# Sparse Sampling Methods for Large Scale Experimental Data

#### Rick Archibald Oak Ridge National Laboratory

#### IPAM January 2017 Big Data Meets Computation

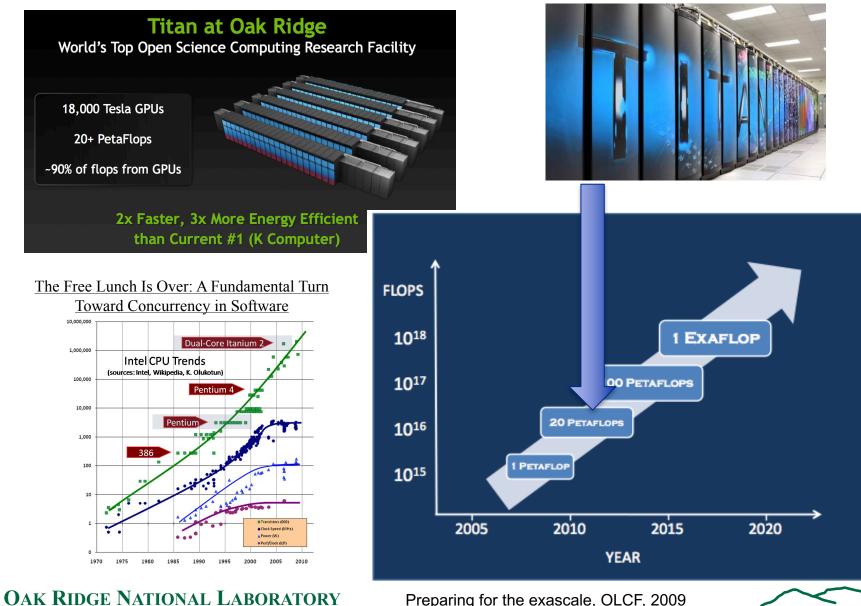




#### Outline

- DOE Facilities
- ACUMEN Project
- Sparse Optimization
  - Tomography
  - Denoising

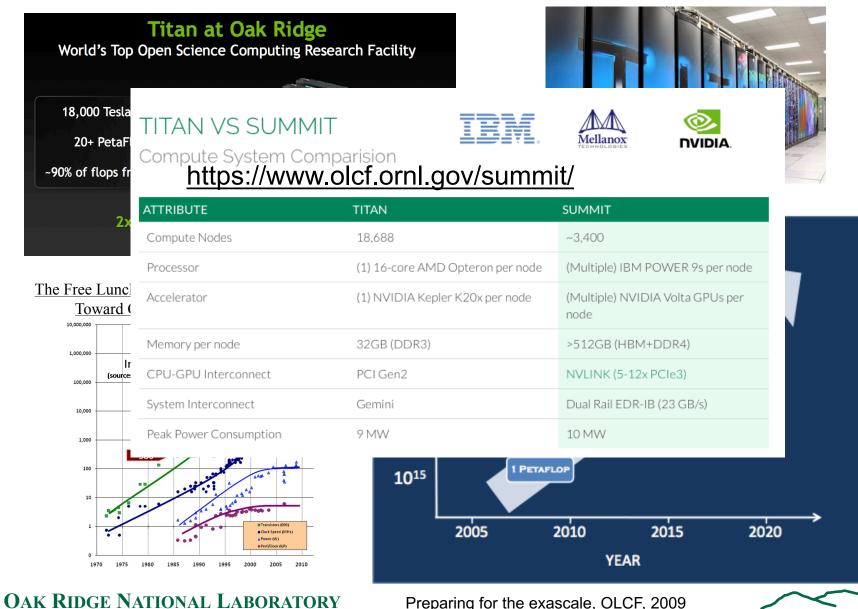
#### **Motivation – Computation Facilities**



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#### **Motivation – Computation Facilities**



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#### **Motivation – Experimental Facilities**





One of the highest steadystate neutron flux research reactor in the world



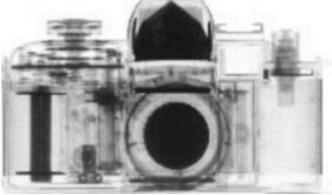
#### Spallation Neutron Source

World's most powerful accelerator-based neutron source

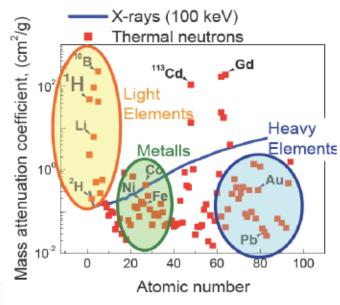


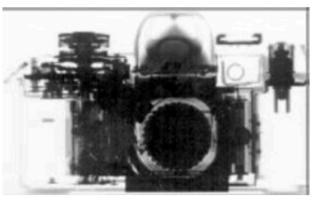


#### **Motivation – Why Neutrons**



#### Neutron



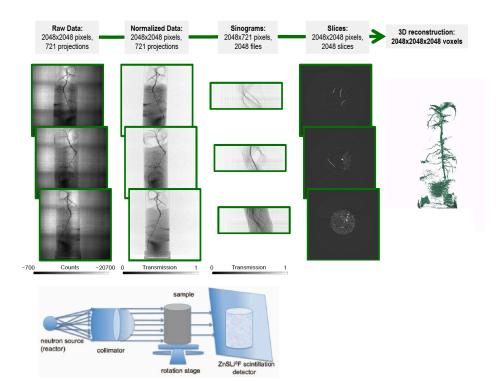


X-ray

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



#### **Motivation – General Equations**



Nueloor >

Tomography  
$$\mathcal{M} = \int F(u)\delta\Omega$$

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# $\begin{aligned} & \text{Scattering} \\ & I_{\{\Phi\}}(\mathbf{Q},\omega) = S_{\{\Phi\}}(\mathbf{Q},\omega) * R(\mathbf{Q},\omega) \end{aligned}$



1

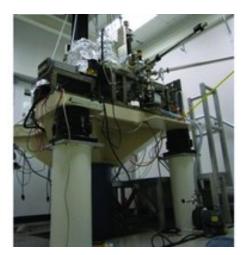
#### **Motivation – Experimental Facilities**





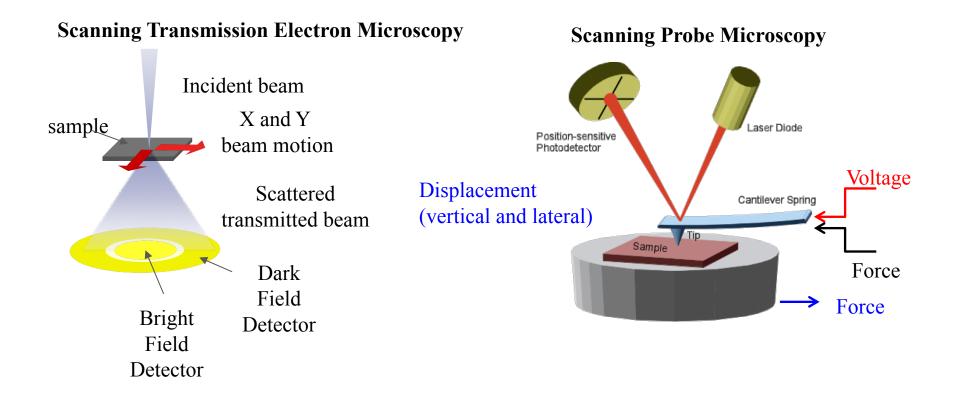
Center for Nanophase Materials Sciences

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





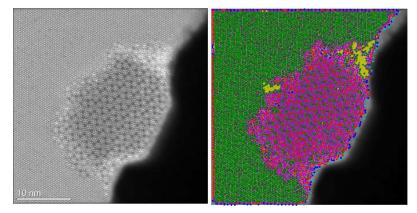
#### **Motivation – Why Electrons**





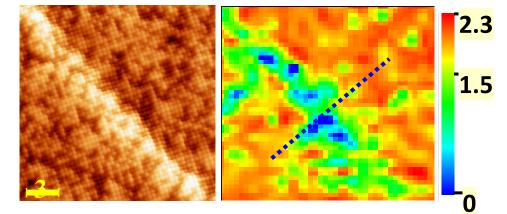
# *Why Electrons?* Understanding of material surface properties.

Atomic resolution of local surface physics and chemistry.



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

Q He, J Woo, A Belianinov, VV Guliants, A Borisevich; ACS nano, DOI: 10.1021/acsnano.5b00271, (2015)
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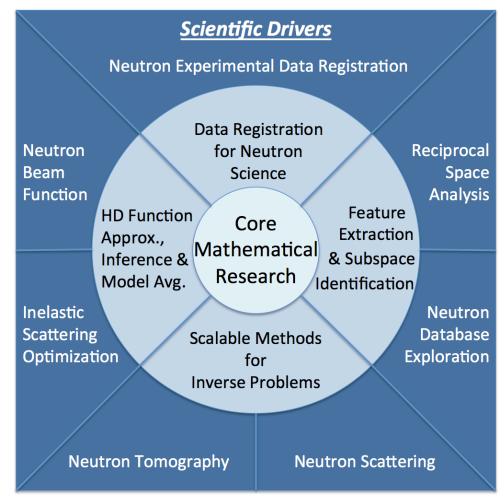


#### Multivariate analysis shows that superconductivity is suppressed in FeSeTe at the defect

A. Gianfrancesco, A. Belianinov, S. Jesse, and S. Kalinin, Microscopy & Microanalysis, DOI:10.1017/S1431927615012507, (2015)



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



ACUMEN will develop scalable mathematical research that will impact neutron science. Focused targets for first year:

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

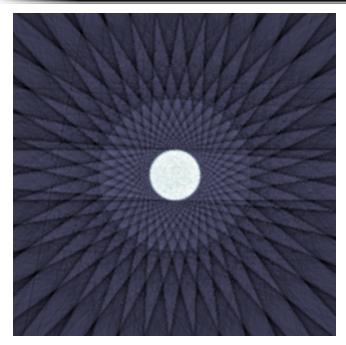
ASCR Funded Project under Dr. Steve Lee.

T-BATTEL

#### **ACUMEN integrates Mathematics with Instruments Scientists**

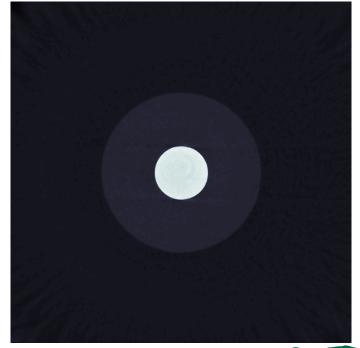
ORNL Facility	Instrument Scientist
CNMS	Dr. Sergei Kalinin Burton Medal, Microscopy Soc. of America Dir. of Inst. Funct. Imaging of Materials
	Dr. Greg Smith NSSA Fellow Structure and Dynamics of Soft Matter GL
SPALLATION NEUTRON SOURCE	Dr. Mark Lumsden Time-of-Flight Spectroscopy GL Mantid Scientific 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
HFIR	Dr. Hassina Bilheux Lead for HFIR Beam line CG-1D Instrument Lead for future SNS VENUS

#### Neutron Tomography Scientist – H. Bilheux Mathematicians – R. Archibald & R. Barnard



- Scalable high order sparse optimization methods provide fast solutions to tomographic images as seen on the *bottom right*.
- Future VENUS tomography instrument at SNS
   will produce majority of total data generated at SNS

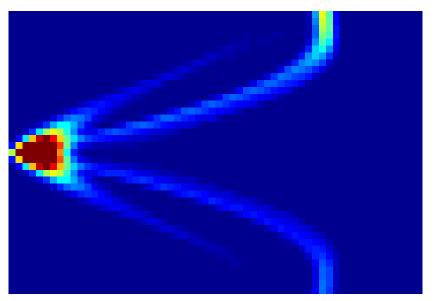
- Standard filtered back projection methods in tomographic reconstruction yields artifacts as seen on the *top left*.
- Image is of Aluminum-Steel Phantom taken at HIFIR - CG1





#### Inelastic Neutron Scattering Scientist – Olivier Delaire Mathematicians – Feng Bao, Ed D'Azvedo & Miro Stoyanov

- 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.



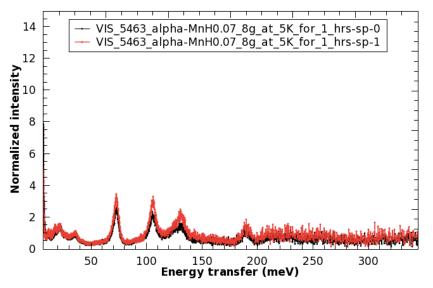
- Theoretical phonon calculation using DFT computationally expensive.
- Developed scalable optimization of DFT with probabilistic bounds of solution.
- Whole S(Q,E) spaced optimized *bottom left*.

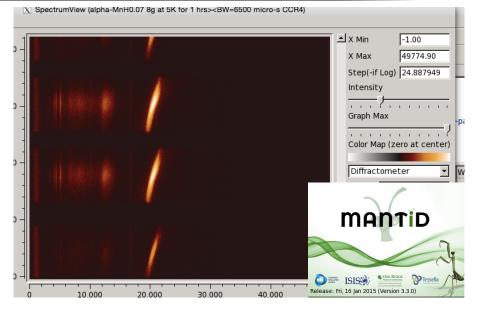


#### VISION Instrument Scientist – Tim Ramirez-Cuesta Mathematicians – Guannan Zhang & Clayton Webster

- Working within the mantid software framework for VISION to embed uncertainty quantification algorithms
- Large amounts of information in raw data of scattering events *top right*.

VIS\_5463\_alpha-MnH0.07\_8g\_at\_5K\_for\_1\_hrs



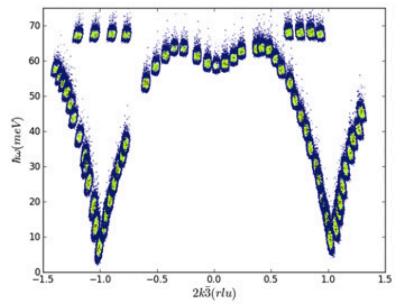


- Resolution at high energies is low for spectrum *bottom left*
- Using Bayesian analysis on the raw data to provide best mean estimate and uncertainty at high energies of spectrum

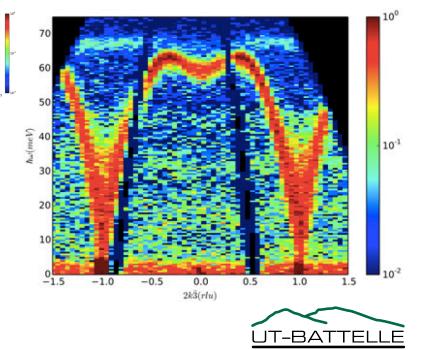


#### High Dimensional Resolution Function Estimation Scientist – Garrett Granroth Mathematicians – Ed D'Azvedo & Miro Stovanov



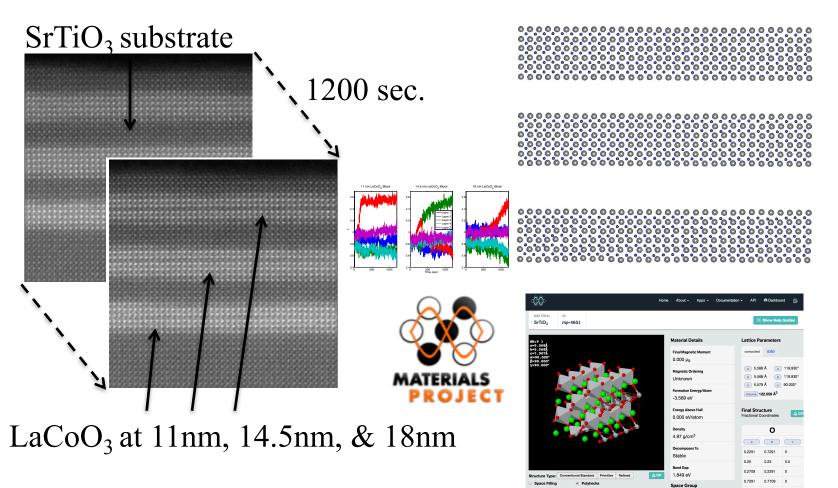


- Need to estimate resolution function is ubiquitous at the DOE experimental facilities
- Often resolution function depends upon many parameters, with different characteristic across parameter space



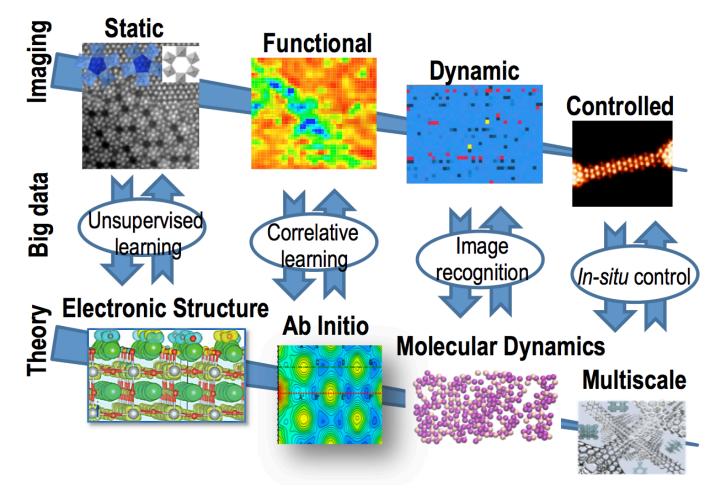
- *McStas (www.mcstas.org)* uses Monte Carlo statistics to simulate resolution function for SEQUOIA
- Building in mathematics from UQ to accelerate resolution function estimation for high dimensional parameter space.
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#### Data Analytics for Microscopy Scientist – Sergei Kalinin Mathematicians – Eirik Endeve & Rick Archibald





#### Connecting with ORNL Institutes and Infrastructure Collaboration - Institute for Functional Imaging of Materials

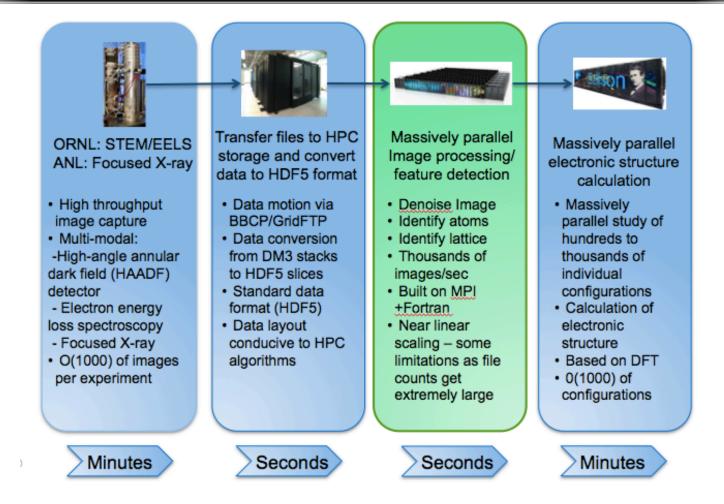


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Institute will bridge imaging and theory using HPC data analytics to reveal local physical, chemical and structureproperties in materials, and use this knowledge to enable the design of new materials with tailored functionalities.

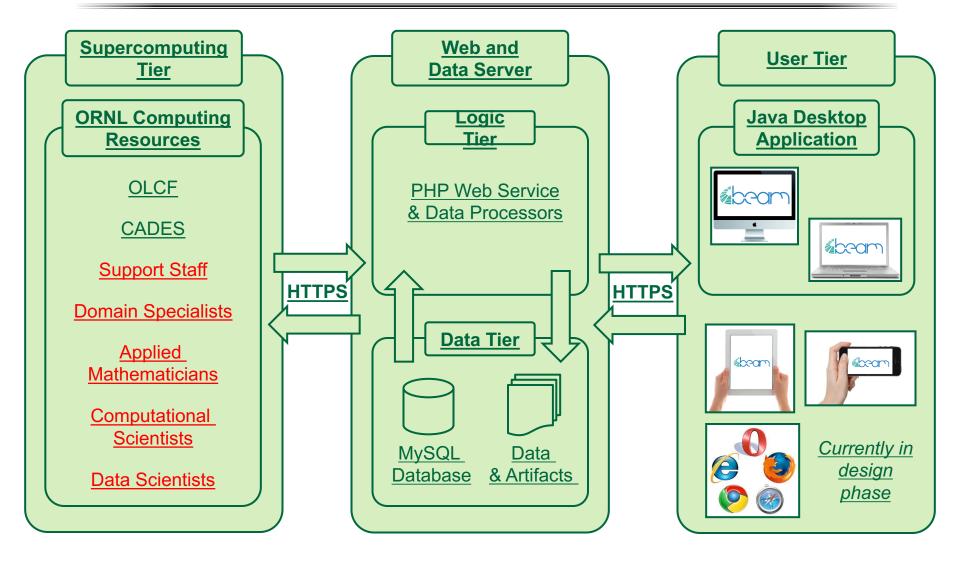


#### Data Analytics for Microscopy Scientist – Sergei Kalinin Mathematicians – Eirik Endeve & Rick Archibald



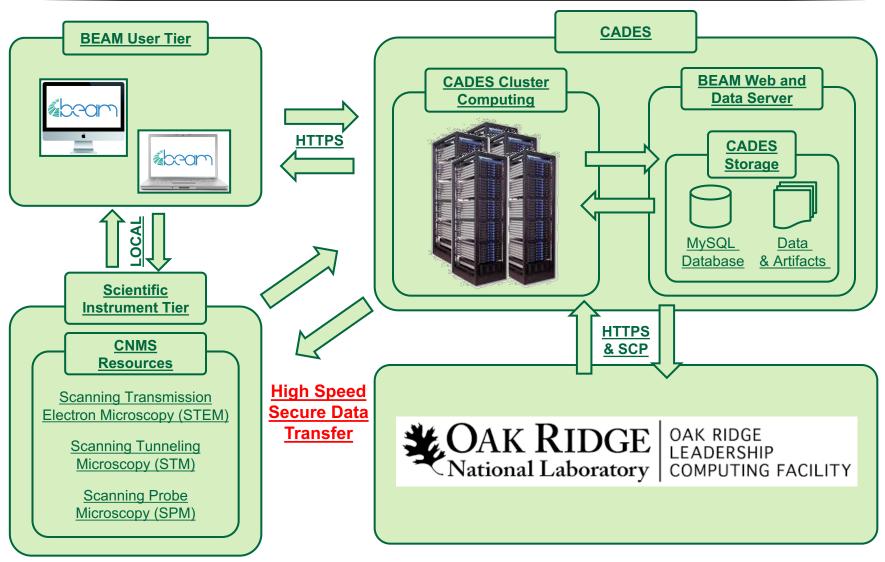


#### Software Integration Strategy





#### Big Data and High Performance Computing



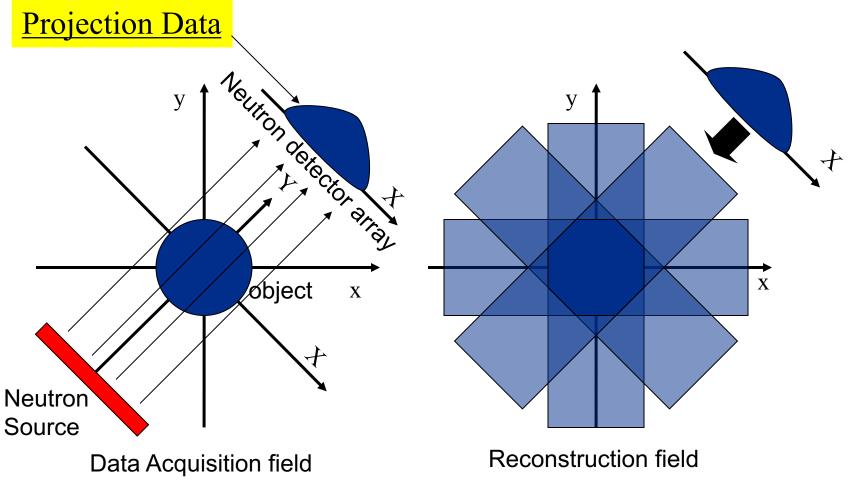


#### Big Data and High Performance Computing

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#### **Basic principle of CT** -Reconstruction of 2 dimensional image-





#### **Reconstruction process**

f(x, y): absorption coefficient (to be reconstructed) [Np/m]  $I_0(x)$ : incident intensity, I(x): attenuated intensity

attenuated intensity: 
$$I(X) = I_0(X)e^{-\int f(x,y)dY}$$

projection data: 
$$p(X,\theta) = \int f(x,y)dY = \ln \frac{I_0(X)}{I(X)}$$

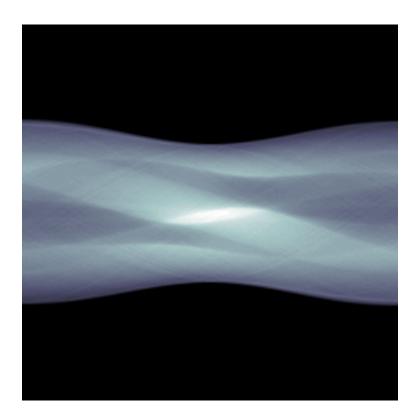
Filtered data: 
$$p_f(X,\theta) = \frac{1}{2\pi} \int_{-\infty}^{\infty} P(U,\theta) \cdot |U| \cdot e^{jUX} dX$$

where  $P(U,\theta)$  is 1D FFT of  $p(X,\theta)$ 

Back projection : 
$$f(x, y) = \int_0^{\pi} p_f(x \cdot \cos \theta + y \cdot \sin \theta, \theta) d\theta$$
  
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J. S. Department of Energy

#### **SL Phantom**

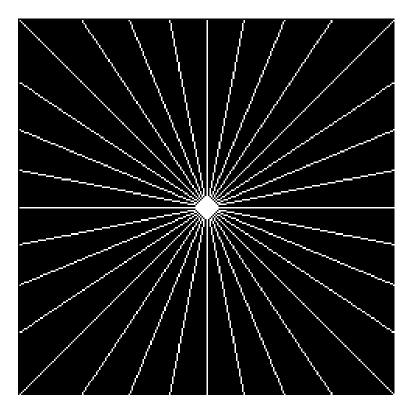




#### True image

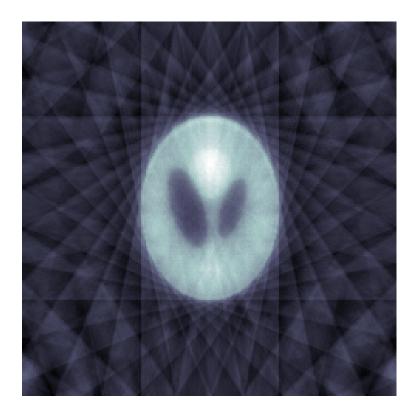


#### **SL Phantom**



#### **Known Fourier Data**

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#### **Partial Reconstruction**



Determine  $\mathbf{f} = \{f(x_i, y_j) : 0 \le i, j \le 2N\}$  that solves the convex optimization problem

minimize 
$$||J_x \mathbf{f}||_1 + ||J_y \mathbf{f}||_1$$
,  
subject to  $||MF\mathbf{f} - \mathbf{\hat{f}}||_2 \le \sigma$ ,

Where the matrix M is a mask that removes unknown Fourier coefficients.



Split Bregman iteration solves the optimization problem using a sequence of two unconstrained problems of the form

$$\mathbf{f}^{k+1} = \min_{\mathbf{f}} ||J_x \mathbf{f}||_1 + ||J_y \mathbf{f}||_1 + \frac{\mu}{2} ||MF\mathbf{f} - \mathbf{\hat{f}}^k||_2,$$
  
$$\mathbf{\hat{f}}^{k+1} = \mathbf{\hat{f}}^k + \mathbf{\hat{f}} - MF\mathbf{f}^{k+1}$$

for optimization parameter  $\mu > 0$ .

Goldstein, T., and Osher, S. The split bregman method for I1-regularized problems. SIAM Journal on Imaging Sciences 2, 2 (2009), 323–343. OAK RIDGE NATIONAL LABORATORY U. S. DEPARTMENT OF ENERGY

Using the total variation operator  $(J_x = \nabla_x \text{ and } J_y = \nabla_y)$ , with the replacements,  $\mathbf{d}_x \leftarrow \nabla_x \mathbf{f}$  and  $\mathbf{d}_y \leftarrow \nabla_y \mathbf{f}$ , using  $||\nabla \mathbf{v}||_1 = \sum_{i,j} \sqrt{|\nabla_x v_{i,j}|^2 + |\nabla_y v_{i,j}|^2}$ , the augmented problem is,

$$\begin{split} \min_{\mathbf{f},\mathbf{d}_x,\mathbf{d}_y} \sum_{i,j} \sqrt{|d_{x,i,j}|^2 + |d_{y,i,j}|^2} &+ \frac{\lambda}{2} ||\mathbf{d}_x - \nabla_x \mathbf{f} - \mathbf{b}_x||_2 \\ &+ \frac{\lambda}{2} ||\mathbf{d}_y - \nabla_y \mathbf{f} - \mathbf{b}_y||_2 + \frac{\mu}{2} ||MF\mathbf{f} - \mathbf{\hat{f}}||_2. \end{split}$$

This augmented problem is done in steps. When **f** is held fixed, the exact optimization of  $\mathbf{d}_x$  and  $\mathbf{d}_y$  can be calculated by,

$$\mathbf{d}_{x}^{opt} = \max(\mathbf{s} - 1/\lambda, 0) \frac{\nabla_{x} \mathbf{f} + \mathbf{b}_{x}}{\mathbf{s}} \quad \text{and} \quad \mathbf{d}_{y}^{opt} = \max(\mathbf{s} - 1/\lambda, 0) \frac{\nabla_{y} \mathbf{f} + \mathbf{b}_{y}}{\mathbf{s}}, \quad (1)$$

where

$$\mathbf{s} = \sqrt{|\nabla_x \mathbf{f} + \mathbf{b}_x|^2 + |\nabla_y \mathbf{f} + \mathbf{b}_y|^2}.$$



When  $\mathbf{d}_x$  and  $\mathbf{d}_y$  are held fixed the  $l^2$  problem

$$\min_{\mathbf{f}} \frac{\lambda}{2} ||\mathbf{d}_x - \nabla_x \mathbf{f} - \mathbf{b}_x||_2 \frac{\lambda}{2} ||\mathbf{d}_y - \nabla_y \mathbf{f} - \mathbf{b}_y||_2 + \frac{\mu}{2} ||MF\mathbf{f} - \mathbf{\hat{f}}||_2.$$

Because this subproblem is differentiable, we can find the optimal solution  $\mathbf{f}$  by differentiating by  $\mathbf{f}$  and setting the result equal to zero to get,

$$(\mu F^T M^T M F + \lambda \nabla_x^T \nabla_x + \lambda \nabla_y^T \nabla_y) \mathbf{f} = rhs,$$

where

$$rhs = \mu F^T M^T \mathbf{\hat{f}} + \lambda \nabla_x^T (\mathbf{d}_x - \mathbf{b}_x) + \lambda \nabla_y^T (\mathbf{d}_y - \mathbf{b}_y).$$



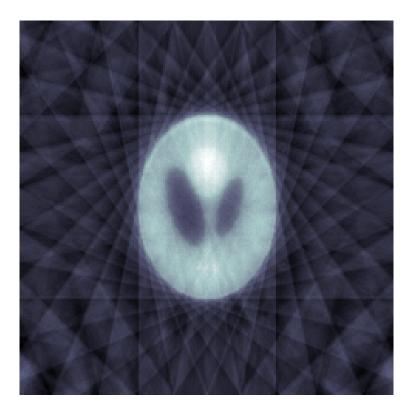
Algorithm: Split Bregmen Optimization of partially sampled Fourier data for the TV operator.

Initialize:  $\mathbf{f}^0 = F^{-1}M^T \mathbf{\hat{f}}$ , and  $\mathbf{b}_x = \mathbf{b}_y = \mathbf{d}_x = \mathbf{d}_y = k = 0$ while  $||MF\mathbf{f}^k - \mathbf{\hat{f}}||_2 > \sigma$  $\mathbf{f}^{k+1} = F^{-1}K^{-1}Frhs^k$  $\mathbf{d}_{x}^{k+1} = \max(\mathbf{s}^{k} - 1/\lambda, 0) \frac{\nabla_{x} \mathbf{f}^{k} + \mathbf{b}_{x}^{k}}{\mathbf{s}^{k}}$  $\mathbf{d}_{u}^{k+1} = \max(\mathbf{s}^{k} - 1/\lambda, 0) \frac{\nabla_{y} \mathbf{f}^{k} + \mathbf{b}_{y}^{k}}{\mathbf{c}^{k}}$  $\mathbf{b}_{x}^{k+1} = \mathbf{b}_{x}^{k+1} + (\nabla_{x} \mathbf{f}^{k+1} - \mathbf{d}_{x}^{k+1})$  $\mathbf{b}_{u}^{k+1} = \mathbf{b}_{u}^{k+1} + (\nabla_{y}\mathbf{f}^{k+1} - \mathbf{d}_{u}^{k+1})$  $\mathbf{\hat{f}}^{k+1} = \mathbf{\hat{f}}^k + \mathbf{\hat{f}} - MF\mathbf{f}^{k+1}$ 

k = k + 1

end





#### **Partial Reconstruction**

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#### **Optimized Reconstruction**



## **Multi-Dimensional Formulation**

- Let  $\mathcal{S}$  be a set of discrete points in the bounded domain  $\Omega \subset \mathbb{R}^d$  and f be a piecewise smooth function known only on  $\mathcal{S}$ .
- We construct a function,  $L_N f$  for  $N \in \mathbb{N}$ , that has the asymptotical convergence property,

$$L_N f(x) \longrightarrow 0,$$

away from jump discontinuities of f.



### **Multi-Dimensional Formulation**

• For any  $x \in \Omega$ , we choose a set

$$\mathcal{S}_x := \mathcal{S}_{x,N} := \{x_1, \dots, x_N\},\$$

which is a local set typically of  $N = m_d := \binom{m+d}{d}$  points around x.



The edge detection method is based on a local polynomial annihilation property and performed in the following two steps:

1. Solve the linear system

$$\sum_{x_j \in \mathcal{S}_x} c_j(x) p_i(x_j) = \sum_{|\alpha|_1 = m} p_i^{(\alpha)}(x), \quad \alpha \in \mathbb{Z}_+^d,$$

where  $p_i$ ,  $i = 1, \dots, m_d$ , is a basis of  $\Pi_m$ . Here  $\Pi_m$  denotes the space of all polynomials of degree  $\leq m$  in  $d \in \mathbb{N}$  variables. Note the dimension of  $\Pi_m$  is  $m_d := \binom{m+d}{d}$ , and therefore the solution exists and is unique.

2. Our edge detector  $L_m f$  is defined as

$$L_m f(x) = \frac{1}{q_{m,d}(x)} \sum_{x_j \in \mathcal{S}_x} c_j(x) f(x_j).$$

Here  $q_{m,d}(x)$  is a suitable normalization factor depending on m, the dimension d, and the local set  $S_x$ .



#### **One Dimension**

• Let f be a piecewise smooth function known only on the set

$$\mathcal{S} := \{ x_j \mid a \le x_1 < x_2 < \dots < x_N \le b \} \subset \mathbb{R}.$$

• Define the local jump function corresponding to f as

$$[f](x) := f(x+) - f(x-),$$

where f(x+) and f(x-) are the right and left side limits of the function f at x.

• Finally define

$$h(x) := \max\{|x_j - x_{j-1}| : x_{j-1}, x_j \in \mathcal{S}_x\},\$$

 $\mathcal{S}_x^+ := \{ x_j \in \mathcal{S}_x | x_j \ge x \}, \text{ and } \mathcal{S}_x^- := \{ x_j \in \mathcal{S}_x | x_j < x \}.$ 



The edge detection method is performed in the following two steps:

1. Solve the linear system

$$\sum_{x_j \in \mathcal{S}_x} c_j(x) p_i(x_j) = p_i^{(m)}(x), \quad i = 1, \cdots, m_1,$$

where  $p_i$ ,  $i = 1, \dots, m_1$ , is a basis of  $\Pi_m$ . Clearly, the coefficients  $c_j(x)$  are uniquely determined by the local set  $S_x$ , and are of order  $\mathcal{O}(h(x)^{-m})$  as h(x) tends to 0.

2. The edge detection method in the one dimensional case is

$$L_m f(x) = \frac{1}{q_m(x)} \sum_{x_j \in \mathcal{S}_x} c_j(x) f(x_j),$$

where the normalization factor is set as

$$q_m(x) := q_{m,1}(x) := \sum_{x_j \in \mathcal{S}_x^+} c_j(x).$$



To further illustrate the linear system consider the following example:

For  $m \in \mathbb{Z}_+$ , consider the following basis of  $\Pi_m$ :

$$p_i(x) = x^{i-1}$$
 for  $i = 1, \cdots, m_1$ .

It follows that becomes

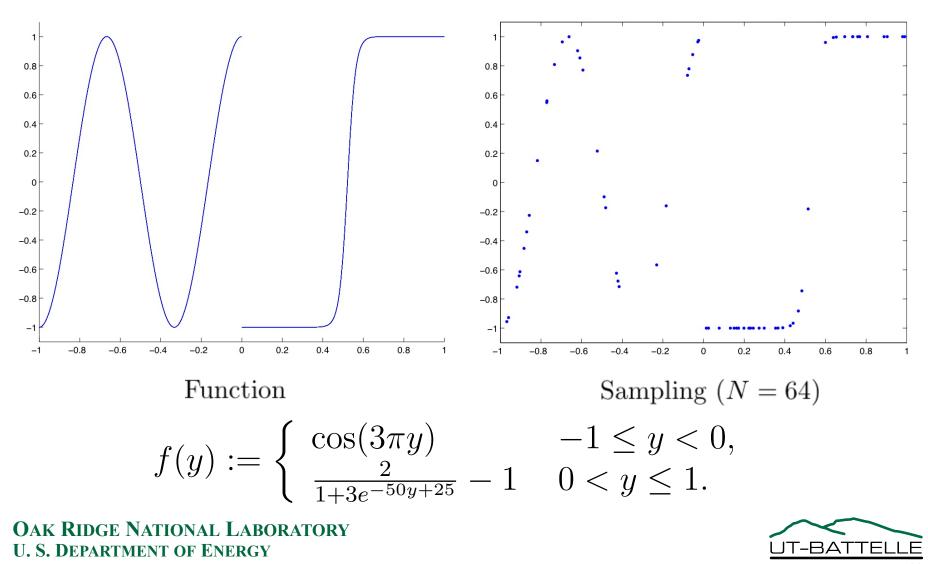
$$\sum_{x_j \in \mathcal{S}_x} c_j(x) x_j^{i-1} = m! \delta_{i,m_1} \quad \text{for } i = 1, \cdots, m_1$$

Specifically, let m = 2 and  $S_x = \{x_1, x_2, x_3\}$ . The linear system can be written in matrix notation as,

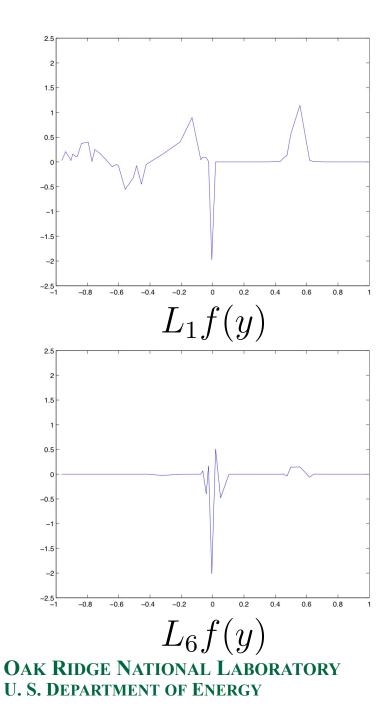
$$\begin{pmatrix} 1 & 1 & 1 \\ x_1 & x_2 & x_3 \\ x_1^2 & x_2^2 & x_3^2 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 2 \end{pmatrix}.$$

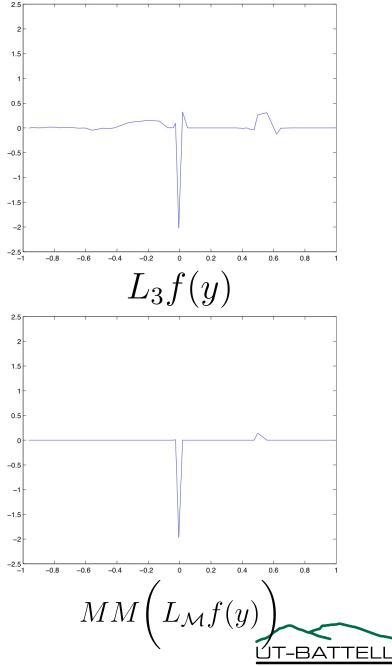


# **Example - 1D Edge Detection**



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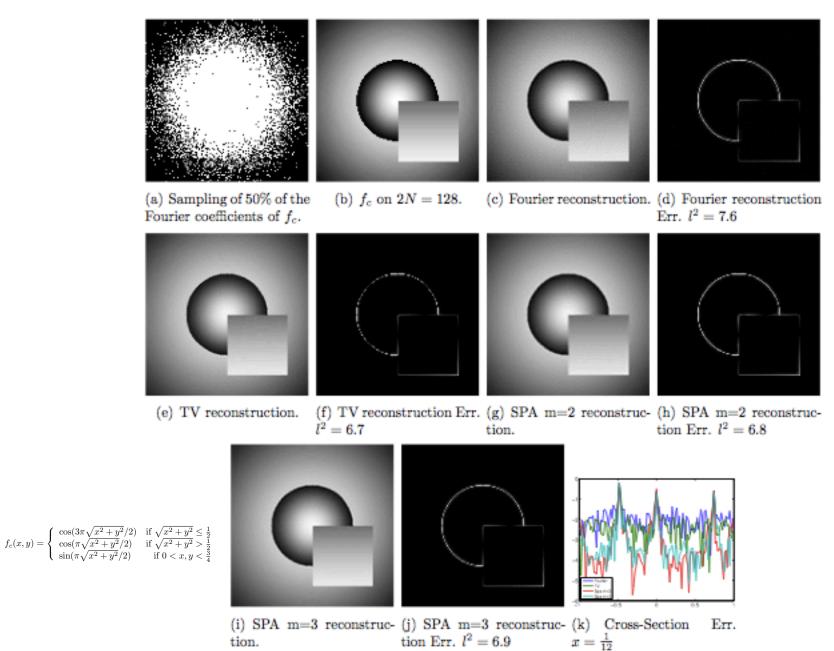
#### **Partially Sampled Fourier Data**

Algorithm: Split Bregmen Optimization of partially sampled Fourier data for the polynomial annihilation operator.

Initialize:  $\mathbf{f}^0 = F^{-1}M^T \mathbf{\hat{f}}$ , and  $\mathbf{b}_x = \mathbf{b}_y = \mathbf{d}_x = \mathbf{d}_y = k = 0$ while  $||MF\mathbf{f}^k - \mathbf{\hat{f}}||_2 > \sigma$  $\mathbf{f}^{k+1} = F^{-1} K_{LM}^{-1} Frhs^k$  $\mathbf{d}_{x}^{k+1} = \max(\mathbf{s}^{k} - 1/\lambda, 0) \frac{L_{m,x} \mathbf{f}^{k} + \mathbf{b}_{x}^{k}}{\mathbf{c}^{k}}$  $\mathbf{d}_{u}^{k+1} = \max(\mathbf{s}^{k} - 1/\lambda, 0) \frac{L_{m,y} \mathbf{f}^{k} + \mathbf{b}_{y}^{k}}{\mathbf{c}^{k}}$  $\mathbf{b}_{x}^{k+1} = \mathbf{b}_{x}^{k+1} + (L_{m_{x}}\mathbf{f}^{k+1} - \mathbf{d}_{x}^{k+1})$  $\mathbf{b}_{u}^{k+1} = \mathbf{b}_{u}^{k+1} + (L_{m,u}\mathbf{f}^{k+1} - \mathbf{d}_{u}^{k+1})$  $\mathbf{\hat{f}}^{k+1} = \mathbf{\hat{f}}^k + \mathbf{\hat{f}} - MF\mathbf{f}^{k+1}$ k = k + 1

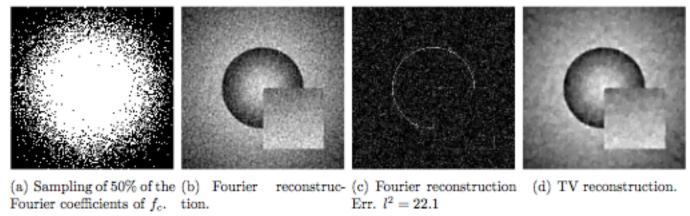
end

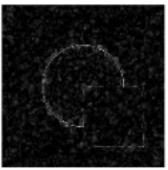


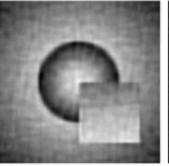


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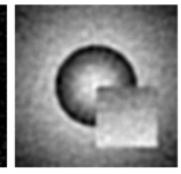






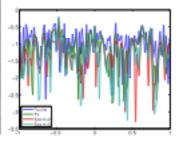






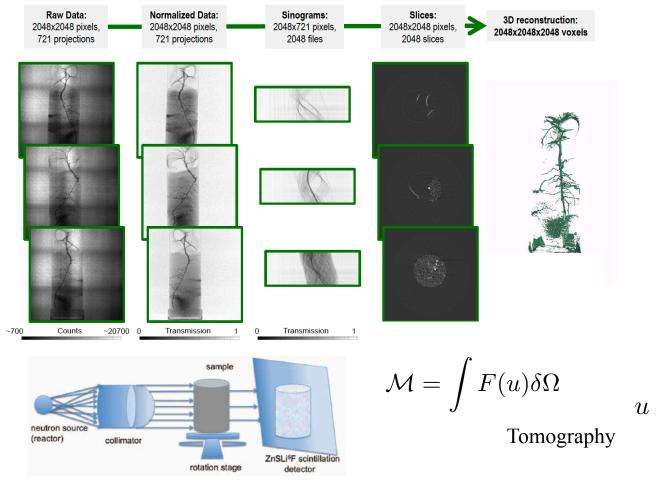
(e) TV reconstruction (f) SPA m=2 reconstruc- (g) SPA m=2 reconstruc- (h) SPA m=3 reconstruc-Err.  $l^2 = 14.4$  tion. tion Err.  $l^2 = 13.0$  tion.



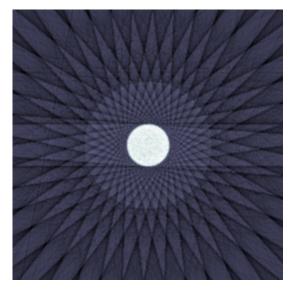


(i) SPA m=3 reconstruc- (j) Cross-Section Err. x =tion Err.  $l^2 = 12.8$   $\frac{1}{12}$ 





$$\mathcal{M} = \int F(u)\delta\Omega$$



- Image is of Aluminum-Steel Phantom taken at HFIR - CG1
- Standard filtered back projection methods in tomographic reconstruction yields artifacts
- Computationally Expensive to reconstruct
- Full 3D dataset is:
   2048×2048×360~30GB

 $\min_{\mathbf{u}\in\mathbf{R}^n}\{\|\Phi(\mathbf{u})-\mathcal{M}_n\|_{\ell^1}+H(\mathbf{u})\}\$ 



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 $\mathcal{M} = \int F(u)\delta\Omega$ 

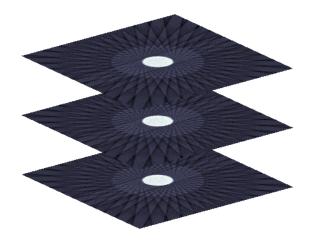
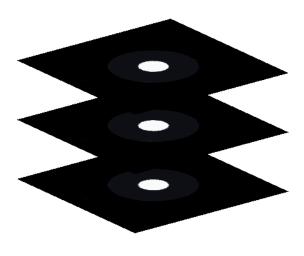


Image is of Aluminum-Steel Phantom taken at HFIR - CG1 Standard filtered back projection methods in tomographic reconstructi yields artifacts Computationally Expensi to reconstruct Full 3D dataset is: 2048 × 2048 × 360 ~30G

 $\min_{\mathbf{u}\in\mathbf{R}^n}\{\|\Phi(\mathbf{u})-\mathcal{M}_n\|_{\ell^1}+H(\mathbf{u})\}\$ 



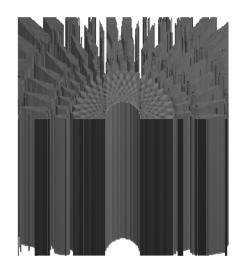
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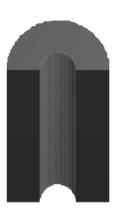
u

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#### $\min_{\mathbf{u}\in\mathbf{R}^n}\{\|\Phi(\mathbf{u})-\mathcal{M}_n\|_{\ell^1}+H(\mathbf{u})\}\$





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# Discussion for Long Program

#### Thank You.

