

Joint image reconstruction of multi-channel X-ray computed tomography data for material science

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Bologna, Italy



The University of Manchester



Project partners and applications

Working together with mathematicians, software developers and imaging scientists

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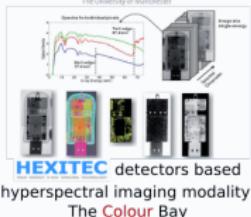
i18, i14 X-ray spectroscopy, diffraction and fluorescence imaging



diamond

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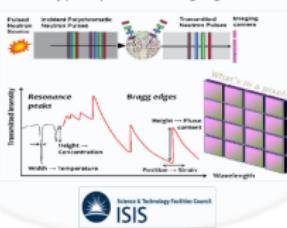
MANCHESTER
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HEXITEC detectors based on hyperspectral imaging modality
The Colour Bay

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The neutron imaging facility IMAT
Hyperspectral imaging



Science & Technology Facilities Council
ISIS

Reconstruction Toolkit for Multichannel CT (RT-MCT)

- Advanced iterative solutions
- Novel multi-channel correlative priors
- Compressed sensing tools
- Fast, efficient and parallelised software

MANCHESTER
1824
The University of Manchester

MINDIA CUDA

Research Complex at Harwell
Working across materials and environmental science

C/C++ python

To be embedded into existing framework (Savu, CCPi)



Academic Impact
Journal publications
Conferences
Workshops
Seminars

Industrial Impact
Important contributions and solutions to materials manufacturing

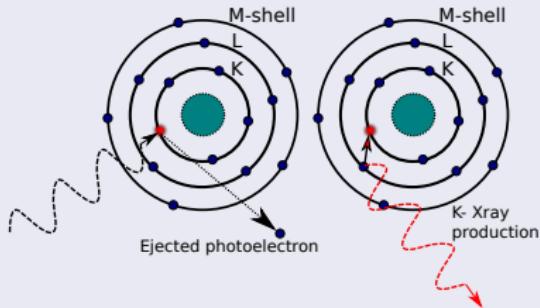
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- 3 Multi-channel regularization approaches
- 4 Numerical Experiments
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The challenges of multi-energetic computed tomography

X-ray matter interactions

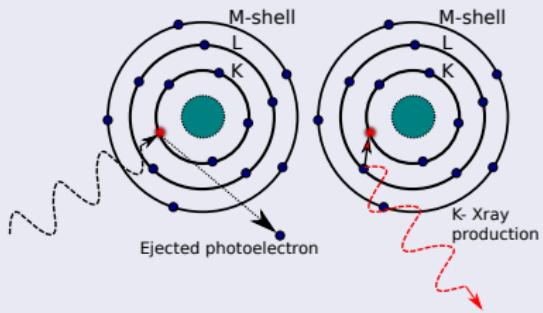
Photoelectric effect



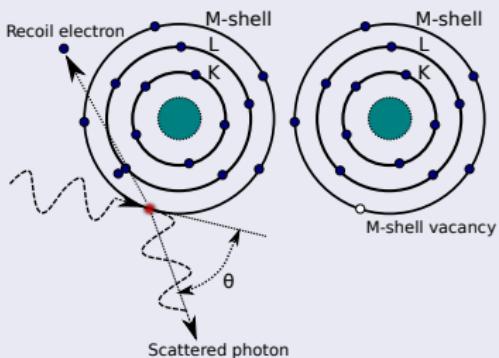
- Inner shell electrons interactions
- Whole of the photon energy is transferred
- To eject, the photon energy must be $>=$ the binding energy

X-ray matter interactions

Photoelectric effect



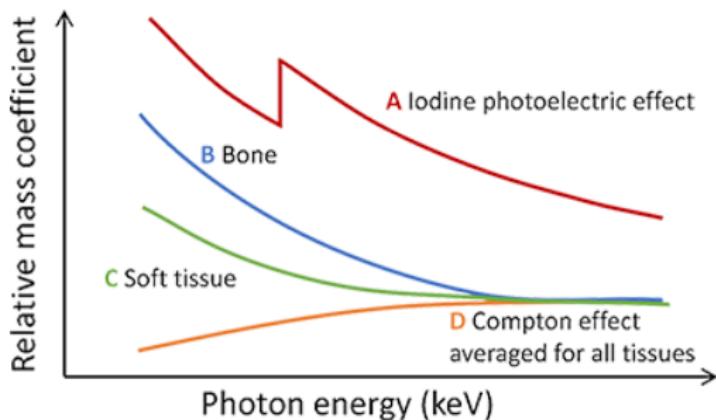
Compton effect



- Inner shell electrons interactions
- Whole of the photon energy is transferred
- To eject, the photon energy must be $>=$ the binding energy

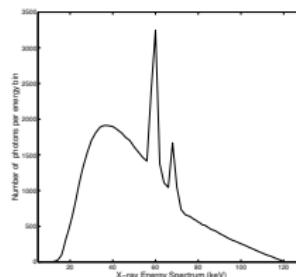
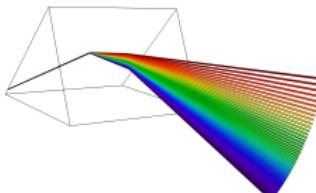
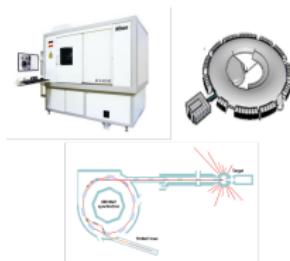
- Outer shell electrons interactions
- Part of the electron energy is transferred
- M-shell is vacant

Search for absorption edges (K-edge imaging)



- When the photon energy is strong enough to match the binding energy of the K-shell of iodine - the **K-edge** appears (a sharp increase in attenuation)
- Specific energy (33keV for iodine) can be used for a greater tissue contrast

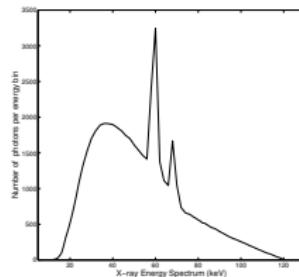
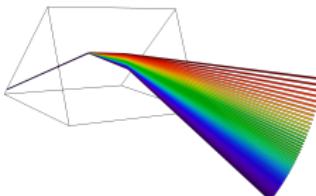
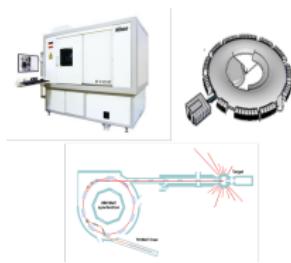
Polychromicity of sources



Challenges

- X-ray sources are polychromatic while detectors still being **energy-integrating** (results in nonlinearity, beam-hardening)
- How one can find the K-edge of an unknown material?

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What is required in order to benefit on poly-beam?

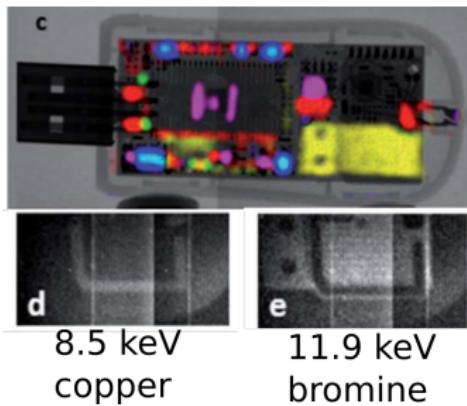
- **Energy-discriminating** detecting systems supporting finer spectral resolution (more than a hundred of energy channels)
- Novel reconstruction approaches employing spectral redundancy
- Efficient, well-written and documented software

On energy-discriminating detectors



HEXITEC¹ spectroscopic hard X-ray imaging detector for K-Edge Enhanced Imaging²

- Pixel size: $250 \mu\text{m} \times 250 \mu\text{m}$
- Number of pixels: $80 \times 80 = 6400$
- Energy Range: 2-200 keV
- Data Rate: 5M photons/second
- Dimensions: $21 \times 5 \times 5 \text{ cm}$

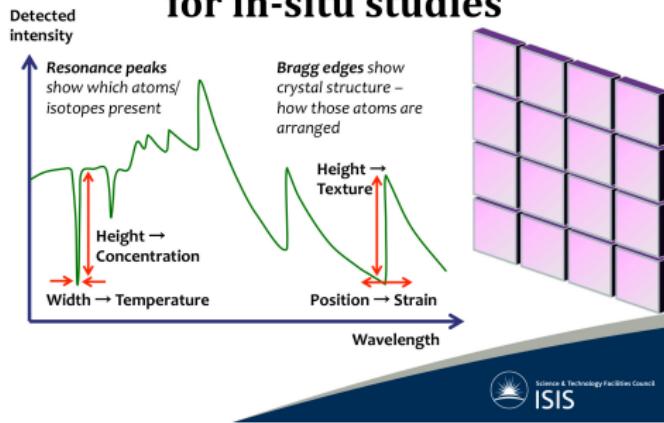


¹<http://quantumdetectors.com/hexitec/>

²S. Jacques et al. A laboratory system for element specific hyperspectral X-ray imaging

Time-of-flight Neutron Imaging

Time-of-flight neutron imaging for in-situ studies



Hyper-spectral X-ray imaging on IMAT ISIS³

- Using the time-of-flight (TOF) technique applied to neutrons, one can get information about the energy (wavelength)
- 4D (x,y,z + energy) imaging with neutrons is possible

³W. Kockelmann, J. Kelleher, T. Minniti, G. Burca and others

Poly-energetic X-ray CT measurement model

Given a poly-energetic X-ray source, the spectral version of Beer's law can be expressed as:

$$\Lambda_i(E) = \sigma_i(E) \exp\left(- \int_{L_i} \mu(\mathbf{r}, E) \, dl\right), \quad i = 1, \dots, M.$$

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With necessary parametrization we write the discrete model:

$$\Lambda_i(E_k) = \sigma_i(E_k) \exp \left(- \sum_{j=1}^N A_{ij} \mu_j(E_k) \right), \quad i = 1, \dots, M, \quad k = 1, \dots, K.$$

This model is an approximation, it tends to be more accurate with finer spectral discretization.

Poly-energetic X-ray CT measurement model

If we define $X_{jk} = \mu_j(E_k)$ and $S_{ik} = \sigma_i(E_k)$, we arrive at the discrete linear model:

$$B_{ik} = -\ln\left(\frac{Y_{ik}}{S_{ik}}\right) \approx \sum_{j=1}^N A_{ij} X_{jk}.$$

To simplify notation, we now define a matrix $\mathbf{X} \in \mathbb{R}^{N \times K}$ with elements X_{jk} , and $\mathbf{x} = \text{vec}(\mathbf{X}) \in \mathbb{R}^{NK}$ denotes the vectorized image (i.e., \mathbf{x} is obtained by stacking the columns of \mathbf{X}). Moreover, \mathbf{X}_k denotes the k th column of \mathbf{X} .

Using new notation for \mathbf{X}, \mathbf{B} we re-write more compactly

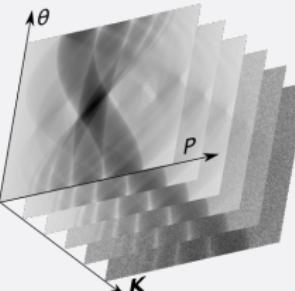
$$\mathbf{b} \approx \bar{\mathbf{A}}\mathbf{x},$$

where $\bar{\mathbf{A}} = \mathbf{A} \otimes \mathbf{I}_{K \times K}$ and $\mathbf{A} \in \mathbb{R}^{M \times N}$ is a sparse projection matrix, \otimes is the Kronecker product, and $\mathbf{I}_{K \times K}$ is the identity matrix of order K .

A generic multi-channel inverse problem

The variety of multi-channel problems

3D spectral dataset (K -channels)
consisting of λ materials



Reconstruction of all K energy channels *without* cross-correlation, i.e.
channel-wise

- + simple implementation, computationally efficient
- not effective to deal with low signal SNR, lots of data to process/analyze

Reconstruction of only λ channels *without* cross-correlation, i.e.
material-wise

- + simple implementation, computationally efficient better than channel-wise
- but still not effective against poor SNR data

Reconstruction of all K energy channels *with* cross-correlation, i.e.
inter-correlated

- + much improved SNR of reconstructed images
- complicated reconstruction algorithms, computational challenges

Basis materials decomposition

- + drastic dimensionality reduction from K to λ , when normally $\lambda \ll K$
- complex and expensive PCA-based methods or ML-based estimations

Reconstruction of only λ channels *with* cross-correlation, i.e.
material-correlated

- + much improved SNR of reconstructed images, less computationally difficult
- complicated reconstruction algorithms

General multi-channel reconstruction problem

The generic objective function for $\boldsymbol{x} \in \mathbb{R}^{NK}$ is:

$$\boldsymbol{x}^* = \arg \min_{\boldsymbol{x}} \{\mathcal{F}(\boldsymbol{x}) + \beta \mathcal{G}(\boldsymbol{x})\},$$

where $\mathcal{F} : \mathbb{R}^{NK} \rightarrow \mathbb{R}_+$ is a smooth convex the **data misfit** term and the **penalty term** $\mathcal{G} : \mathbb{R}^{NK} \rightarrow \mathbb{R}_+$ defines a regularization penalty with $\beta > 0$ as a trade-off parameter.

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Choosing the data fidelity term $\mathcal{F}(\bar{\boldsymbol{A}}\boldsymbol{x}, \boldsymbol{b})$

- $\mathcal{F}(\cdot) = \|\cdot\|_2^2$ - the Least-Squares misfit (Gaussian noise in data \boldsymbol{b})

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- Other nonlinear/nonconvex terms can be employed, such as, ℓ_1 , Huber, Student's t misfit^a, and others.

^aK. et al. *A novel tomographic reconstruction method based on the robust Student's t function for suppressing data outliers*, IEEE TCI, 2017

Multi-channel regularization approaches

Channel-wise regularization strategies

The total variation (TV) penalty⁴ for a (single-channel) image $\mathbf{v} \in \mathbb{R}^N$:

$$\text{TV}(\mathbf{v}) = \sum_{j=1}^N \|\mathbf{D}_j \mathbf{v}\|_2,$$

where \mathbf{D}_j is a $2 \times N$ matrix such that $\mathbf{D}_j \mathbf{v}$ is a finite-difference approximation of the gradient of \mathbf{v} at pixel j .

⁴L. Rudin et al., *Nonlinear total variation based noise removal algorithms*, 1992

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For multi-channel CT, one can consider using **channel-wise TV**:

$$\mathcal{G}_{\text{TV}}(\mathbf{x}) = \sum_{k=1}^K \text{TV}(\mathbf{X}_k), k = 1, \dots, K$$

The significant disadvantage of channel-wise TV is that there is no correlation between channels k .

⁴L. Rudin et al., *Nonlinear total variation based noise removal algorithms*, 1992

Why one needs correlative regularization?

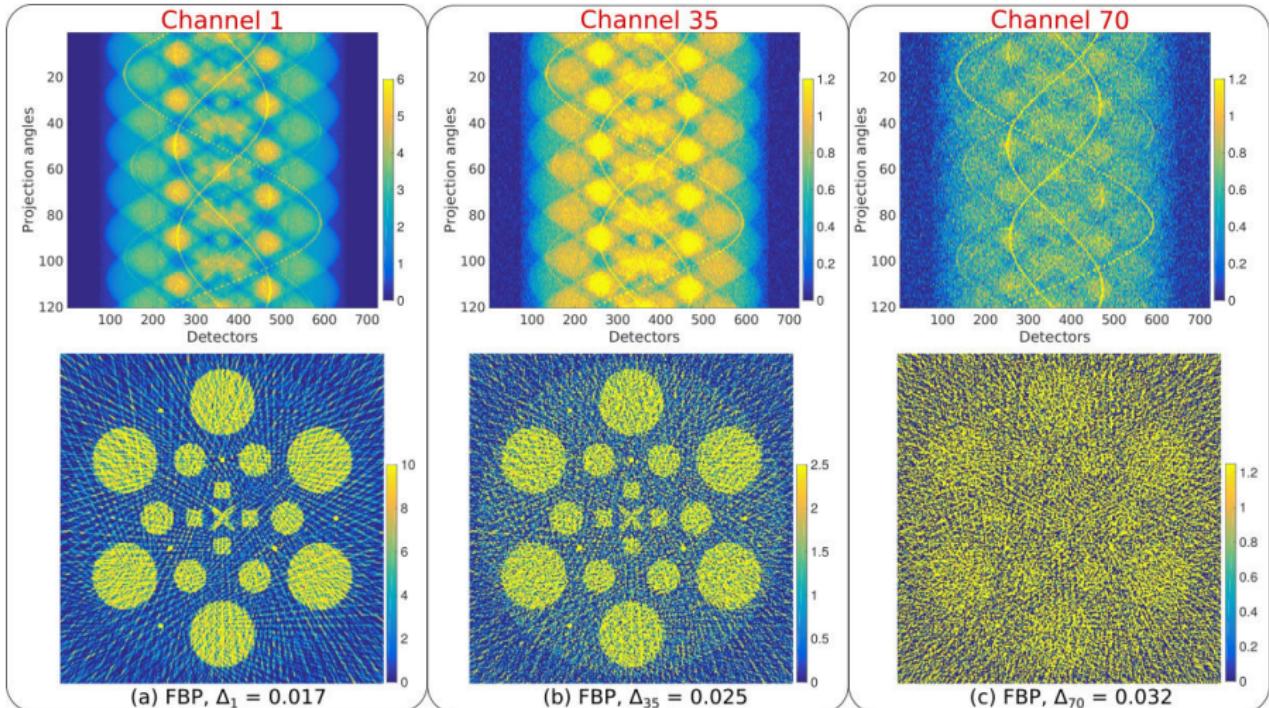
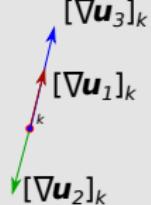
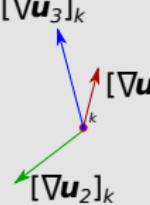
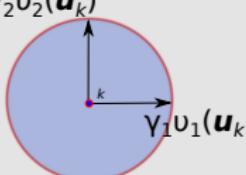
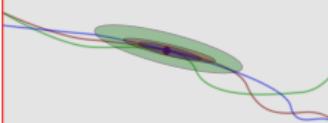
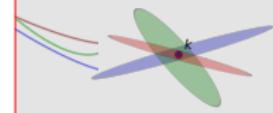


Image reconstruction using Filtered-Backprojection (FBP) method

Introducing vector-valued correlative strategies

Uniform (constant) area	Correlated channels	Uncorrelated channels
<p>Vectorial (level sets) framework</p> $[D\mathbf{u}]_k = 0$  <p>All singular values of Jacobian (J) are zero</p>	<p>Vectorial (level sets) framework</p>  <p>Parallel level sets at point k One singular value is non-zero (\mathbf{u}_2)</p>	<p>Vectorial (level sets) framework</p>  <p>Unique gradient directions Nonzero singular values</p>
<p>Tensor-based framework</p>  <p>Mixture of isotropic tensors</p>	<p>Tensor-based framework</p>  <p>Three anisotropic (diffusion) tensors with the same eigenvectors, yet different eigenvalues</p> <p>eigenvectors (\mathbf{u}): direction of diffusion eigenvalues (γ): strength of diffusion</p>	<p>Tensor-based framework</p>  <p>Unique diffusion directions and diffusive forces</p> <p>One can interpolate between tensors to obtain an averaged tensor</p> <p>?</p>

Total Nuclear Variation functional

One can consider of penalizing Jacobian which is obtained by applying the finite difference operator at pixel j to all channels simultaneously, i.e., $\mathbf{D}_j \mathbf{X}$ for $j = 1, \dots, N$. In particular the Total Nuclear Variation (TNV)⁵ is defined as

$$\mathcal{G}_{\text{TNV}}(\mathbf{x}) = \sum_{j=1}^N \|\mathbf{D}_j \mathbf{X}\|_*,$$

where $\|\cdot\|_*$ denotes the nuclear norm, i.e., the sum of the singular values. Singular value analysis shows that TNV encourages the gradient vectors of each energy channels to be aligned which is equivalent to a low rank Jacobian.

⁵D.S. Rigue et al. *Joint reconstruction of multi-channel, spectral CT data via constrained total nuclear variation minimization*, PMB, 2015

K. Holt, *Total nuclear variation and Jacobian extensions of total variation for vector fields*, IEEE, 2014

Diffusion-based interpretation of TNV model

Regularization functional for vectorial image \mathbf{u} :

$$E(\mathbf{u}) = \int_{\Omega} \psi(\lambda^+, \lambda^-) d\Omega,$$

where $\lambda^{+,-}$ are the larger and smaller eigenvalues of the structure tensor $k_\rho * (\nabla \mathbf{u}_\sigma^\top \nabla \mathbf{u}_\sigma)$, respectively.

⁶S. Lefkimiatis et al. *Structure tensor total variation*, SIAM Imaging Sciences, 2015
J. Duran et al. *Collaborative Total Variation*, SIAM Imaging Sciences, 2016

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One chooses: $\psi(\lambda^+, \lambda^-) = \|(\sqrt{\lambda^+}, \sqrt{\lambda^-})\|_p$ and $p = 1$ for the nuclear norm⁶.

The E-L equations then given as:

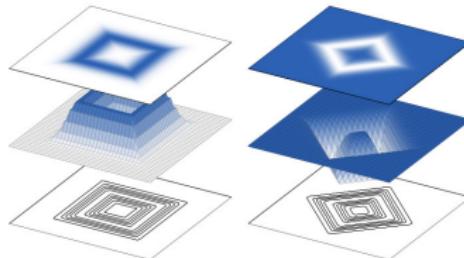
$$\frac{\partial \mathbf{u}}{\partial t} = \nabla \cdot (\mathbf{D} \nabla \mathbf{u}), \text{ s.t. BCS,}$$

with the diffusion tensor: $\mathbf{D} = K_\sigma * \left(\frac{1}{\sqrt{\lambda^+}} \theta^+ \otimes \theta^+ + \frac{1}{\sqrt{\lambda^-}} \theta^- \otimes \theta^- \right)$

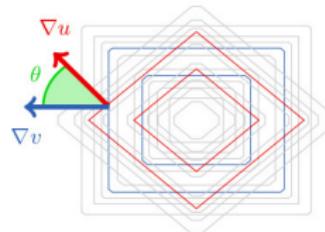
⁶S. Lefkimiatis et al. *Structure tensor total variation*, SIAM Imaging Sciences, 2015
 J. Duran et al. *Collaborative Total Variation*, SIAM Imaging Sciences, 2016

Parallel level sets to drive diffusivity

One can also consider the level sets of images



and introduce correlation between channels through **parallel level sets**⁷



⁷M.J. Ehrhardt, Joint Reconstruction for Multi-Modality Imaging with Common Structure, Ph.D. Thesis, UCL, UK

M.J. Ehrhardt, S.R. Arridge, *Vector-valued image processing by parallel level sets.*

dTV regularization with known reference

The directional TV regularizer (dTV)⁸ is introduced as:

$$\text{dTV}(\mathbf{v}, \mathbf{z}) = \sum_{j=1}^N \|P_{\mathbf{z}} \mathbf{D}_j \mathbf{v}\|_2, \quad (1)$$

where:

$$P_{\mathbf{z}} = \begin{cases} \mathbf{I}_{2 \times 2} - \frac{\mathbf{D}_j \mathbf{z} \mathbf{z}^\top \mathbf{D}_j^\top}{\mathbf{z}^\top \mathbf{D}_j^\top \mathbf{D}_j \mathbf{z}} & \mathbf{D}_j \mathbf{z} \neq 0 \\ \mathbf{I}_{2 \times 2} & \mathbf{D}_j \mathbf{z} = 0. \end{cases}$$

The regularization function (1) is the *directional diffusion* of the channel \mathbf{v} , given a known reference \mathbf{z} .

⁸M.J. Ehrhardt M.M. Betcke, *Multicontrast MRI reconstruction with structure-guided total variation* SIAM Journal on Imaging Sciences, 2016

Multiple channels with unknown reference

The proposed⁹ dTV-type probabilistic regularizer for multi-channel case:

$$\mathcal{G}_{\text{dTV-p}}(\boldsymbol{x}^{[s]}) = \sum_{k=1}^K \text{dTV}\left(\boldsymbol{X}_k^{[s]}, \boldsymbol{X}_{k^*(s,k)}^{[s-1]}\right), \quad (2)$$

where the *reference* channel (previous estimate) is chosen according to the probability mass function:

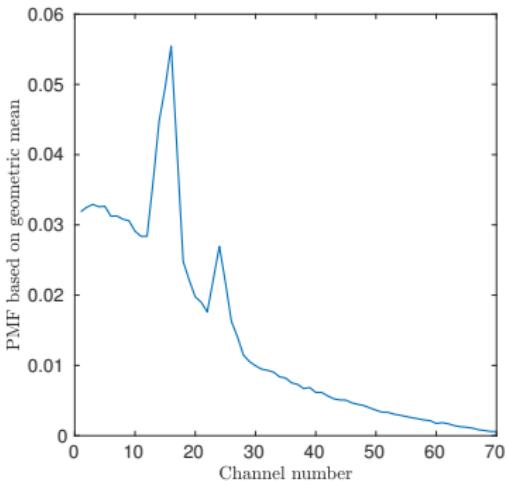
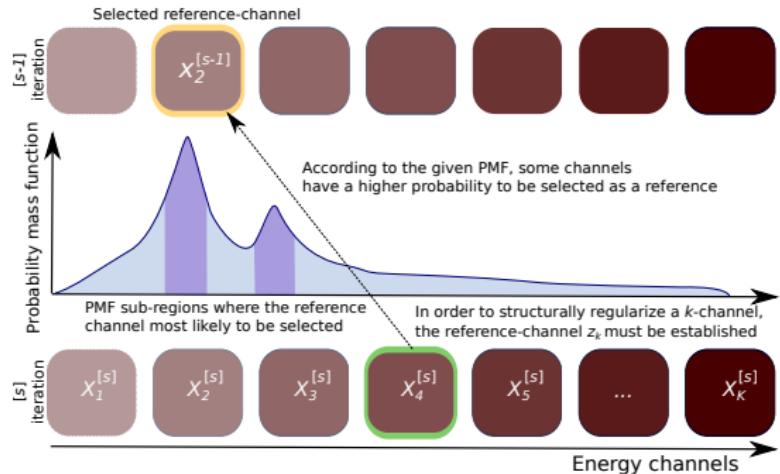
$$\bar{\rho}_{k^*} = \frac{\rho_{k^*}}{\sum_{k=1}^K \rho_k}, \quad (3)$$

where channel-wise geometric mean of the approximate SNR is

$$\rho_k = \left(\prod_{i=1}^M B_{ik} \sqrt{Y_{ik}} \right)^{1/M}.$$

⁹K. et al. *Joint image reconstruction method with correlative multi-channel prior for x-ray spectral computed tomography*, Inverse Problems, 2018

Multiple channels with unknown reference



The reference-channel $z_k^{[s]} = X_{k^*}^{[s-1]}$ is selected by randomly drawing a sample (index $k^* \in \{1, \dots, K\}$) of a channel) from the given probability mass function (PMF). The PMF specific to our experiment is depicted in the right figure.

Multi-channel reconstruction algorithm

Algorithm 1 Multi-channel FISTA-based reconstruction scheme

Input: \mathbf{b} , $\mathbf{x}^{[0]}$, β , S , L

Output: $\mathbf{x}^{[S]}$

$$\mathbf{y}^{[1]} = \mathbf{x}^{[0]}, t^{[1]} = 1$$

for all $s = 1, \dots, S$ do

$$1: \mathbf{u}^{[s]} = \mathbf{y}^{[s]} - L^{-1} \nabla \mathcal{F}(\mathbf{y}^{[s]})$$

$$2: \mathbf{x}^{[s]} = \text{prox}_{\beta/L}[\mathcal{G}](\mathbf{u}^{[s]})$$

$$3: t^{[s+1]} = \left(1 + \sqrt{1 + 4(t^{[s]})^2}\right) / 2$$

$$4: \mathbf{y}^{[s+1]} = \mathbf{x}^{[s]} + (t^{[s]} - 1)/t^{[s+1]} \cdot (\mathbf{x}^{[s]} - \mathbf{x}^{[s-1]})$$

end for

FISTA outer iterations

PWLS gradient step

Regularization proximal step

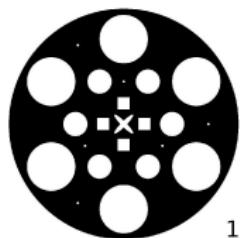
Where the data fidelity is used $\nabla \mathcal{F}(\mathbf{v}) = \bar{\mathbf{A}}^\top \mathbf{W}(\bar{\mathbf{A}}\mathbf{v} - \mathbf{b})$ with the Lipschitz constant of $\nabla \mathcal{F}$, $L = \|\bar{\mathbf{A}}^\top \mathbf{W} \bar{\mathbf{A}}\|_2$. The proximal operator¹⁰ in step 2 is given generally as

$$\text{prox}_{\beta/L}[\mathcal{G}](\mathbf{v}) = \arg \min_{\mathbf{u}} \left\{ \frac{\beta}{L} \mathcal{G}(\mathbf{u}) + \frac{1}{2} \|\mathbf{u} - \mathbf{v}\|_2^2 \right\}.$$

¹⁰A. Beck, *First-Order Methods in Optimization*, SIAM, 2017

Numerical Experiments

Four materials synthetic phantom



(a) Quartz



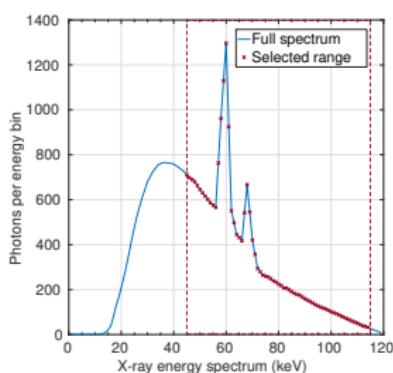
(b) Pyrite

3

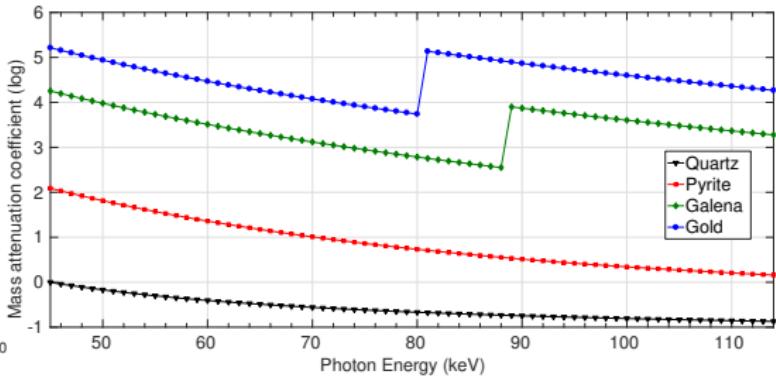
(c) Galena

4

(d) Gold



(e) Energy spectr.



(f) Mass attenuation curves material-wise

Image reconstruction with TV

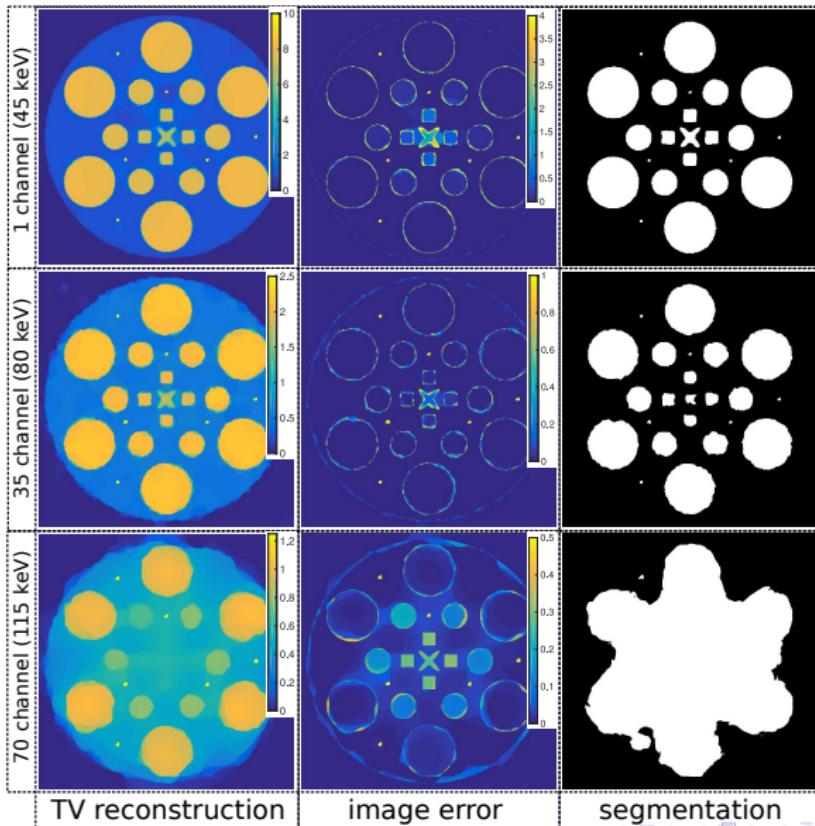


Image reconstruction with TNV

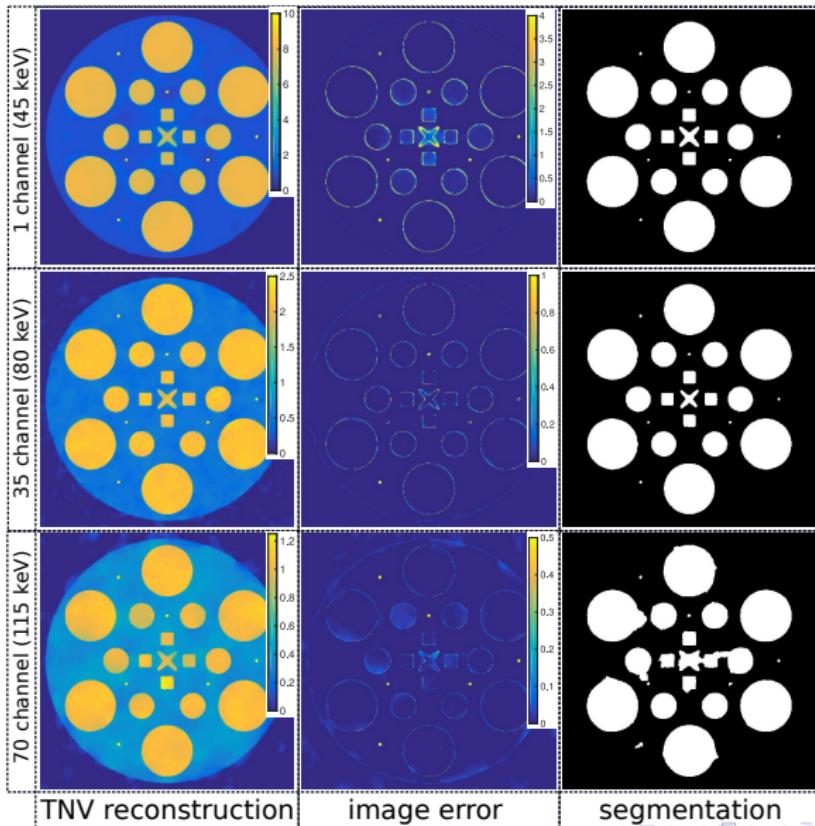
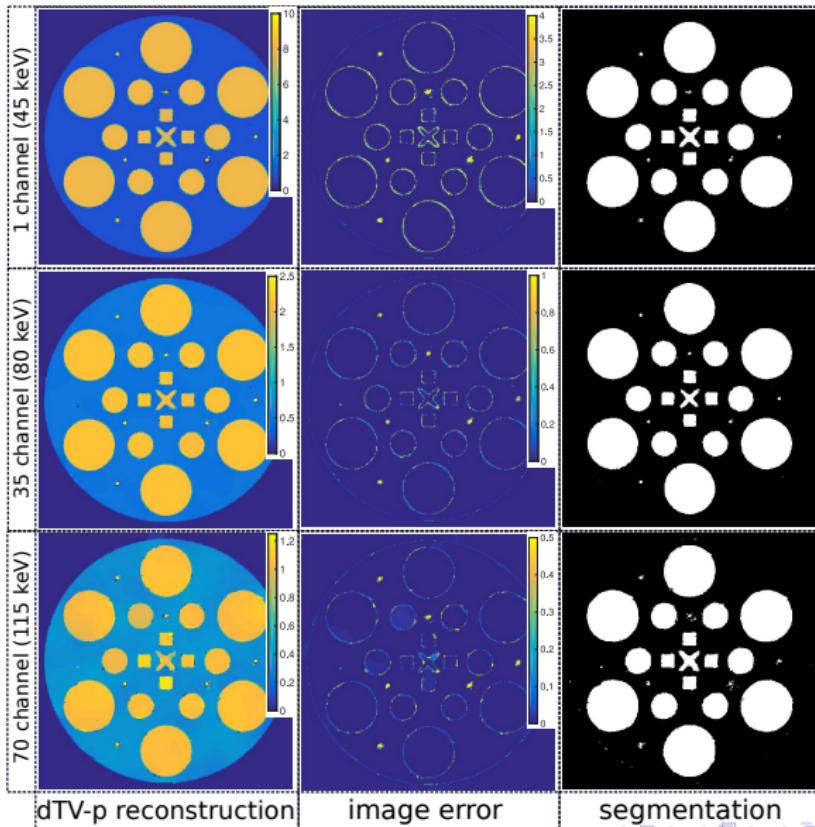
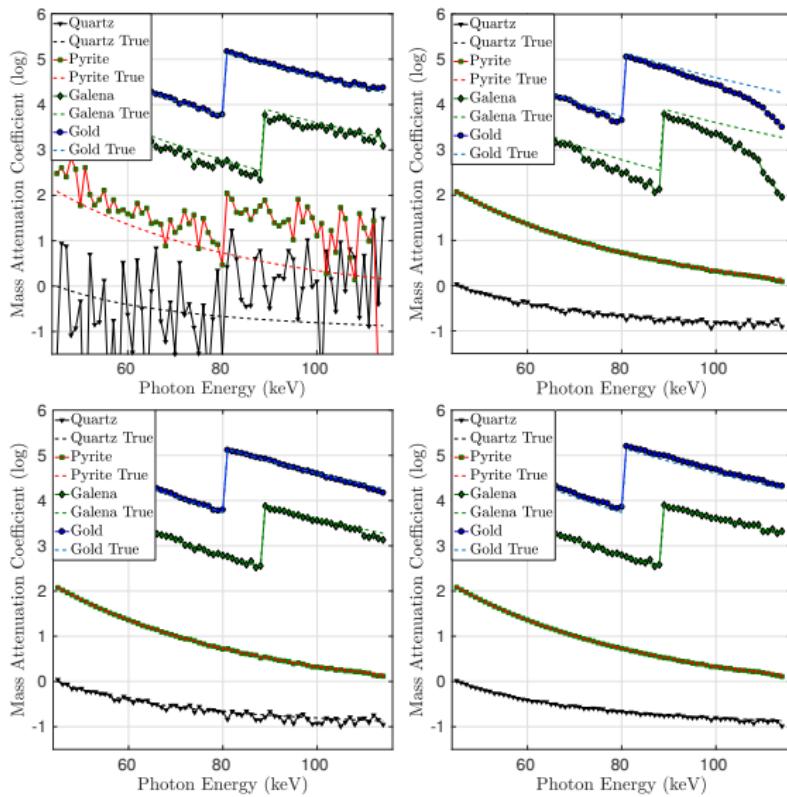


Image reconstruction with dTV-p



Reconstructed energy profiles



SNR data invariance possible solutions

Proposed: Choose a reference-channel based on SNR of data. Other parameters kept fixed to simplify comparisons.

SNR data invariance possible solutions

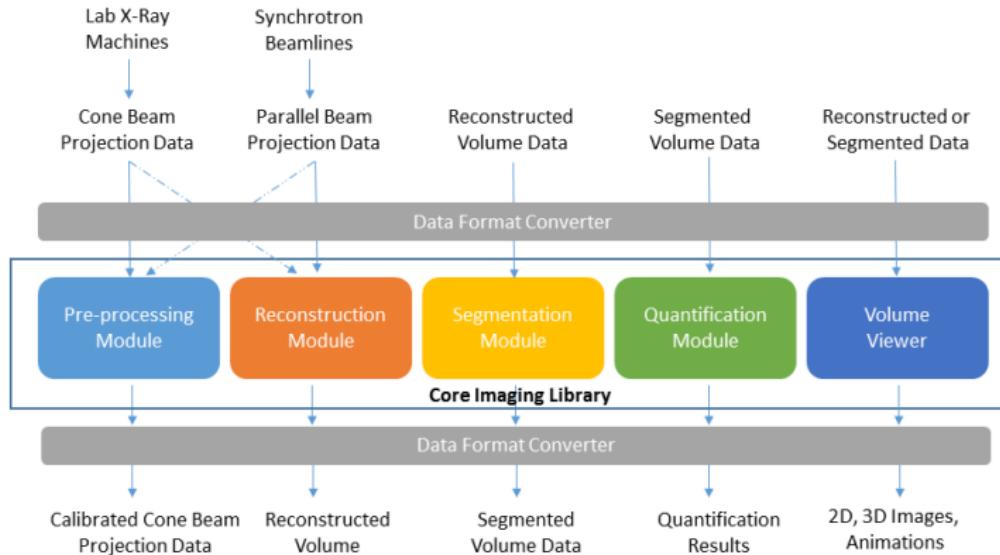
Proposed: Choose a reference-channel based on SNR of data. Other parameters kept fixed to simplify comparisons.

Other approaches to compensate for variable SNR

- Data normalization (D. Rigie, Phys. Med. Biol. 2015)
- Variable regularization parameters (A. Sawatzky et al, IEEE TMI 2014)
- Variable smoothing constant to establish gradient of the reference (preliminary tested to improve dTV-p method)
- Variable convergence parameters (methods normally converge with different rates)

Some software references

CCPi Core Imaging Library (CIL)



- CCPi website: <https://www.ccpι.ac.uk/>
- Open-source software: <https://github.com/vais-ral>
- Software supporting publication: <https://github.com/dkazanc>

CCPi Regularisation Toolkit

CCPi - Regularisation Toolkit (2D/3D CPU/GPU)

Regularisers (single-channel)

- ROF Total Variation (TV)
- Fast Gradient Projection TV
- Split Bregman TV
- Total Generalised Variation
- LLT-ROF (Higher order)
- Nonlinear Diffusion
- Anisotropic Diffusion (HO)
-

Regularisers (multi-channel)

- FGP directional TV
- Total Nuclear Variation

Inpainters

- Linear/Nonlinear diffusion
- Nonlocal vertical marching

Regularisers (time-lapse)

- to be added...

Python

Cython

Access to
High-level platforms

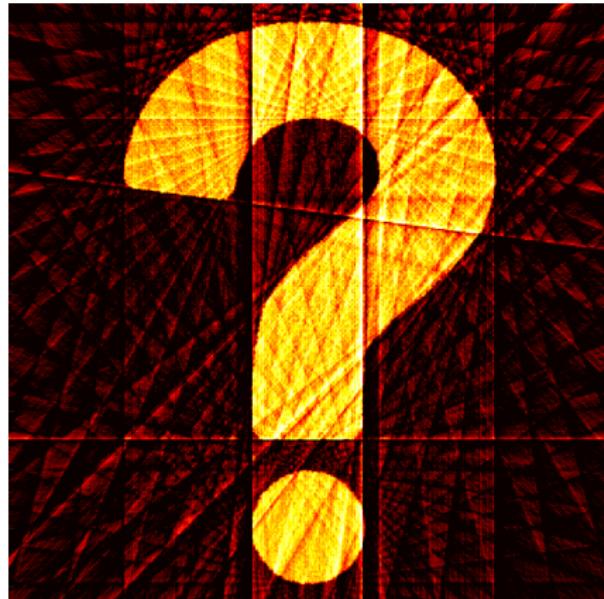
MATLAB

C-MEX

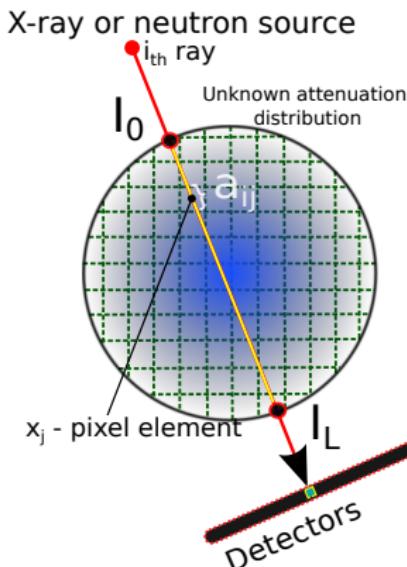
- <https://github.com/vais-ral/CCPi-Regularisation-Toolkit>
- Multi-threaded software for CPU/GPU architectures.

Questions

**Thank you!
Questions**



Collecting tomographic projection data



The basic CT measurement model: A **line** integral through the dense media

Forward (acquisition) model assumptions:

- ① No refraction or diffraction
- ② The X-rays are **monochromatic**
- ③ The linearity of Beer-Lamberts law

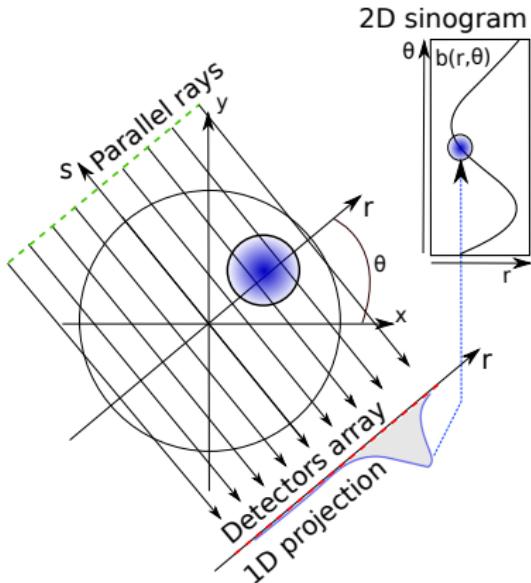
The exit beam intensity measured as:

$$\Lambda_i = I_{0,i} \exp\left(- \int_{L_i} \mu(\mathbf{r}) dl\right), \quad i = 1, \dots, m,$$

where $\mathbf{r} \in \mathbb{R}^2$ is the spatial position. Then:

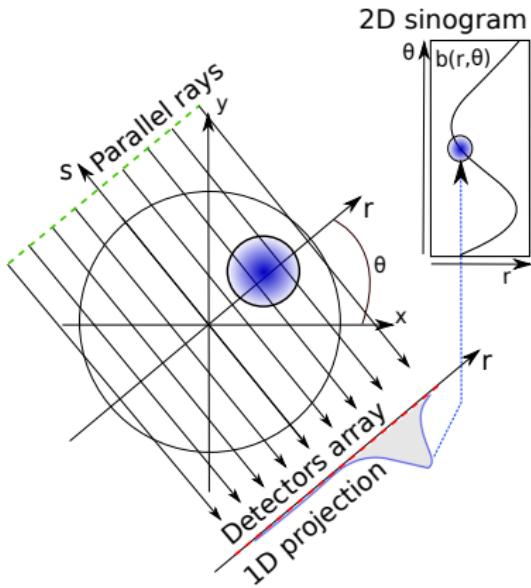
$$\int_{L_i} \mu(\mathbf{r}) dl = - \ln\left(\frac{\Lambda_i}{I_{0,i}}\right).$$

Collecting tomographic projection data

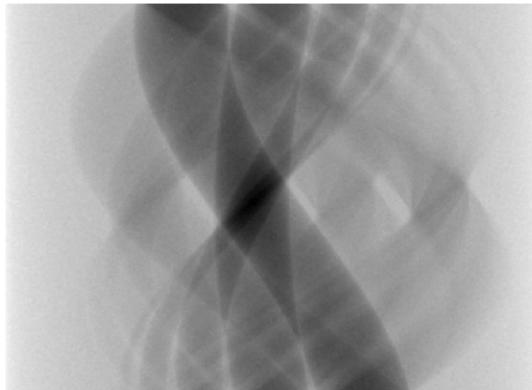


Sinogram $b(r, \theta)$ is a function of the detector's position r and the angle of acquisition θ .

Collecting tomographic projection data



Sinogram $b(r, \theta)$ is a function of the detector's position r and the angle of acquisition θ .



The measured data Y_i is modelled as a Poisson random variable with parameter Λ_i :

$$Y_i \sim \text{Poiss}\{\bar{\Lambda}_i\} = \text{Poiss}\{I_{0,i} e^{-[\mathbf{A}\mu]_i}\},$$

where attenuation coefficient on a square grid of n pixels: $\mu(\mathbf{r}) = \sum_{j=1}^n x_j \chi_j(\mathbf{r})$.