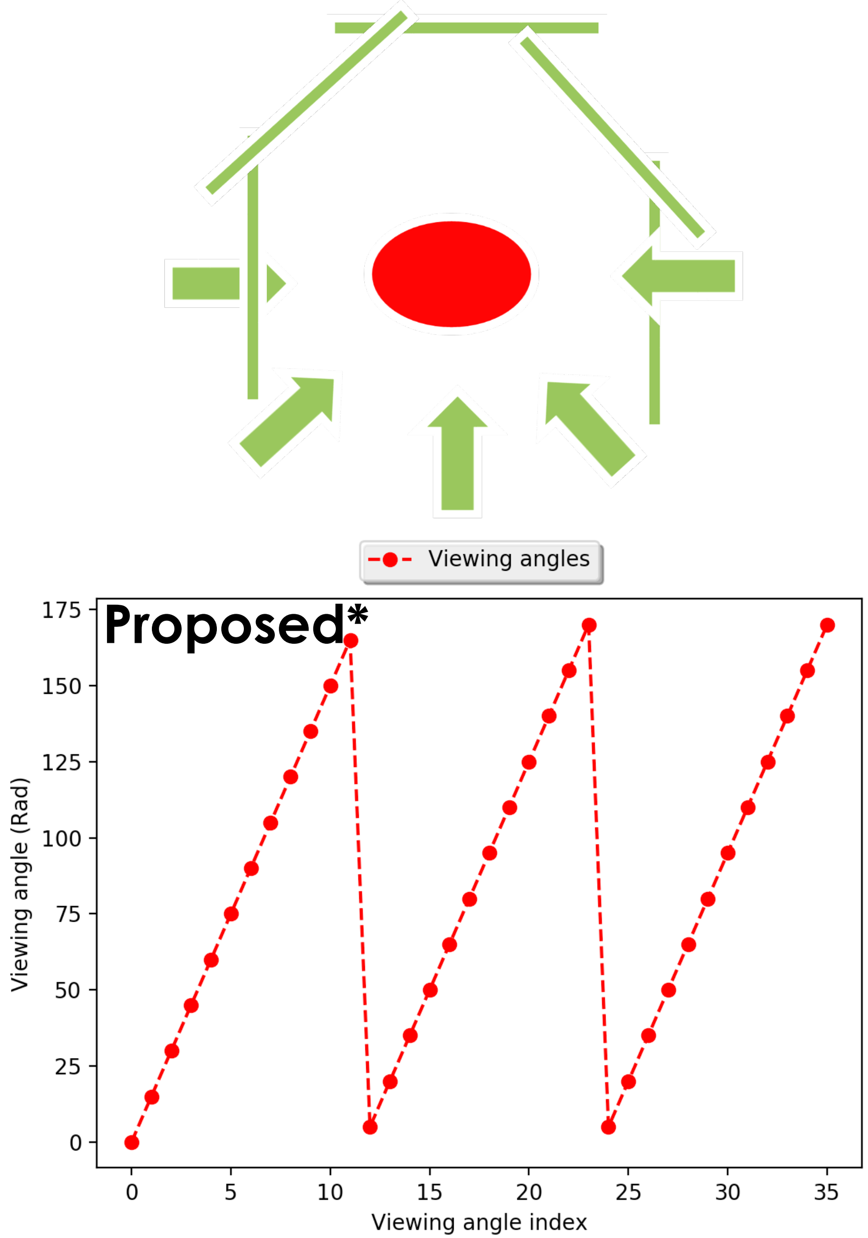
$$Q_T(x;x') = \begin{cases} x^2 & |x'| < T \\ T^2 & |x'| \geq T \end{cases}$$ is a surrogate to $\beta_T(x)$.



*S. V. Venkatakrishnan, L.F. Drummy, M. Jackson, M. De Graef, J.P. Simmons, and C.A. Bouman (IEEE TCI, Vol. 1, No. 1, Mar. 2015

Streaming CT: Acquisition for Better Feedback





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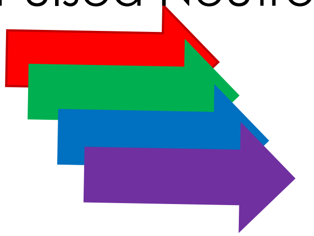
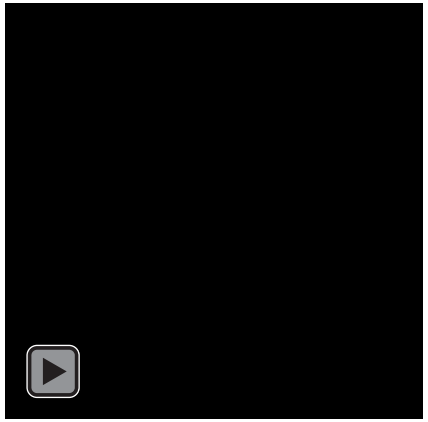
* **K. A. Mohan**, **S**. *V*. *Venkatakrishnan, John W. Gibbs, E. Begum Gulsoy, Xianghui Xiao, Marc De Graef, Peter W. Voorhees, and Charles A. Bouman, "TIMBIR – A reconstruction method for space-time reconstructions from interlaced views", IEEE TCI, Vol. 1, No. 2, 2015*

Comparing Acquisition + Reconstruction*

Pulsed Neutrons

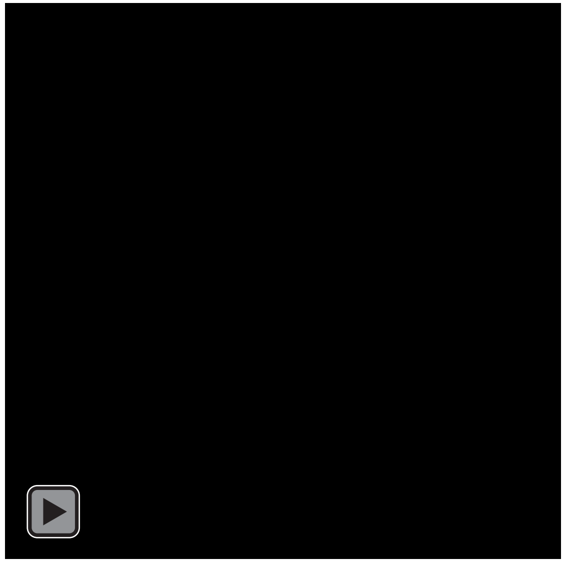


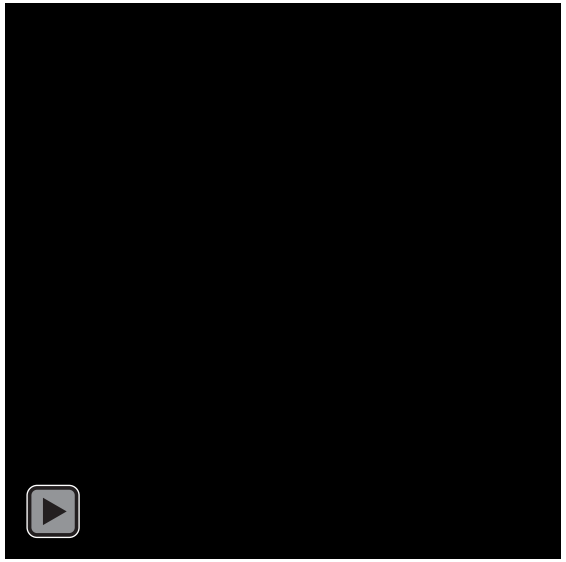


- ~1500 wavelength/ToF Bins
- 512 X 512 pixels per image
- 30 projections acquired (~36 h)

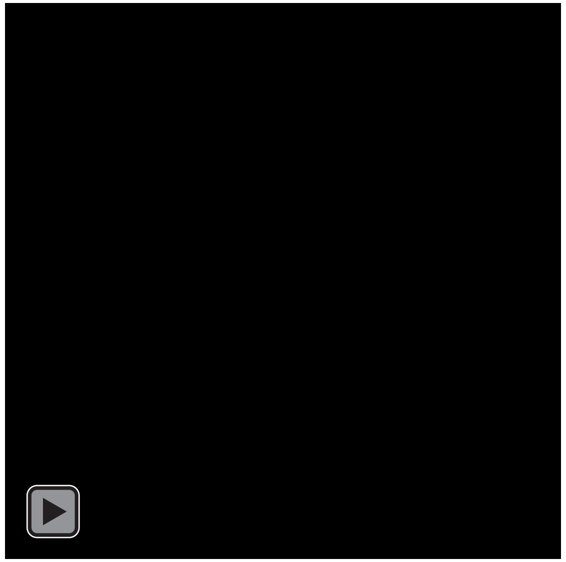
Conventional | **Interlaced**

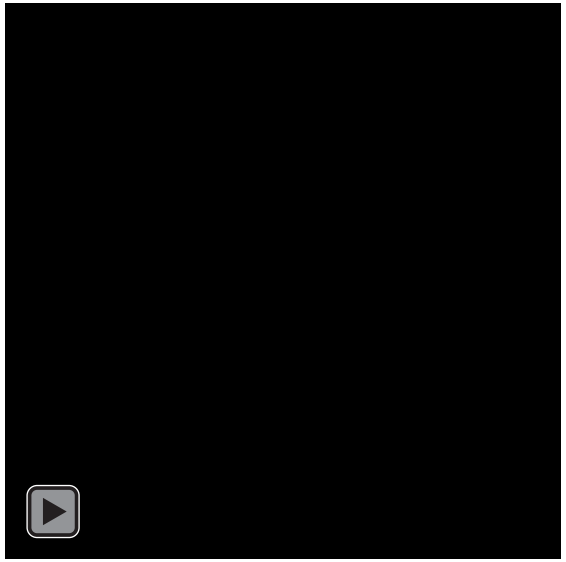
FBP





MBIR





[* https://github.com/svvenkatakrishnan/pyMBIR](https://github.com/svvenkatakrishnan/pyMBIR)

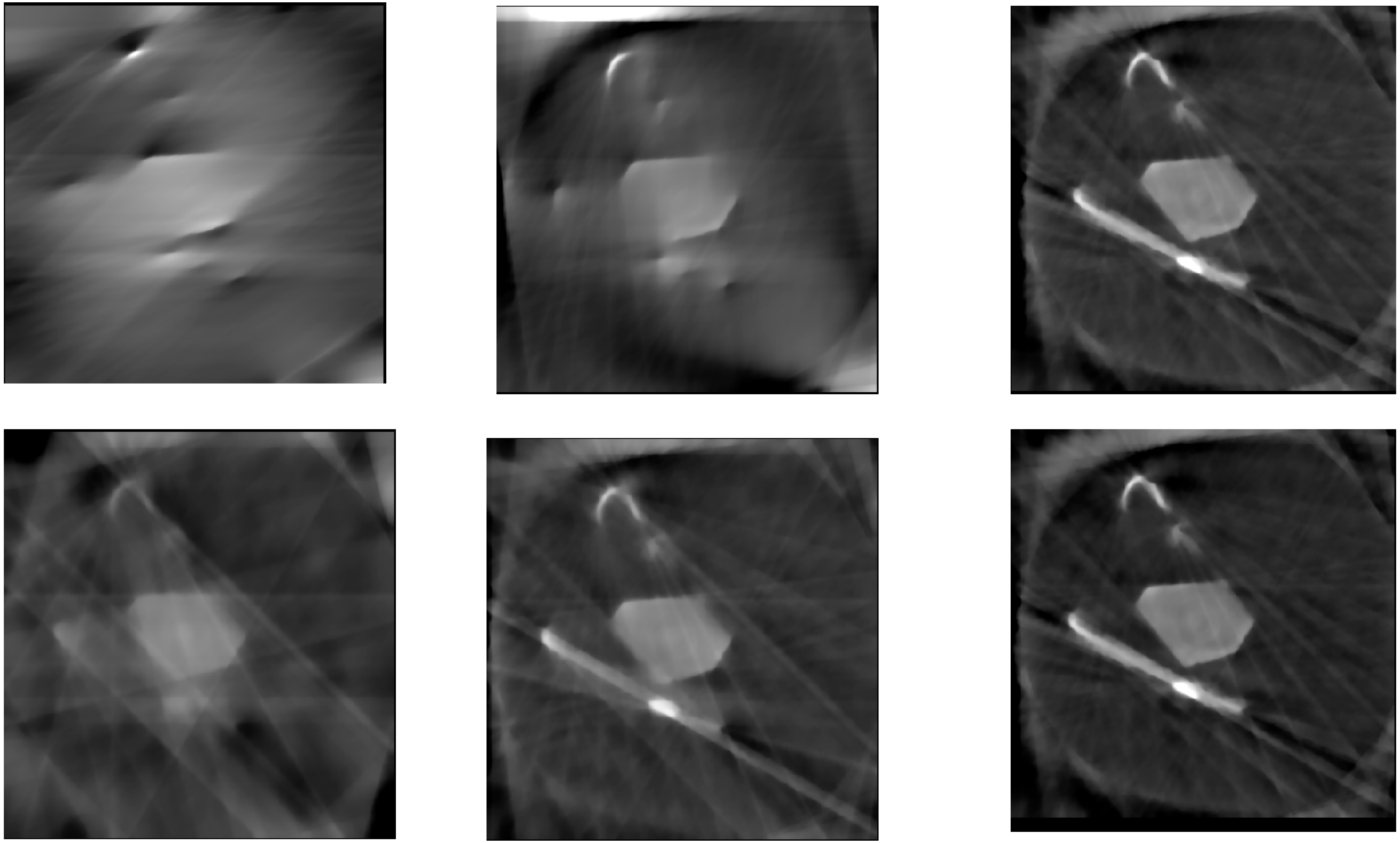
* Singanallur Venkatakrishnan, Yuxuan Zhang, Luc Dessieux, Christina Ho<man , Philip Bingham, and Hassina Bilheux, “Improved Acquisition and Reconstruction for Wavelength-Resolved Neutron Tomography” Journal of Imaging 2021

Impact of Different Acquisition Schemes + MBIR

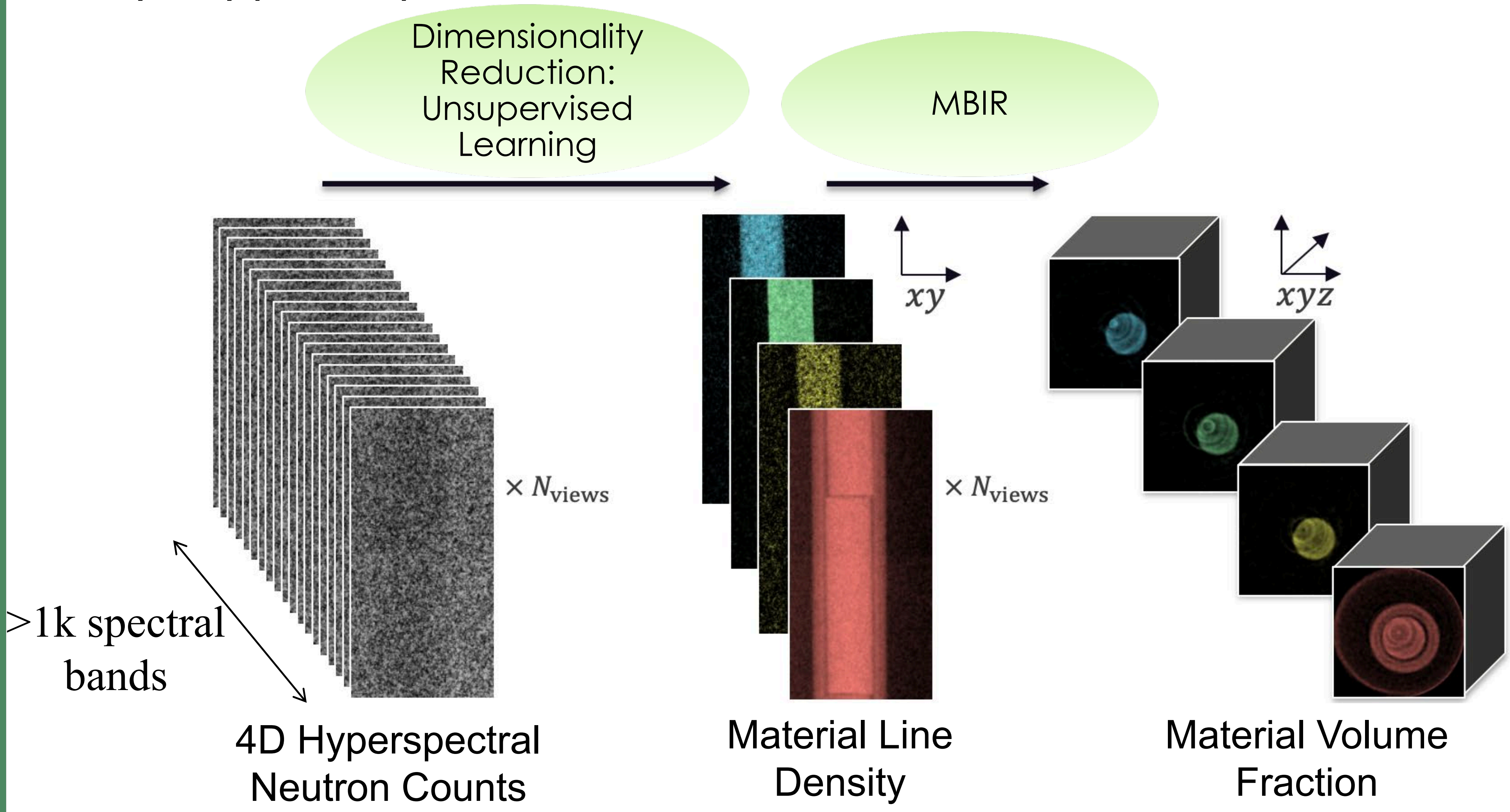
10 views (~12 hours) | **20 views (~24 hours)** | **30 views (~36 hours)**

Conventional

Interlaced



Fully Hyper-Spectral CT Reconstruction*



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Courtesy: Prof. Charles Bouman, Samin Nur Chowdhury (Purdue University)

Dimensionality Reduction : Non-Negative Matrix Factorization

- NNMF goal

$$\left(\widetilde{M}, \widetilde{D}\ \right) = \arg \min_{M \geq 0, D \geq 0} \|p - MD^t\|^2$$

    - where M and D have non-negative elements
    - You can select the number of material bases you prefer

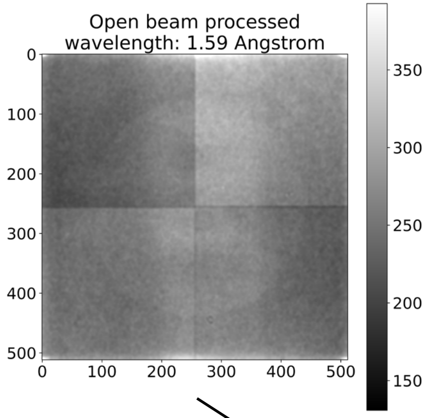
- Basic algorithm
    - Repeat {

$$\widehat{M} \leftarrow \arg \min_{M \geq 0} \left\| p - M\widetilde{D}^t \right\|^2$$

$$\widehat{D} \leftarrow \arg \min_{D \geq 0} \left\| p - \widetilde{M}D^t \right\|^2$$

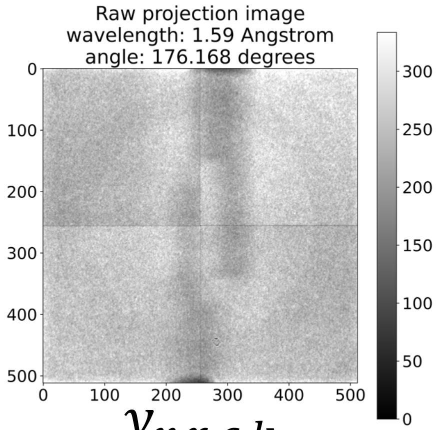
}

Experiment : Ni-Cu Sample Wrapped With Aluminum



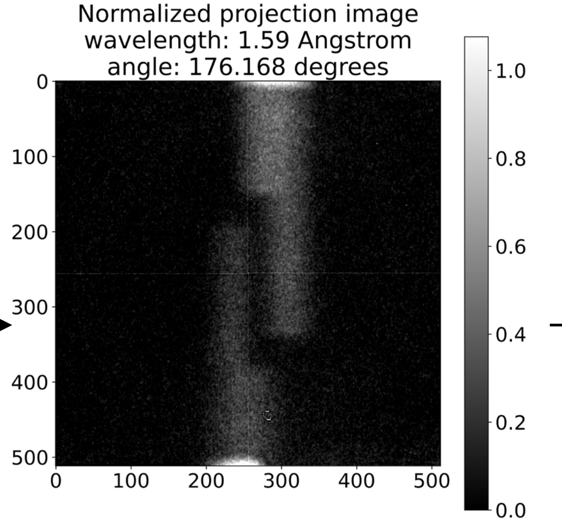
$\bar{y}^{o}_{r,c,k}$

Open beam



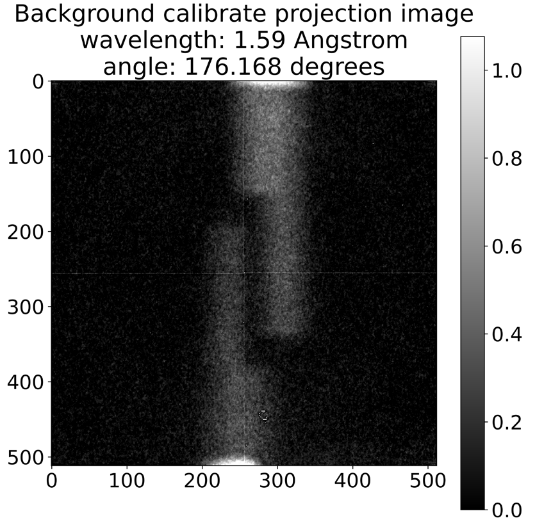
$y_{v,r,c,k}$

Raw projection



$$\hat{p}^{*}_{v,r,c,k} = -log\left(\frac{y_{v,r,c,k}}{\bar{y}^{o}_{r,c,k}}\right)$$

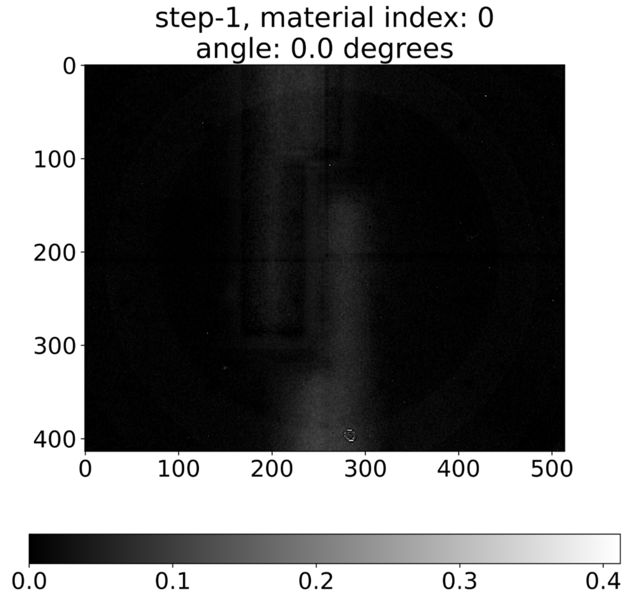
Log normalized



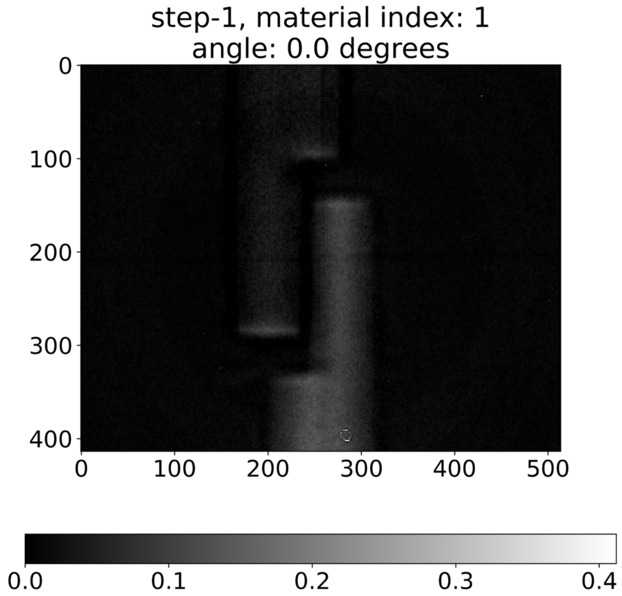
$$\hat{p}_{v,r,c,k} = \hat{p}^{*}_{v,r,c,k} - b_{v,k}$$

Background offset corrected

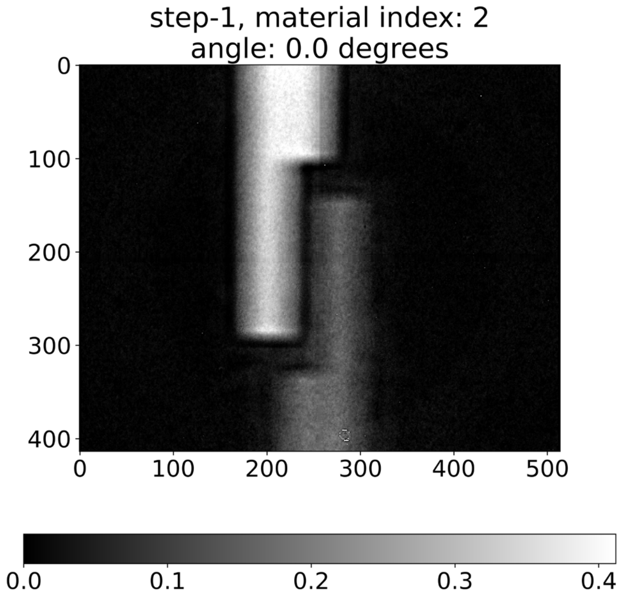
Result: NMF Dimensionality Reduction



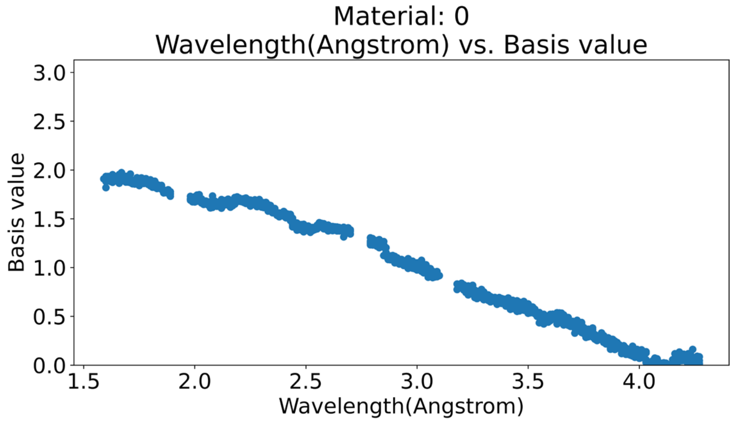
Material 0

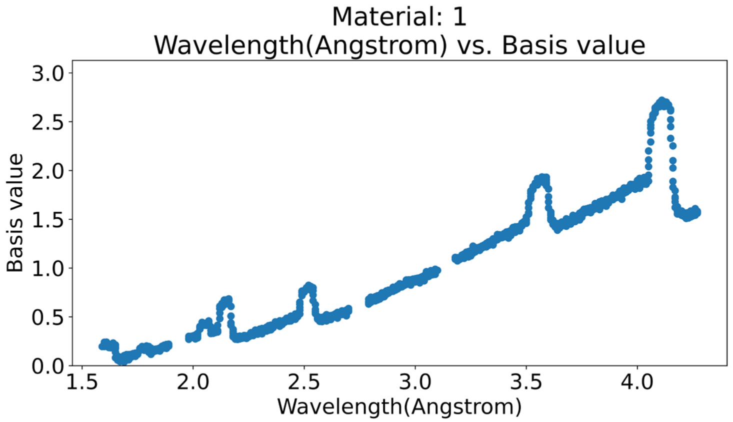


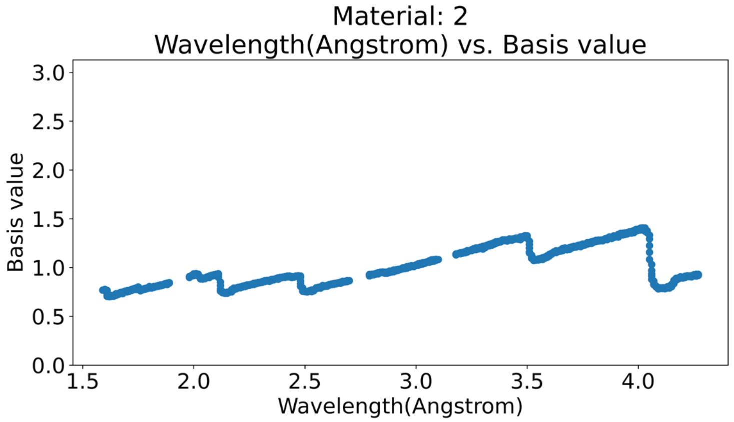
Material 1



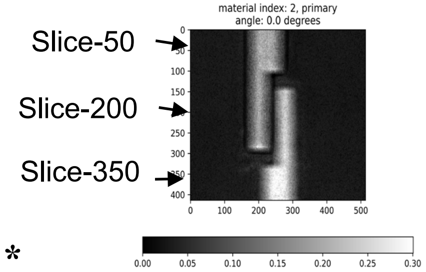
Material 2







Final reconstruction

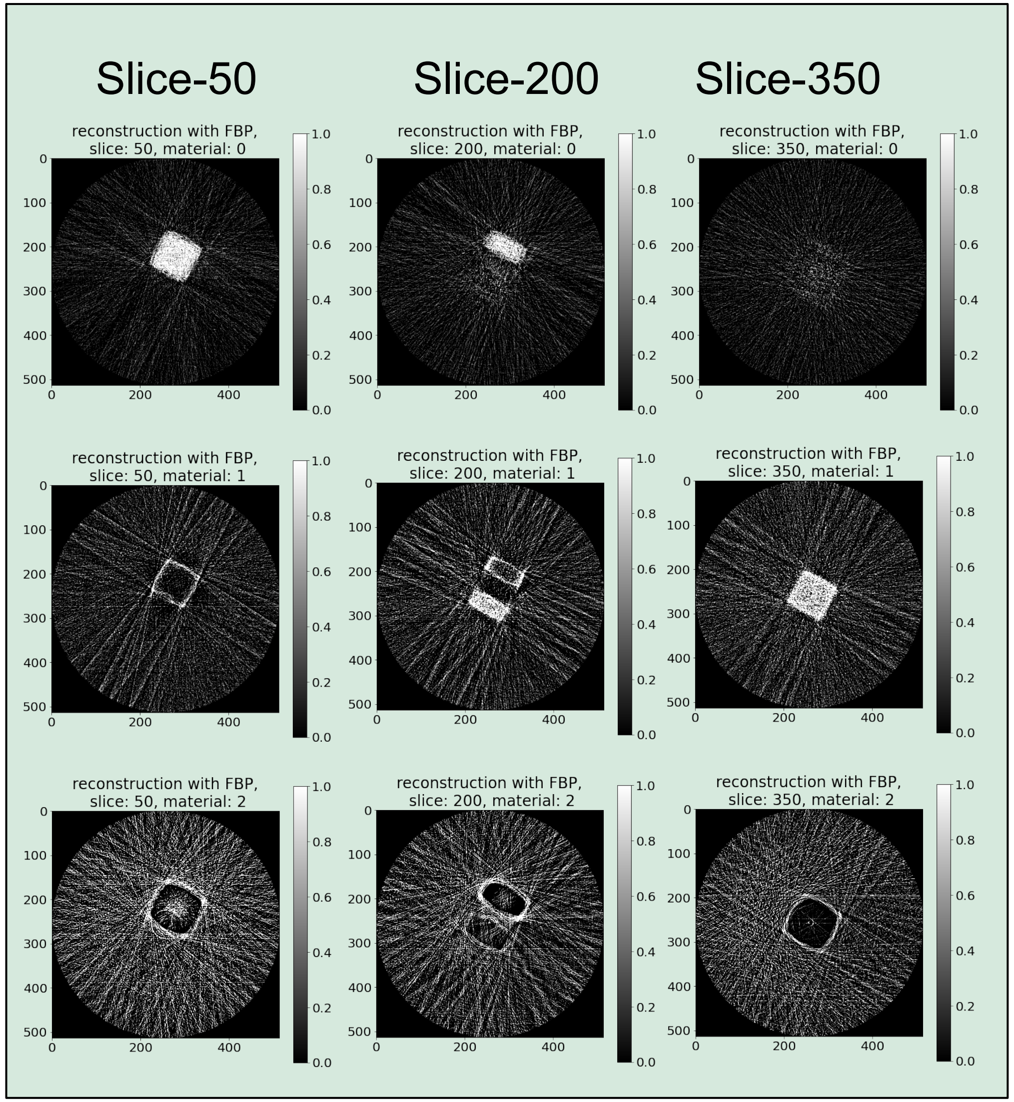


FBP

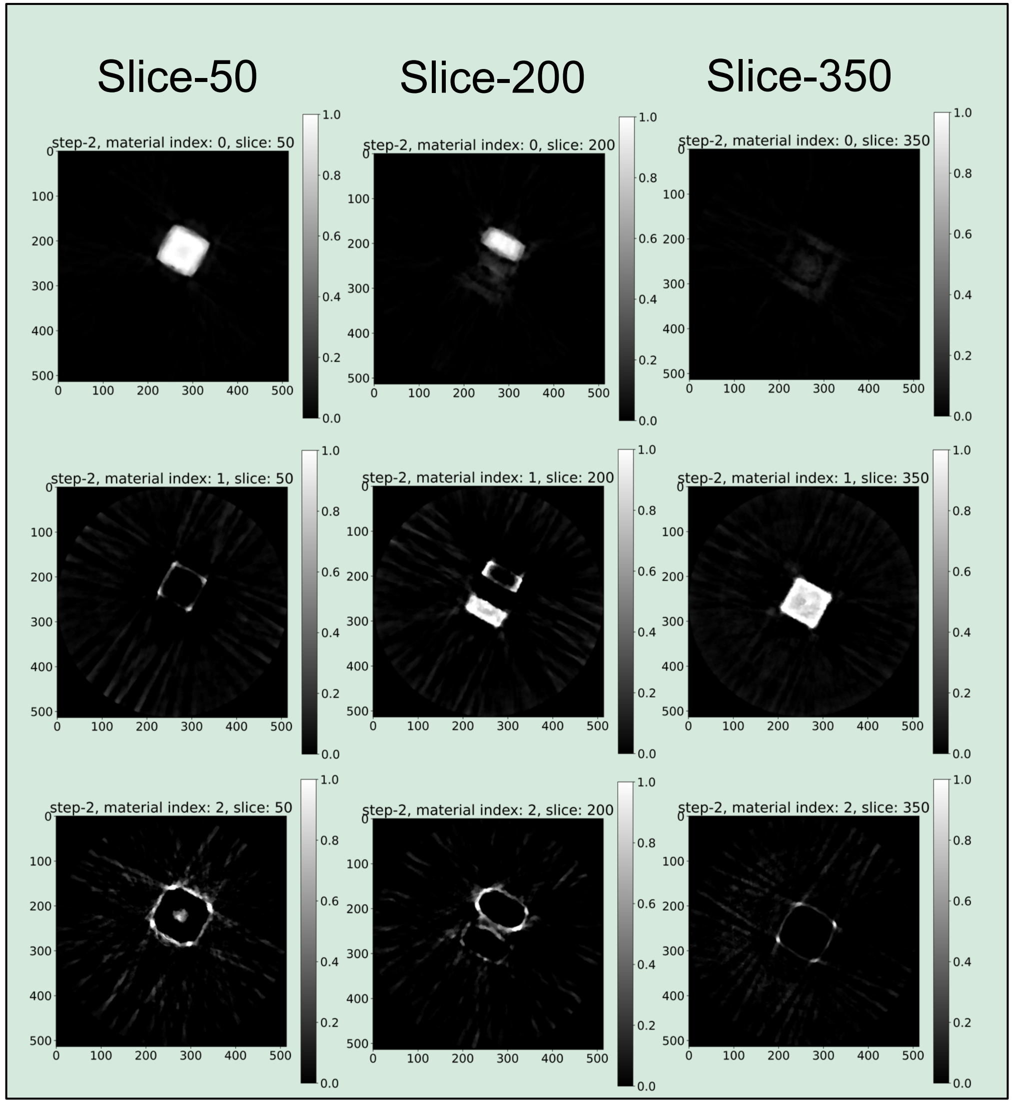
Material-0

Material-1

Material-2



SVMBIR*



* https://github.com/cabouman/svmbir

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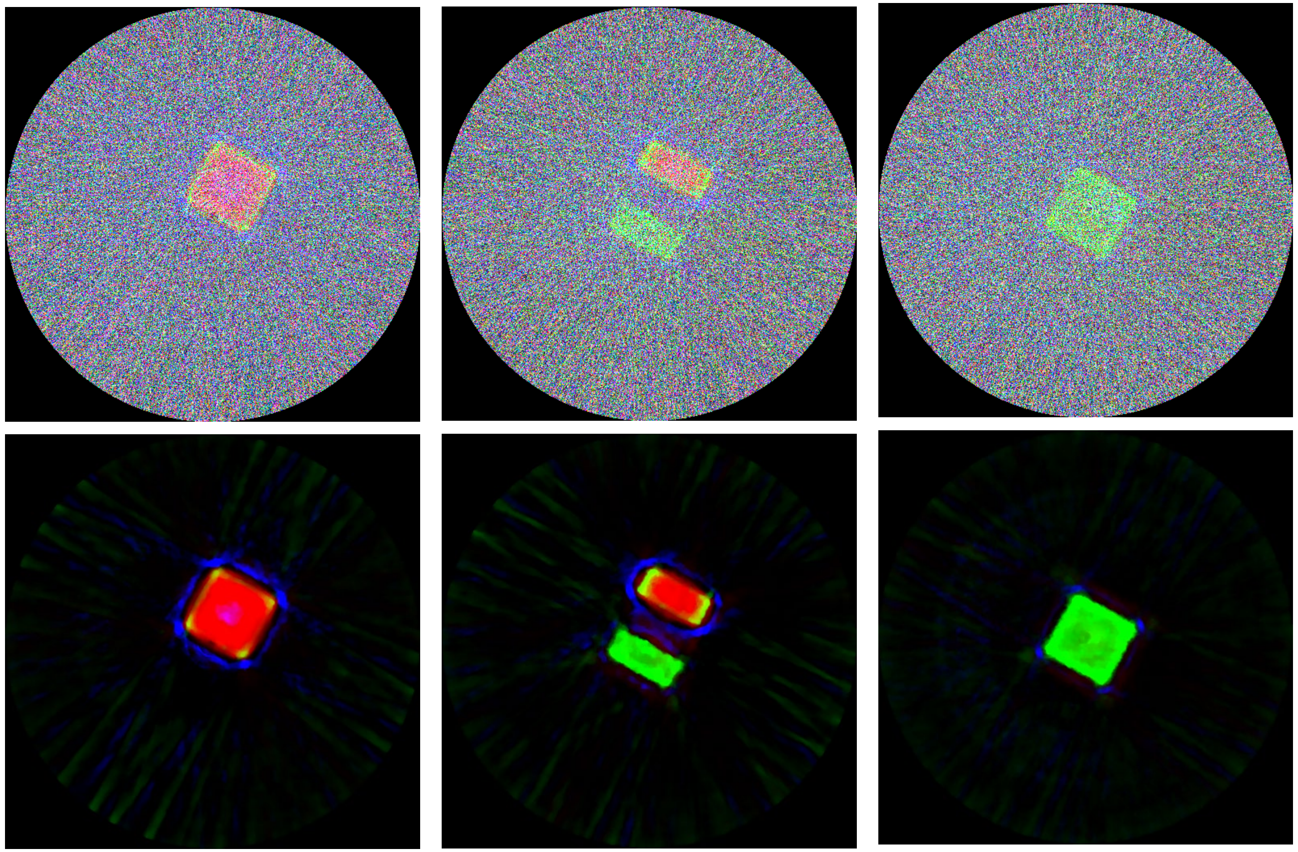
RGB Representation of Reconstruction

Slice-50 Slice-200 Slice-350

FBP

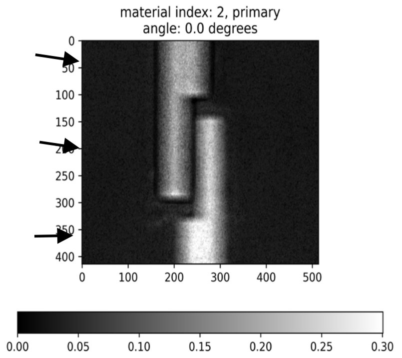
SVMBIR



Slice-50

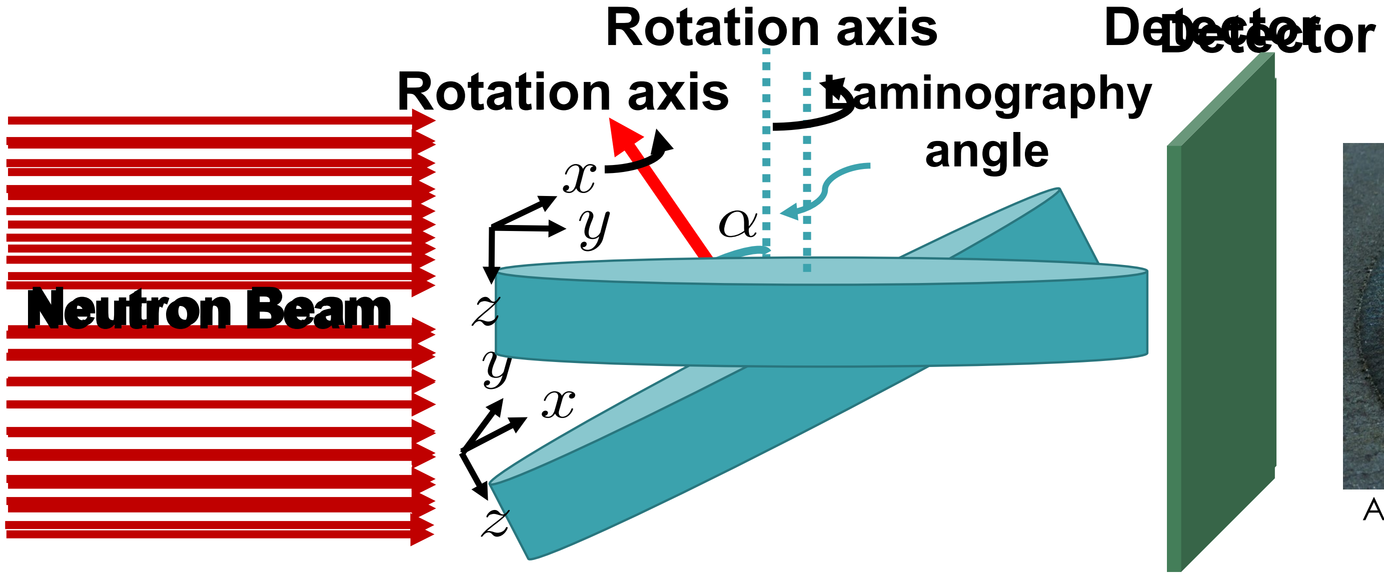
Slice-200

Slice-350

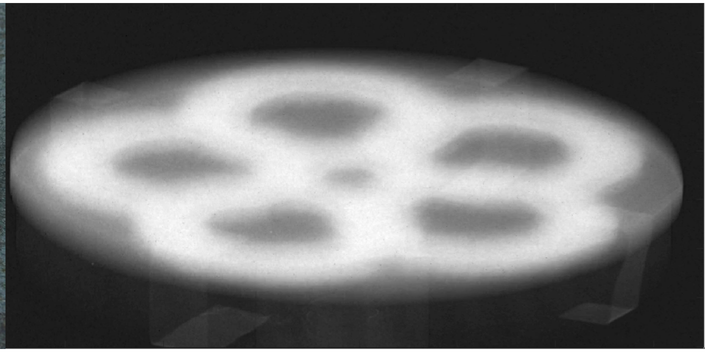


Red: 255 = 100% Ni, 0 = 0% Ni
Green: 255 = 100% Cu, 0 = 0% Cu
Blue: 255 = 100% Al, 0 = 0% Al

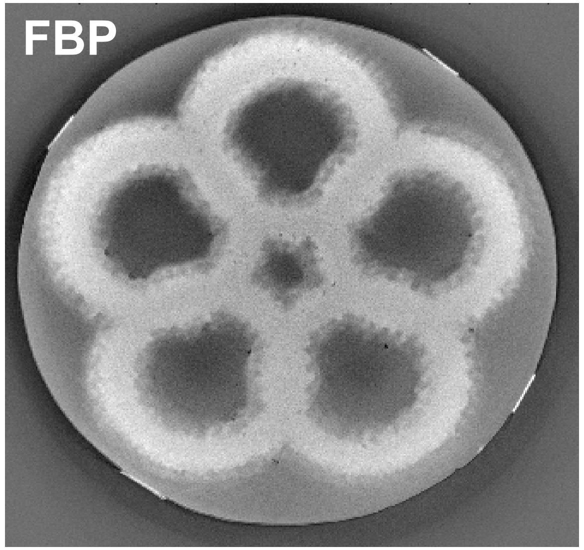
New Geometries: Neutron Laminography*

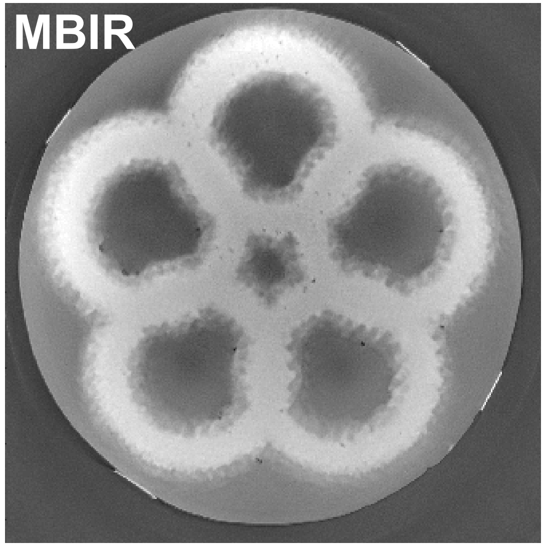


Additively manufactured part



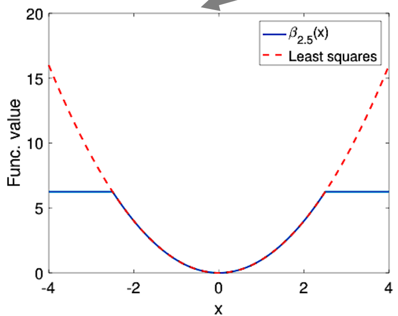
Neutron laminography data (Normalized)





Low flux (noisy), gamma-hits and geometry of set-up make it challenging to invert

$$c(f) = \frac{1}{2}\sum_{i=1}^{M} \beta_T\left((g_i - [Af]_i)\sqrt{W_{ii}}\right) + s(f)$$



Forward projector for laminography geometry

*S.V. Venkatakrishnan, Ercan Cakmak, Hassina Billheux, Philip Bingham, Richard Archibald, "Model-based iterative reconstruction for neutron laminography", ***Proc. of IEEE Asilomar Conference on Signals, Systems and Computer 2017***

** Ercan Cakmak, Niyanth Sridharan, Singanallur V. Venkatakrishnan, Hassina Z. Bilheux, Louis J. Santodonato, Amit Shyam, Sudarsanam S. Babu, "Feasibility Study of Making Metallic Hybrid Materials Using Additive Manufacturing" ***Metallurgical and Materials Transactions A, 2018***

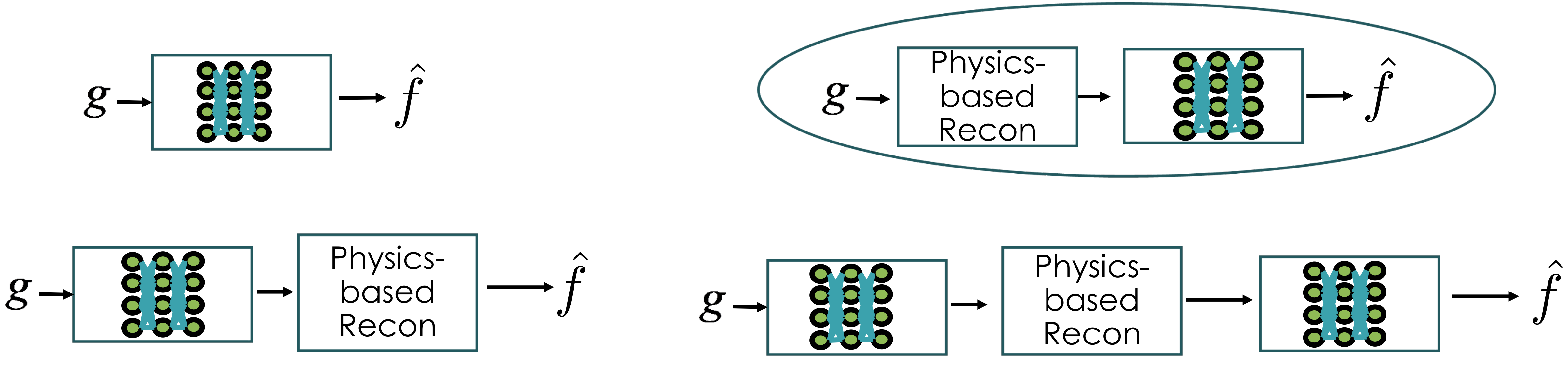
Oak Ridge National Laboratory

Non-Iterative Deep Learning for Neutron CT

This work has been supported in part by the Artificial Intelligence Initiative at Oak Ridge National Laboratory.

Non-Iterative Deep Learning for Inverse Problems

$$\hat{f} = H_\theta(g)$$ Learnt inversion operator



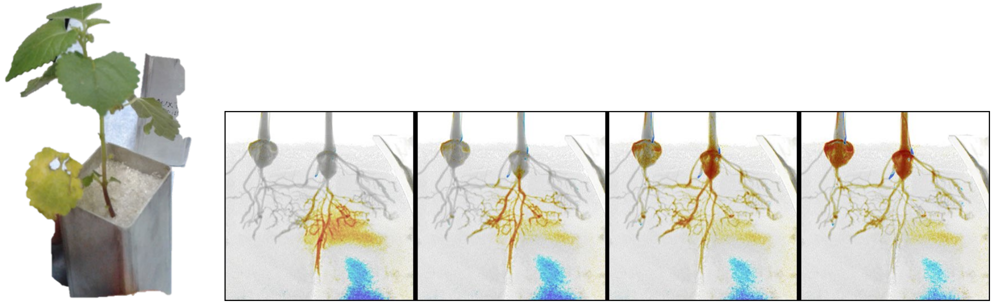
Hypothesis : Best of both worlds – speed of analytic methods and quality of MBIR

When Are Data-Driven Methods Useful ?

- Sequence of samples

Meteorites [Courtesy: Andrew Needham, NASA]

- Time-resolved CT

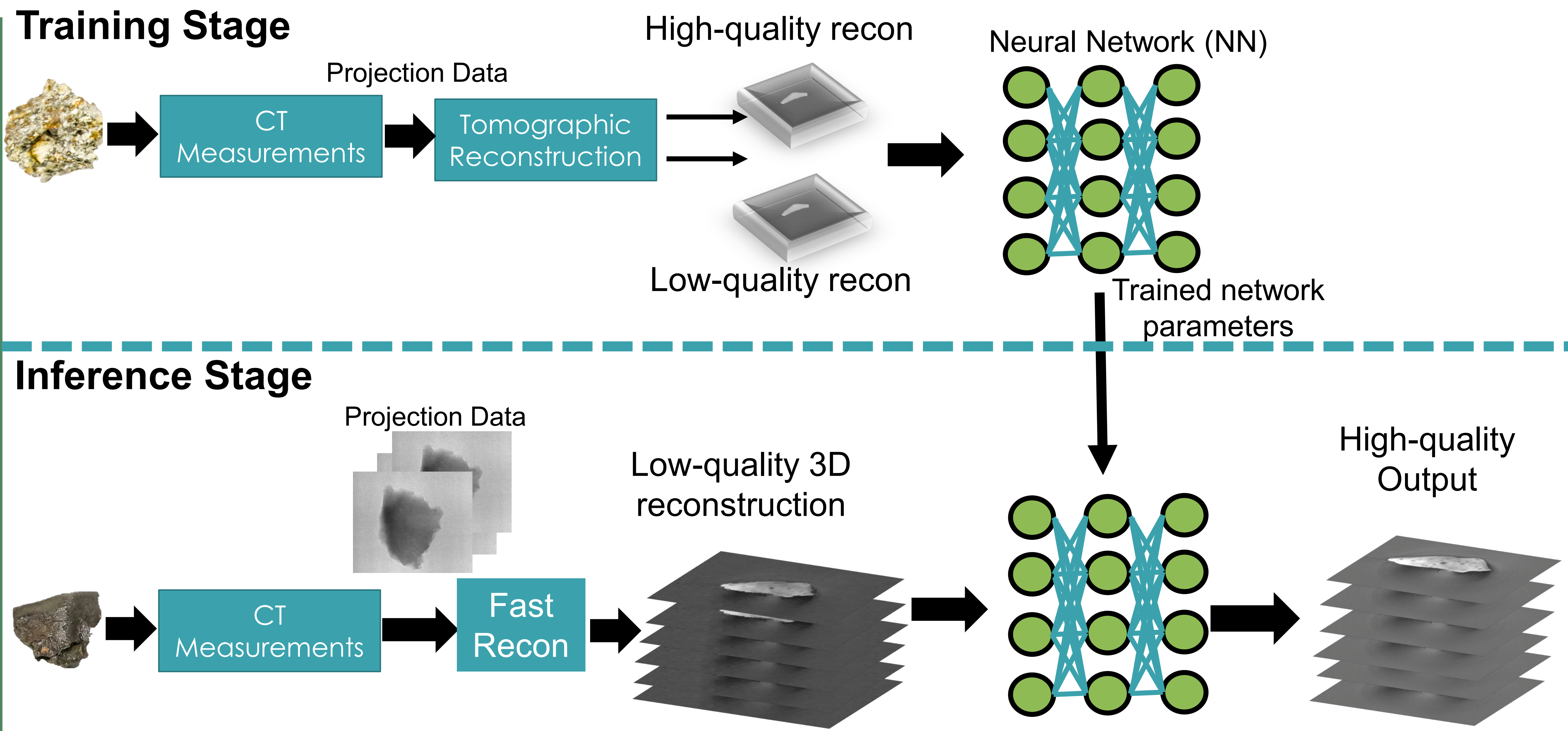


- CAD-model

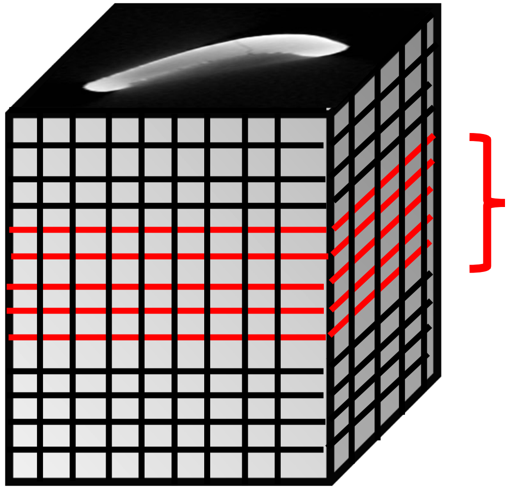
3D Printer

Jet Engine Turbine Blades

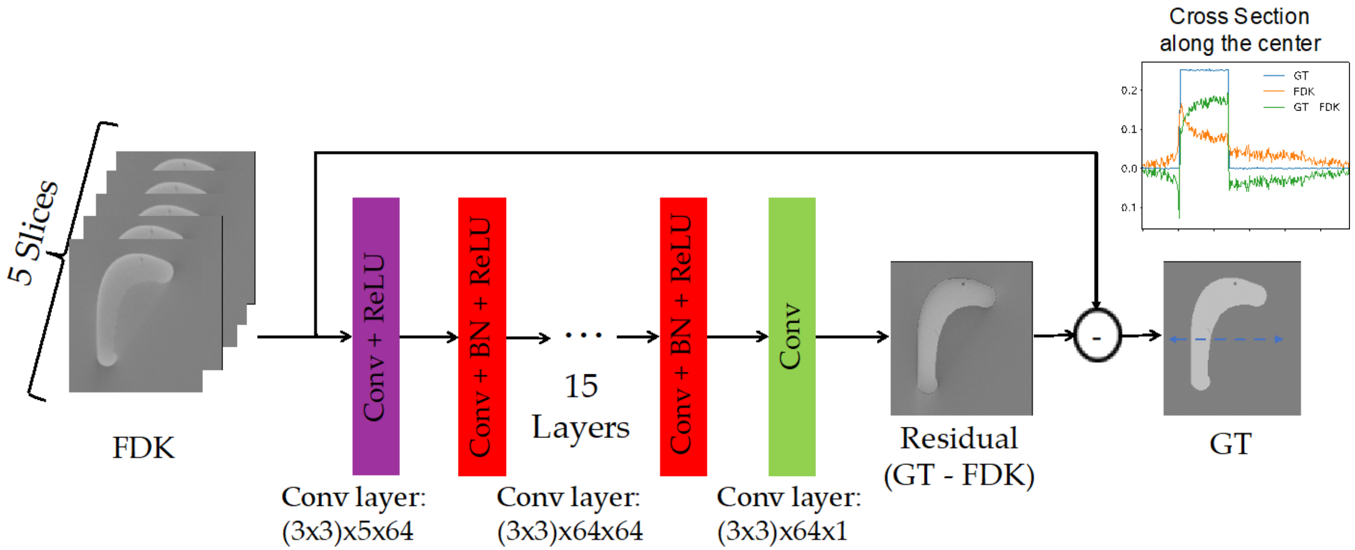
Courtesy: ORNL Manufacturing Demonstration Facility


Training Stage
Projection Data
CT Measurements
Tomographic Reconstruction
High-quality recon
Low-quality recon
Neural Network (NN)
Trained network parameters
Inference Stage
Projection Data
CT Measurements
Fast Recon
Low-quality 3D reconstruction
High-quality Output

Dealing With 3D Data+



Use adjacent slices from the 3D volume as input

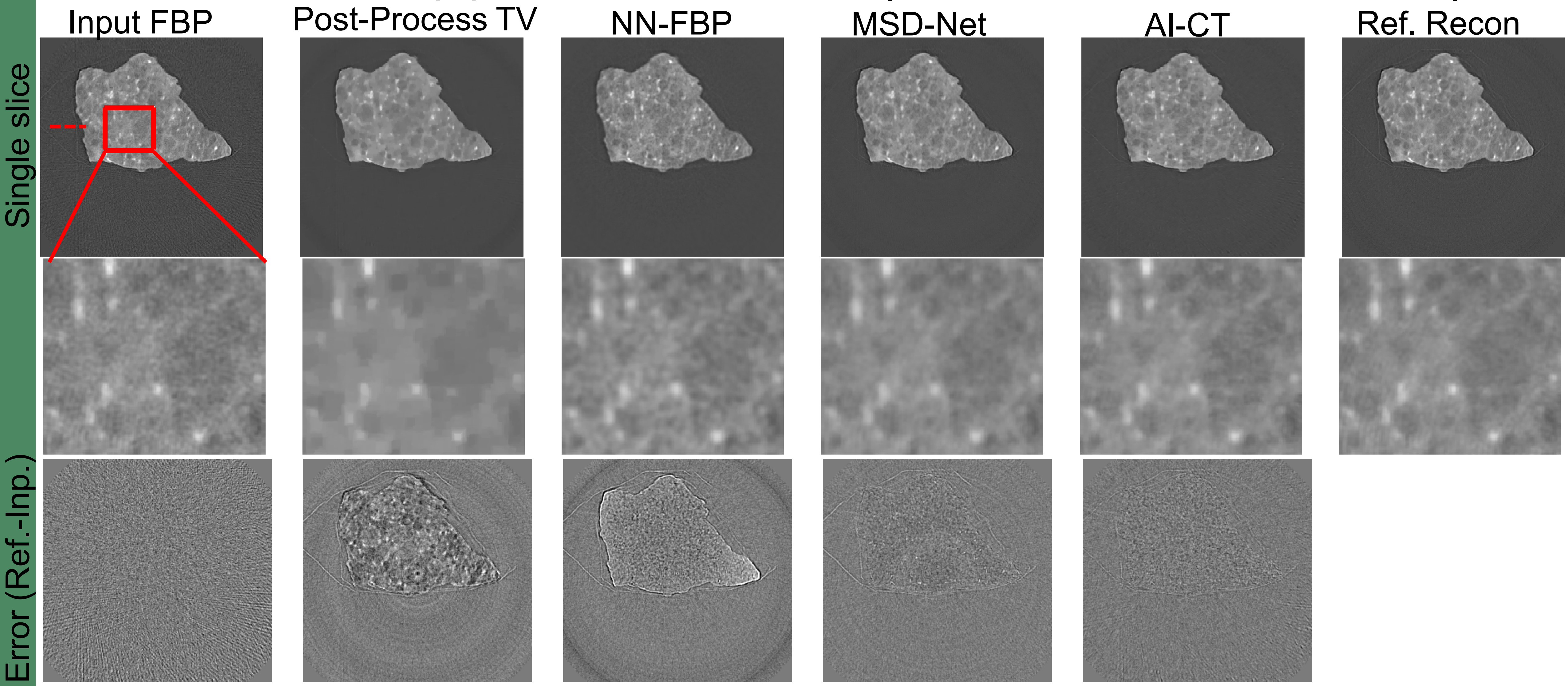


AI-CT+
17 layers

$$c(\theta; y, x) = \frac{1}{N}\sum_{i=1}^{N} l(y_i, f_\theta(x_i))$$

+ Ziabari, et al. 2.5D Deep Learning for CT Image Reconstruction Using A Multi-GPU Implementation. IEEE Asilomar On Signals, Systems and Computers 2018
+ S.V.Venkatakrishnan, Amirkoushyar Ziabari, Jacob Hinkle, Andrew W. Needham, Jeffrey M. Warren, Hassina Z. Bilheux, "Convolutional Neural Network Based Non-Iterative Reconstruction for Accelerating Neutron Tomography", Machine Learning: Science and Technology 2021

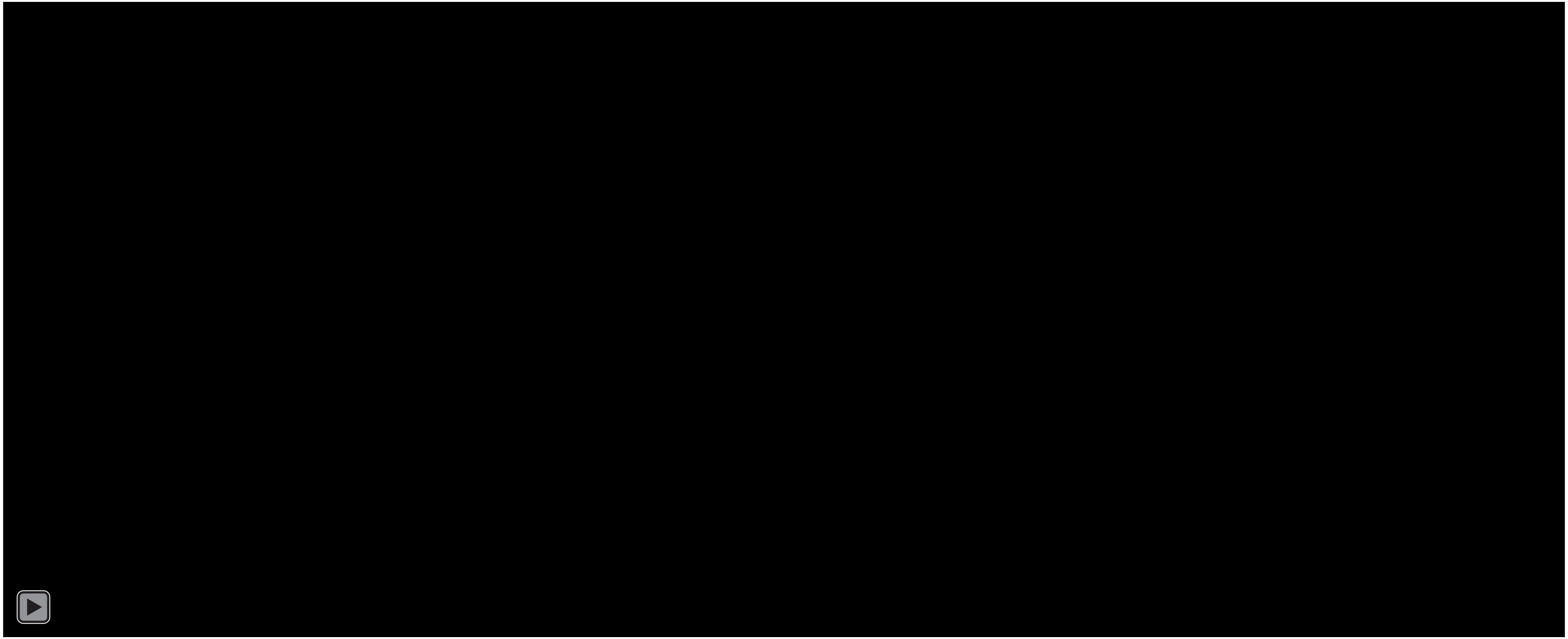
Results of NN Applied to Test Set (**4X Scan Acceleration**)



Approximate Inference Time (8 A-100 GPUs) 512 X 1280 X 1280 volume	56s	64s

ML-Based Time-Resolved Reconstruction (90s/CT scan)

Input FBP CNN



Single reconstructed slice as a function of time after D20 injection into plant

Oak Ridge National Laboratory

Summary

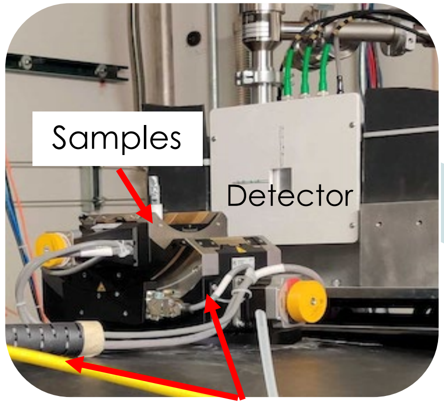
- Advanced algorithms + implementation + compute allow:
  - High quality reconstruction from partial, low SNR data (reduced time)
  - Reconstructions from new scanning geometries
  - Reconstructions in real time

OAK RIDGE National Laboratory

Autonomous Control for Neutron CT

Courtesy: Shimin Tang,
Hassina Bilheux

First completely autonomous neutron experiment at ORNL



Goniometers

Harley Skorpenske, Jamie Molaison, Jiao Lin, Jean Bilheux, Hassina Bilheux

Contributions also from:
Bogdan Vacaliuc
Xiasong Geng
Alex Groff
Bino and team
S&A
And others!

Ray Gregory
API serves new motor positions to EPICS which moves the beamline to the **next beamline configuration**

Networks:
- Beamline
- Open Research

Acquisition starts with new motor and pCharge values, new file and directory names, etc.

Jeeeeeem Khol
ADARA archives raw data on SNS analysis server
ADARA triggers auto reduction

Data reduced on reduction node (analysis server)

Peter Peterson, Jean Bilheux

Rich Crompton
Matt Bedynek

START

Via **algorithms, Imaging GPU computer** communicates with the Application Program Interface (API) to provide **new motor positions**

HyperCT

Jean Bilheux

Algorithm monitors reduced data and **triggers data reconstruction on imaging GPU computer**

Shimin Tang

Experiment is done. No new command sent.

YES

NO

Autonomous decision based on comparison between reconstructions of two consecutive scans: Continue?

Hyperspectral reconstruction on imaging GPU

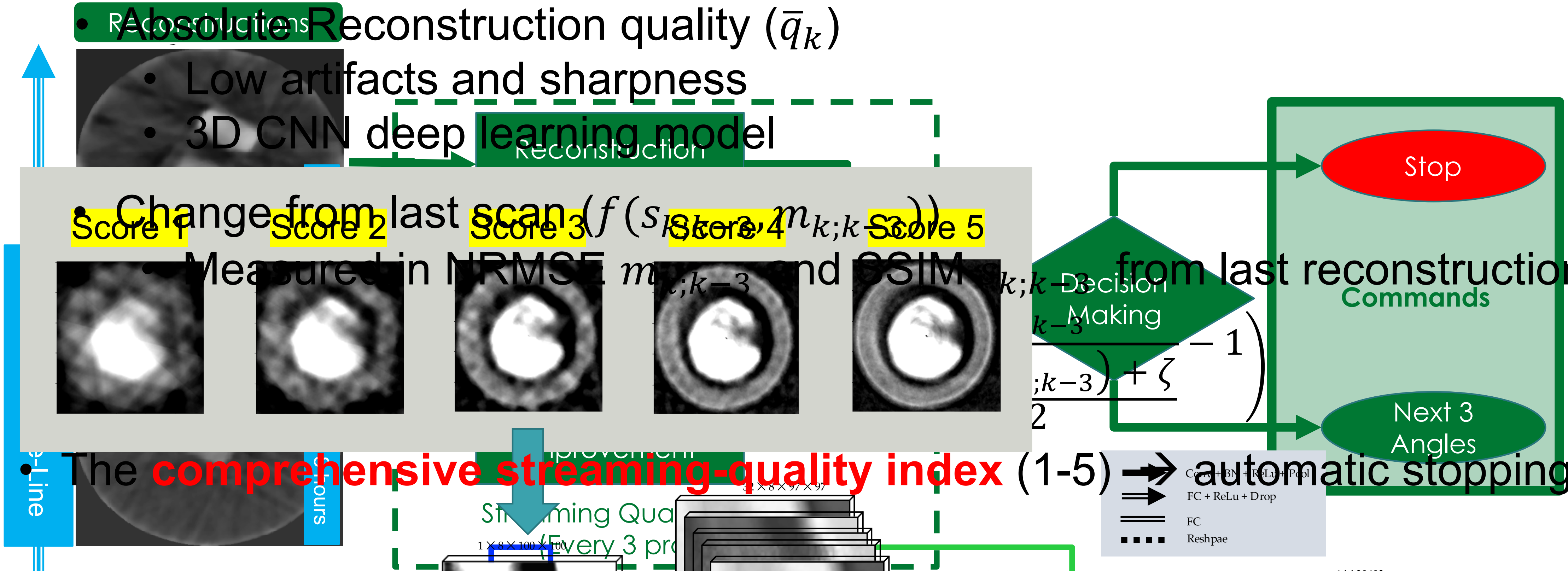
Rich Crompton
Matt Bedynek

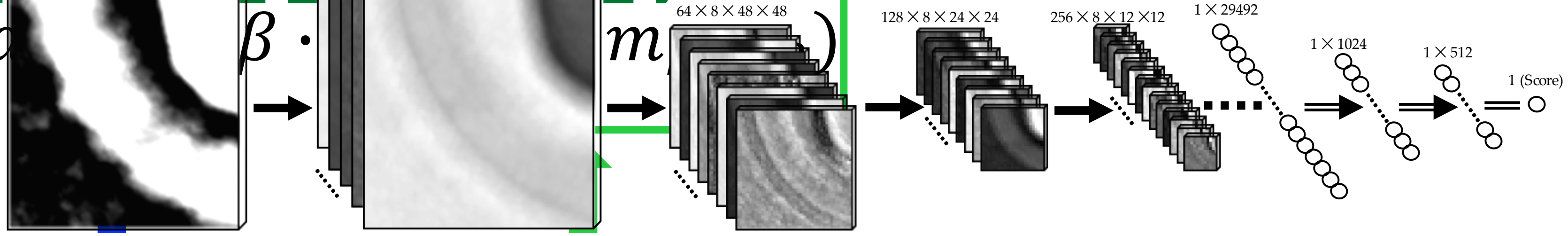
Users can access the reconstructed data and the decision-making algorithms on GPU imaging computer via ThinLinc

Automated Stopping Criteria Design

- Reconstruction quality evaluated using 2 criteria :
  - Absolute Reconstruction quality ($\bar{q}_k$)
    - Low artifacts and sharpness
    - 3D CNN deep learning model
  - Change from last scan ($f(s_{k;k-3}, m_{k;k-3})$)
    - Measured in NRMSE $m_{k;k-3}$ and SSIM $s_{k;k-3}$ from last reconstruction.
- The **comprehensive streaming-quality index** (1-5) → automatic stopping criteria

$QI = \alpha \cdot \ldots \beta \cdot \ldots m \ldots)$

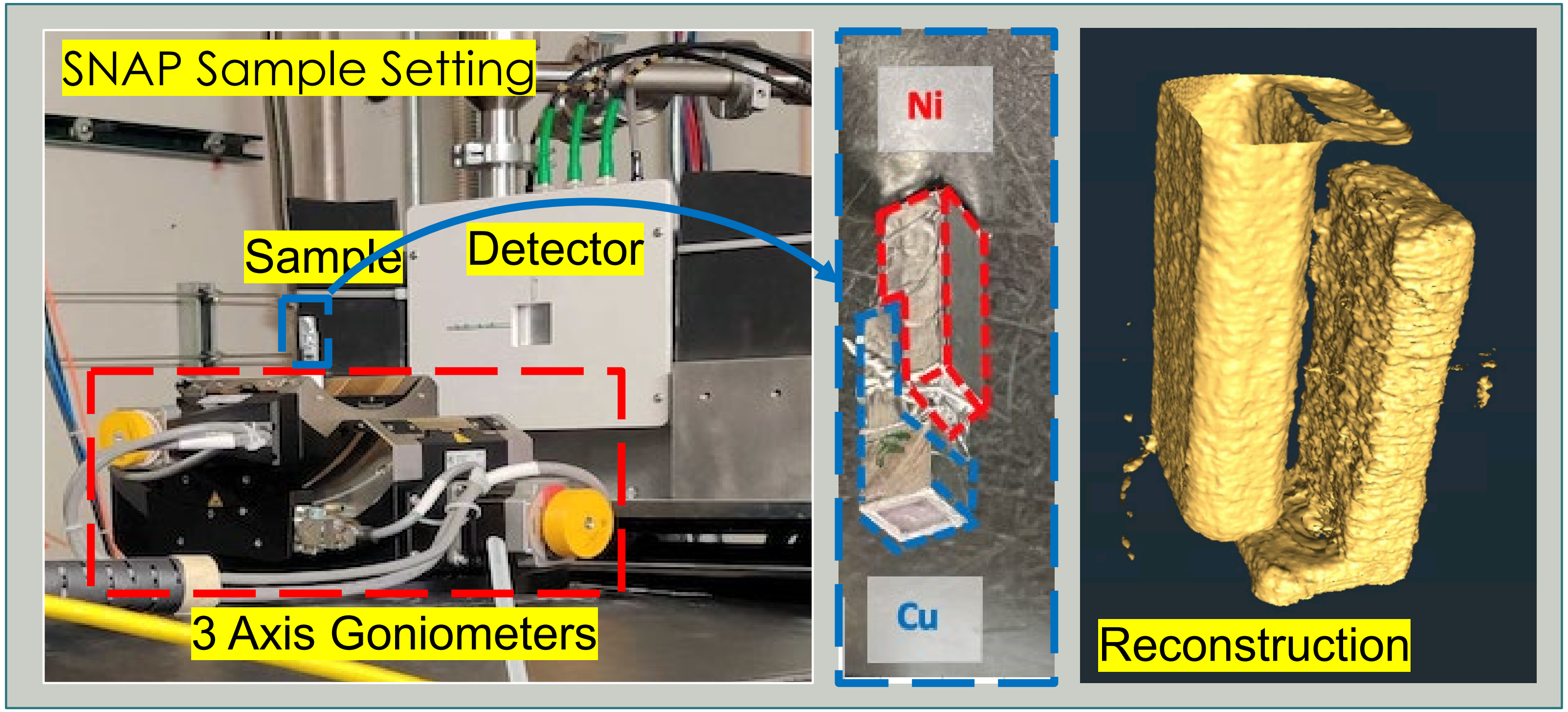


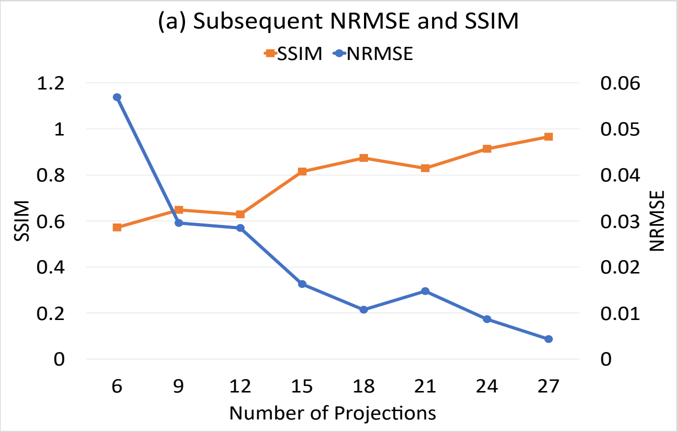


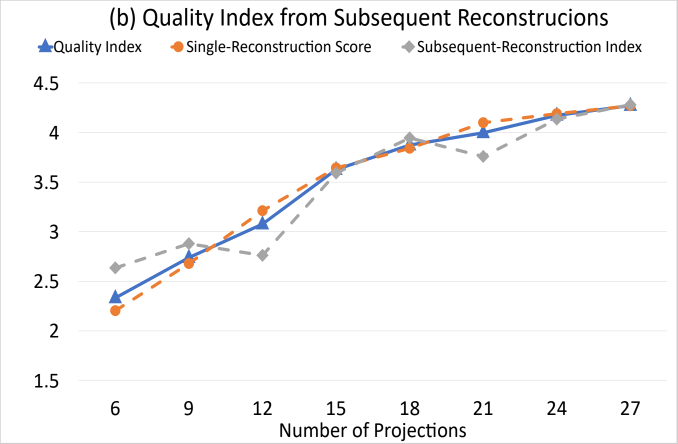
Reference-Free Quality score

Quality Improvement

Real automatic measurement demo







Streaming Time-Line

Take Home Message

- Advanced reconstruction methods (MBIR, DL) :
  - Dramatic increase in image quality
  - Accelerate scan time
  - Real-time user feedback

- AI/ML methods -> reduction, reconstruction and control

- Joint design of hardware + compute for next gen instruments

Thank You!

https://sites.google.com/view/svenkata