

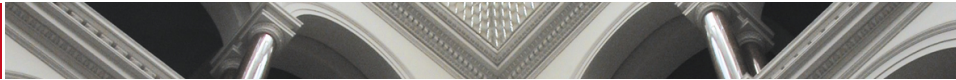
SFB F68  
Tomography Across the Scales



## Generalized Fourier Diffraction Theorem and Filtered Backpropagation for Tomographic Reconstruction

Michael Quellmalz | TU Berlin | GIP Meeting, Siegen, 25 September 2024  
joint work with Clemens Kirisits, Eric Setterqvist

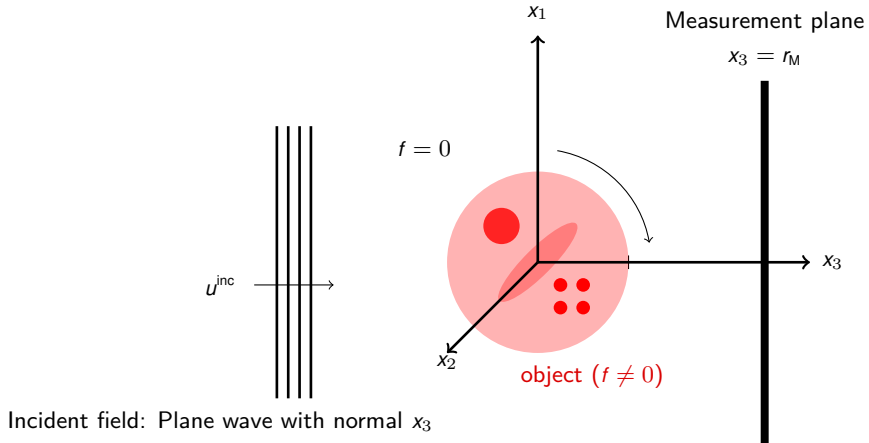
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## Outline

- 1 Introduction**
- 2 Helmholtz Equation and Fourier Diffraction Theorem
- 3 Motion of the Object
- 4 Reconstruction of the Object

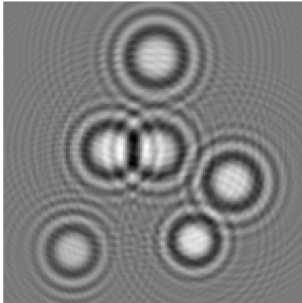
## Optical Diffraction Tomography (ODT)





## Optical Diffraction

Optical diffraction occurs when the wavelength of the incident wave is large  
 $\approx$  the size of the object ( $\mu\text{m}$  scale)



Simulation of the scattered field from  
spherical particles (size  $\approx$  wavelength)

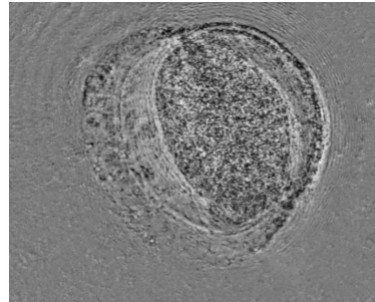


Image with diffraction  
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## Model of Optical Diffraction Tomography (for one direction)

- **We have:** field  $u^{\text{tot}}(\tilde{\mathbf{x}}, r_M)$ ,  $\tilde{\mathbf{x}} \in \mathbb{R}^{d-1}$ , at measurement plane  $x_d = r_M$
- **We want:** scattering potential  $f$  on  $\mathbb{R}^d$  with compact support
- Illumination by plane wave  $u^{\text{inc}}(\mathbf{x}) = e^{ik_0 \mathbf{x} \cdot \mathbf{s}}$  with direction  $\mathbf{s} \in \mathbb{S}^{d-1}$  and wave number  $k_0$
- Total field  $u^{\text{tot}}(\mathbf{x}) = u(\mathbf{x}) + u^{\text{inc}}(\mathbf{x})$  solves the **wave equation**

$$-(\Delta + f(\mathbf{x}) + k_0^2) u^{\text{tot}}(\mathbf{x}) = 0$$

- Rearranging yields

$$-(\Delta + k_0^2) u(\mathbf{x}) - \underbrace{(\Delta + k_0^2) u^{\text{inc}}(\mathbf{x})}_{=0} = f(\mathbf{x}) (u(\mathbf{x}) + u^{\text{inc}}(\mathbf{x}))$$

### Born approximation

Assuming  $|u| \ll |u^{\text{inc}}|$ , we obtain the Helmholtz equation

$$-(\Delta + k_0^2) u(\mathbf{x}) = f(\mathbf{x}) u^{\text{inc}}(\mathbf{x})$$



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- Helmholtz equation

$$-(\Delta + k_0^2)u(\mathbf{x}) = g(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^d \quad (1)$$

- The **outgoing solution** satisfies the Sommerfeld radiation condition

$$\lim_{r \rightarrow \infty} r^{\frac{d-1}{2}} \left( \frac{\partial u(\mathbf{x})}{\partial r} - ik_0 u(\mathbf{x}) \right) = 0$$

uniformly in  $\mathbf{s}$ , where  $\mathbf{x} = r\mathbf{s}$ ,  $r = |\mathbf{x}|$ , and  $\partial/\partial r$  denotes the radial derivative

- It has the **fundamental solution**

$$G(\mathbf{x}) = \frac{i}{4} \left( \frac{k_0}{2\pi|\mathbf{x}|} \right)^{\frac{d-2}{2}} H_{\frac{d-2}{2}}^{(1)}(k_0 |\mathbf{x}|),$$

where  $H_a^{(1)}$  is the Hankel function of the first kind and order  $a$ .

### Lemma

For  $g \in L^1(\mathbb{R}^d)$  with compact support,

$$u = g * G \in L_{loc}^1(\mathbb{R}^d) \cap S'(\mathbb{R}^d)$$

is the unique outgoing solution of the Helmholtz equation (1).

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## Some Auxiliary Lemmas

### Lemma

If  $g_n \rightarrow 0$  in  $L^1(\mathbb{R}^d)$  and  $\bigcup_n \text{supp } g_n$  is bounded, then  $g_n * G \rightarrow 0$  in  $\mathcal{S}'(\mathbb{R}^d)$ .

- Set  $\tilde{\mathcal{F}}$  as partial Fourier transform in the first  $d - 1$  coordinates
- For  $\mathbf{x} \in \mathbb{R}^d$ , set  $\tilde{\mathbf{x}} = (x_1, \dots, x_{d-1})$
- $\kappa(\mathbf{x}) := \sqrt{k_0^2 - |\mathbf{x}|^2}$ ,  $\mathbf{x} \in \mathbb{R}^{d-1}$

### Lemma

Let  $d \geq 2$ . Then  $\tilde{\mathcal{F}}G$  is given by the locally integrable function

$$\tilde{\mathcal{F}}G(\mathbf{x}) = (2\pi)^{\frac{1-d}{2}} \frac{e^{i\kappa(\tilde{\mathbf{x}})|x_d|}}{2\kappa(\tilde{\mathbf{x}})}.$$

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Define  $\mathbf{h}^\pm(\mathbf{x}) := \begin{pmatrix} \mathbf{x} \\ \pm\kappa(\mathbf{x}) \end{pmatrix} = \begin{pmatrix} \mathbf{x} \\ \pm\sqrt{k_0^2 - |\mathbf{x}|^2} \end{pmatrix}$ ,  $\mathbf{x} \in \mathbb{R}^{d-1}$  (hemisphere)

## Generalized Fourier Diffraction Theorem

[Kirisits, Q, Setterqvist 2024]

Let  $d \geq 2$  and  $g \in L^1(\mathbb{R}^d)$  has compact support. Then  $\tilde{\mathcal{F}}u$ , where  $u = g * G$ , is given by the locally integrable function

$$\tilde{\mathcal{F}}u(\mathbf{x}) = \sqrt{\frac{\pi}{2}} \frac{i}{\kappa(\tilde{\mathbf{x}})} \left( e^{i\kappa(\tilde{\mathbf{x}})x_d} \mathcal{F}((1 - \chi_{x_d})g)(\mathbf{h}^+(\tilde{\mathbf{x}})) + e^{-i\kappa(\tilde{\mathbf{x}})x_d} \mathcal{F}(\chi_{x_d}g)(\mathbf{h}^-(\tilde{\mathbf{x}})) \right),$$

where  $\tilde{\mathbf{x}} = (x_1, \dots, x_{d-1})$ ,  $\tilde{\mathcal{F}}$  is the  $d - 1$  dimensional partial Fourier transform and  $\chi_{x_d}$  is the indicator function of  $\{\mathbf{y} \in \mathbb{R}^d : y_d \geq x_d\}$ .

If  $x_d$  is sufficiently large or sufficiently small such that

$$\pm(x_d - y_d) > 0 \quad \text{for all } \mathbf{y} \in \text{supp } g,$$

then

$$\tilde{\mathcal{F}}u(\mathbf{x}) = \sqrt{\frac{\pi}{2}} \frac{ie^{\pm i\kappa(\tilde{\mathbf{x}})x_d}}{\kappa(\tilde{\mathbf{x}})} \hat{g}(\mathbf{h}^\pm(\tilde{\mathbf{x}})).$$

## (Classical) Fourier Diffraction Theorem

Additional assumptions:

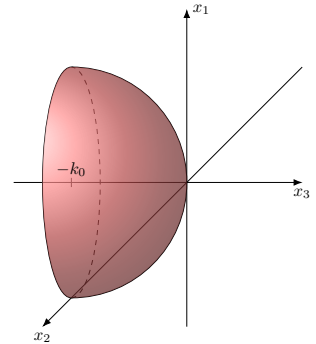
- the incident field is a plane wave  $u^{\text{inc}}(\mathbf{x}) = e^{ik_0 \mathbf{x} \cdot \mathbf{s}}$
- the measurement plane  $x_d = r_M$  not intersect  $\text{supp } f$

Then

$$\sqrt{\frac{2}{\pi}} \kappa i e^{-i\kappa r_M} \underbrace{\tilde{\mathcal{F}} u(\tilde{\mathbf{x}}, r_M)}_{\text{measured}} = \mathcal{F}f(\mathbf{h}(\tilde{\mathbf{x}}) - k_0 \mathbf{s}), \quad \tilde{\mathbf{x}} \in \mathbb{R}^{d-1},$$

where  $\mathbf{h}(\tilde{\mathbf{x}}) := \begin{pmatrix} \tilde{\mathbf{x}} \\ \kappa \end{pmatrix}$  and  $\kappa = \sqrt{k_0^2 - |\tilde{\mathbf{x}}|^2}$ .

Formula well-known from [Wolf 1969] [Natterer Wuebbeling 2001] [Kak Slaney 2001]



Semisphere  $\mathbf{h}(\mathbf{k})$  of available data in Fourier space

## Focused Beams

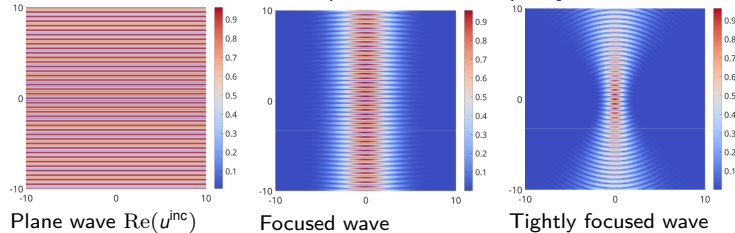
- The generalized version allows for other incidence fields
- For an incident Herglotz wave

$$u^{\text{inc}}(\mathbf{r}) = \int_{\mathbb{S}^{d-1}} a(\mathbf{s}) e^{ik_0 \mathbf{s} \cdot \mathbf{r}} d\mathbf{s}(\mathbf{s}), \quad \text{where } a \in L^2(\mathbb{S}^{d-1}),$$

it yields

$$\tilde{\mathcal{F}}u(\mathbf{x}, r_M) = \sqrt{\frac{\pi}{2}} \frac{ie^{\pm i\kappa(\mathbf{x})r_M} k_0^2}{\kappa(\mathbf{x})} \int_{\mathbb{S}^{d-1}} a(\mathbf{s}) \hat{f}(\mathbf{h}^\pm(\mathbf{x}) - k_0 \mathbf{s}) d\mathbf{s}(\mathbf{s}).$$

- Reconstruction algorithms for focused beams (see images below) in [\[Kirisits Naujoks Scherzer 2024\]](#)





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## Moving the Object and Incidence Direction

- Rigid motion of the object causes scattering potential  $f(R_t(\mathbf{x} - \mathbf{d}_t))$  with
  - Rotation  $R_t \in \text{SO}(d)$  (with  $R_0 := \text{id}$ )
  - Translation  $\mathbf{d}_t \in \mathbb{R}^d$  (with  $\mathbf{d}_0 := \mathbf{0}$ )
- Incidence direction  $\mathbf{s}_t \in \mathbb{S}^{d-1}$
- Position of the measurement plane is kept fixed (equivalent to moving object and incidence simultaneously)

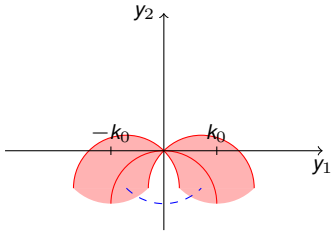
## Fourier diffraction theorem (with motion)

The quantity

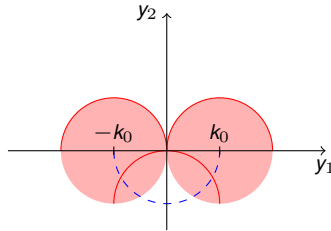
$$\mu_t(\mathbf{x}) := \sqrt{\frac{2}{\pi}} \kappa_t e^{-i\kappa_t r_M} \tilde{\mathcal{F}}u(\mathbf{k}, r_M) = \mathcal{F}f(\underbrace{R_t \mathbf{h}(\mathbf{x}) - k_0 \mathbf{s}_t}_{\text{Fourier cover}}) e^{-i\langle \mathbf{d}_t, \mathbf{h}(\mathbf{x}) \rangle}, \quad \|\mathbf{x}\| < k_0,$$

depends only on the measurements of  $u$ .

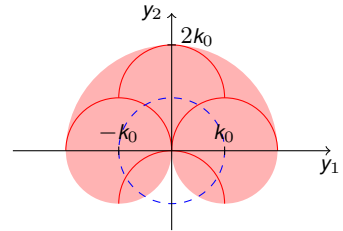
## Fourier Cover: Angle Scan



Quarter turn  $t \in [\pi/4, 3\pi/4]$



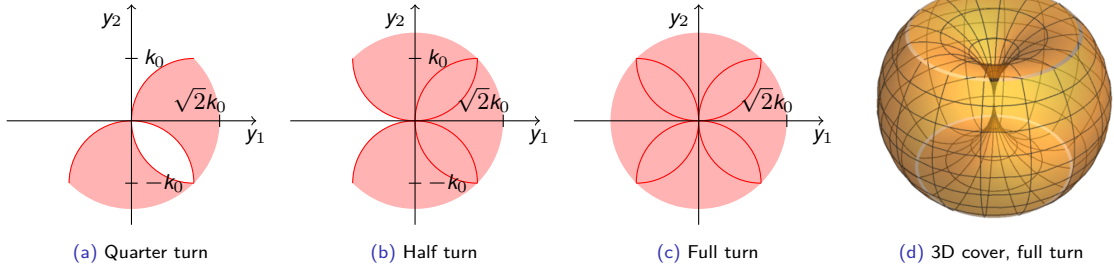
Half turn  $t \in [0, \pi]$



Full turn  $t \in [0, 2\pi]$

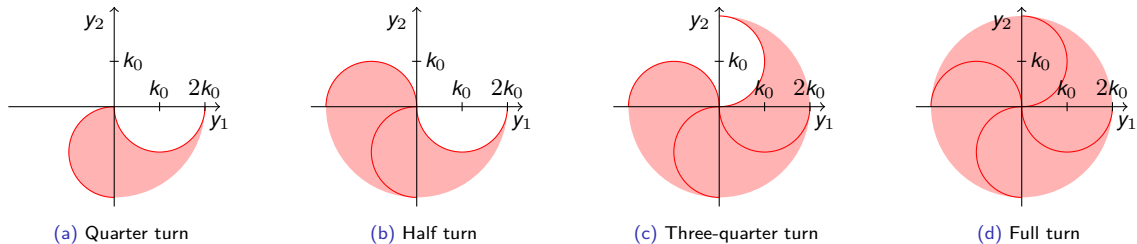
2D Fourier coverage for incidence direction  $\mathbf{s}(t) = (\cos t, \sin t)$ . Measurements are taken at  $r_2 = r_M$ . The Fourier coverage (light red) is a union of infinitely many semicircles, whose centers lie on the dashed blue curve.

## Fourier coverage: Object Rotation (Incidence Parallel to Measurement Plane)

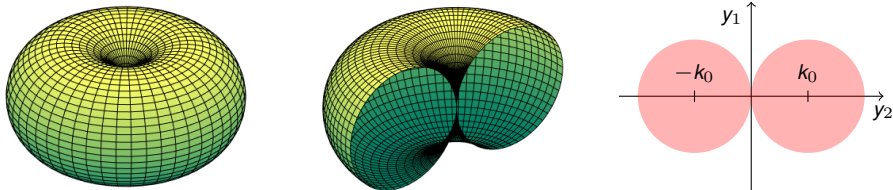


**Figure:** 2D Fourier coverage for a rotating object, incidence direction  $\mathbf{s} = (0, 1)$  and measurements taken at  $r_2 = r_M$ . The Fourier coverage (light red) is a union of infinitely many semicircles, some of which are depicted in red.  
 (d): 3D Fourier coverage for incidence  $\mathbf{s} = (0, 0, 1)$  and rotation around first axis.

## Fourier Cover: Object Rotation (Incidence Perpendicular to Measurement Plane)

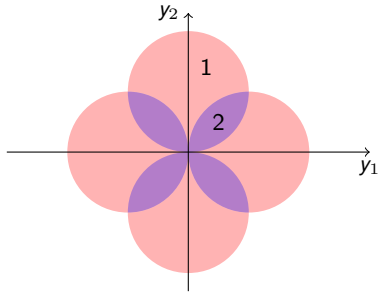


**Figure:** 2D Fourier coverage for a rotating object, incidence direction  $\mathbf{s} = (1, 0)$  and measurements taken at  $r_2 = r_M$ .

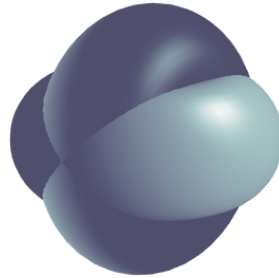


**Figure:** 3D Fourier coverage for a full rotation of the object about the  $r_1$ -axis with incidence direction  $\mathbf{s} = (0, 1, 0)$ .

## Fourier cover: Angle scan & Rotation



2D Fourier cover  
(colors represent Banch indicatrix)



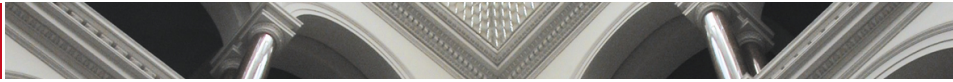
3D Fourier cover

- Incidence is rotated along a half circle
- and the experiment is repeated with the object rotated by  $90^\circ$ .



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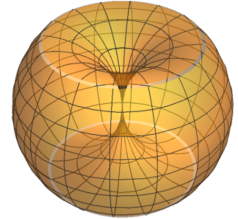


## Approach 1: Filtered Backpropagation

**Idea:** Inverse Fourier transform of  $\mathcal{F}f$  restricted to the set of available data  $\mathcal{Y}$ ,

$$f_{\text{bp}}(\mathbf{r}) := (2\pi)^{-\frac{d}{2}} \int_{\mathcal{Y}} \mathcal{F}f(\mathbf{y}) e^{i\mathbf{y}\cdot\mathbf{r}} d\mathbf{y}$$

with the transformation  $T(\mathbf{x}, t) := R_t \mathbf{h}(\mathbf{x})$



### Theorem

[Kirisits, Q, Setterqvist 2024]

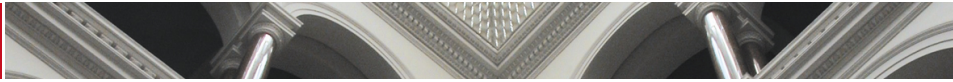
Let the rotation  $R_t \in SO(d)$ , translation  $\mathbf{d}_t$  and incidence  $\mathbf{s}_t \in \mathbb{S}^{d-1}$  be piecewise  $C^1$ . Then

$$f_{\text{bp}}(\mathbf{r}) = (2\pi)^{-\frac{d}{2}} \int_0^T \int_{B_{\kappa_0}} \mathcal{F}f(T(\mathbf{x}, t)) e^{i\mathcal{T}(\mathbf{x}, t)\cdot(\mathbf{r}+\mathbf{d}_t)} \frac{|\det \nabla T(\mathbf{x}, t)|}{\text{Card } T^{-1}(T(\mathbf{x}, t))} d\mathbf{x} dt,$$

where  $\det \nabla T(\mathbf{x}, t) = \frac{k_0(t)k_0'(t) - R_t \mathbf{h}(\mathbf{x}, t) (k_0(t)R_t \mathbf{s}_t)'}{\kappa}$ .

Banach indicatrix  $\text{Card}(T^{-1}(\mathbf{y}))$  needs to be estimated (except for special cases).

Well-known for rotation around coordinate axis [Devaney 1982]

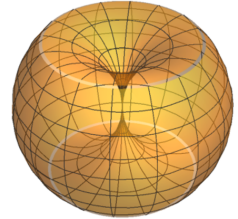


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where  $\det \nabla T(\mathbf{x}, t) = \frac{k_0(t)k_0'(t) - R_t \mathbf{h}(\mathbf{x}, t) (k_0(t)R_t \mathbf{s}_t)'}{\kappa}$ .

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## Discretization

- Object  $f(\mathbf{x}_k)$  with  $\mathbf{x}_k = \mathbf{k} \frac{2L_S}{K}$ ,  $\mathbf{k} \in \mathcal{I}_K^d := \{-K/2, \dots, K/2 - 1\}^d$
- Measurements  $u_{t_m}^{\text{tot}}(\mathbf{y}_n, r_M)$  with  $\mathbf{y}_n = \mathbf{n} \frac{2L_M}{N}$ ,  $\mathbf{n} \in \mathcal{I}_N^{d-1}$
- discrete Fourier transform (DFT)

$$[\mathbf{F}_{\text{DFT}} u_{t_m}]_{\boldsymbol{\ell}} := \sum_{\mathbf{n} \in \mathcal{I}_N^{d-1}} u_{t_m}(\mathbf{y}_n, r_M) e^{-2\pi i \mathbf{n} \cdot \boldsymbol{\ell} / N}, \quad \boldsymbol{\ell} \in \mathcal{I}_N^{d-1},$$

- Non-uniform discrete Fourier transform (NDFT)

$$[\mathbf{F}_{\text{NDFT}} \mathbf{f}]_{m, \boldsymbol{\ell}} := \sum_{\mathbf{k} \in \mathcal{I}_K^d} f_{\mathbf{k}} e^{-i \mathbf{x}_{\mathbf{k}} \cdot (R_{t_m} \mathbf{h}(\mathbf{y}_{\boldsymbol{\ell}}))}, \quad m \in \mathcal{J}_M, \boldsymbol{\ell} \in \mathcal{I}_N^{d-1}$$

## Discretized forward operator

$$\mathbf{D}^{\text{tot}} \mathbf{f} := \mathbf{F}_{\text{DFT}}^{-1}(\mathbf{c} \odot \mathbf{F}_{\text{NDFT}} \mathbf{f}) + e^{i k_0 r_M}, \quad \mathbf{f} \in \mathbb{R}^{K^d},$$

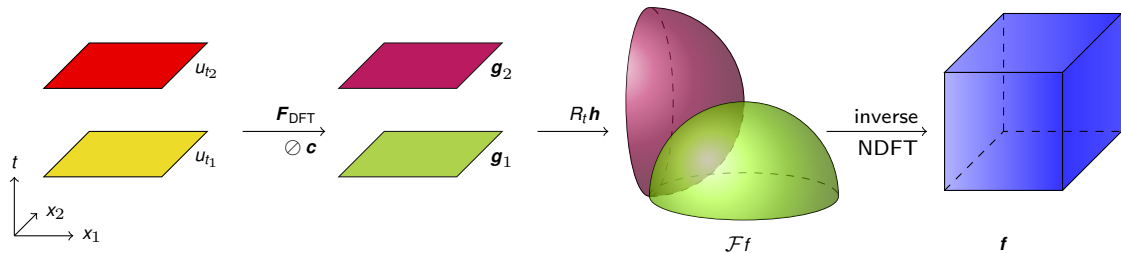
where  $\mathbf{c} = \left[ \frac{i}{\kappa(\mathbf{y}_{\boldsymbol{\ell}})} e^{i \kappa(\mathbf{y}_{\boldsymbol{\ell}}) r_M} \left(\frac{N}{L_M}\right)^{d-1} \left(\frac{L_S}{K}\right)^d \right]_{\boldsymbol{\ell} \in \mathcal{I}_N^{d-1}}$

## Reconstruction of $f$

Inverse

$$f \approx \mathbf{F}_{\text{NDFT}}^{-1} \left( (\mathbf{F}_{\text{DFT}} \mathbf{u}^{\text{tot}} - e^{ik_0 r_M}) \oslash \mathbf{c} \right)$$

Crucial part: inversion of NDFT  $\mathbf{F}_{\text{NDFT}}^{-1}$



## Approach 2: Conjugate Gradient (CG) Method

- Conjugate Gradients (CG) on the normal equations

$$\arg \min_{\mathbf{f} \in \mathbb{R}^{K^3}} \|\mathbf{F}_{\text{NDFT}}(\mathbf{f}) - \mathbf{g}\|_2^2$$

- NFFT (Non-uniform fast Fourier transform) for computing  $\mathbf{F}_{\text{NDFT}}(\mathbf{f})$  in  $\mathcal{O}(N^3 \log N)$  steps

[Dutt Rokhlin 93], [Beylkin 95], [Potts Steidl Tasche 01], [Potts Kunis Keiner 04+]

## Approach 3: TV (Total Variation) Regularization

- Regularized inverse

$$\arg \min_{\mathbf{f} \in \mathbb{R}^{K^3}} \chi_{\mathbb{R}_{\geq 0}^{K^3}}(\mathbf{f}) + \frac{1}{2} \|\mathbf{F}_{\text{NDFT}}(\mathbf{f}) - \mathbf{g}\|_2^2 + \lambda \text{TV}(\mathbf{f}),$$

- Primal-dual (PD) iteration [Chambolle & Pock 2010]
- Adaptive selection of step sizes [Yokota & Hontani 2017]

## Approach 2: Conjugate Gradient (CG) Method

- Conjugate Gradients (CG) on the normal equations

$$\arg \min_{\mathbf{f} \in \mathbb{R}^{K^3}} \|\mathbf{F}_{\text{NDFT}}(\mathbf{f}) - \mathbf{g}\|_2^2$$

- NFFT (Non-uniform fast Fourier transform) for computing  $\mathbf{F}_{\text{NDFT}}(\mathbf{f})$  in  $\mathcal{O}(N^3 \log N)$  steps

[Dutt Rokhlin 93], [Beylkin 95], [Potts Steidl Tasche 01], [Potts Kunis Keiner 04+]

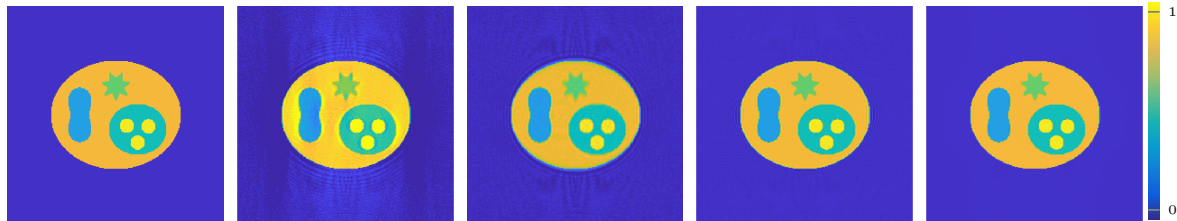
## Approach 3: TV (Total Variation) Regularization

- Regularized inverse

$$\arg \min_{\mathbf{f} \in \mathbb{R}^{K^3}} \chi_{\mathbb{R}_{\geq 0}^{K^3}}(\mathbf{f}) + \frac{1}{2} \|\mathbf{F}_{\text{NDFT}}(\mathbf{f}) - \mathbf{g}\|_2^2 + \lambda \text{TV}(\mathbf{f}),$$

- Primal-dual (PD) iteration [Chambolle & Pock 2010]
- Adaptive selection of step sizes [Yokota & Hontani 2017]

## 3D Reconstruction: Moving Rotation Axis



Ground truth  $f$   
( $240 \times 240 \times 240$  grid)

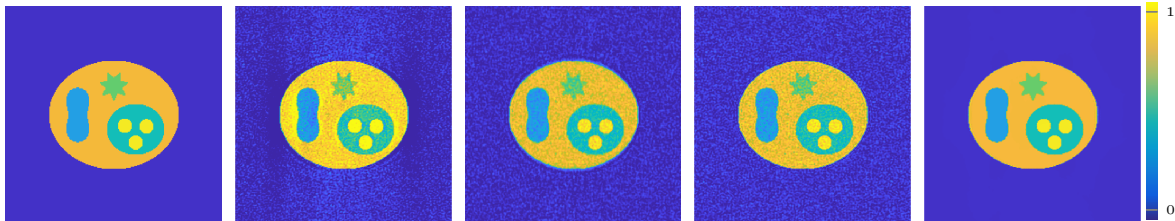
Backpropagation  
PSNR 24.17  
SSIM 0.171  
5 s

Backpropagation  
(with inticatrix estimation)  
PSNR 31.84  
SSIM 0.350  
5 s + 22 s precompute

CG Reconstruction  
PSNR 35.84  
SSIM 0.962  
82 s

TV ( $\lambda = 0.02$ )  
PSNR 40.95  
SSIM 0.972  
1395 s

## 3D Reconstruction: Moving Rotation Axis and 5% Gaussian Noise



Ground truth  $f$

Backpropagation  
PSNR 21.19  
SSIM 0.075

Backpropagation  
(with indicatrix estimation)  
PSNR 25.50  
SSIM 0.157

CG Reconstruction  
PSNR 24.10  
SSIM 0.193

TV ( $\lambda = 0.05$ )  
PSNR 38.01  
SSIM 0.772

## Conclusions

- Generalized Fourier diffraction theorem on  $L^1(\mathbb{R}^d)$
- Filtered backpropagation formula for a wide range of experimental setups
- Compared image reconstruction methods






## Conclusions

- Generalized Fourier diffraction theorem on  $L^1(\mathbb{R}^d)$
- Filtered backpropagation formula for a wide range of experimental setups
- Compared image reconstruction methods

Thank you for your attention!



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## Estimation of the Banach indicatrix

- Banach indicatrix  $\text{Card}(T_{\pm}^{-1}(\mathbf{y}))$  counts how often a point  $\mathbf{y} \in \mathbb{B}_{2k_0}^d$  is “hit” by  $T_+$ .
- In a discrete setting, it is unlikely that a point  $\mathbf{y}$  is exactly hit by any grid point  $T_+(\tilde{\mathbf{x}}_m, t_n)$ .
- The coverage for fixed time  $t$  is the hemisphere

$$\{T_+(\tilde{\mathbf{x}}, t) : \tilde{\mathbf{x}} \in \mathbb{B}_{k_0}^{d-1}\} = \{\mathbf{z} \in \mathbb{R}^d : \|\mathbf{z} + k_0(t)R_t\mathbf{s}_t\| = k_0(t), \mathbf{z} \cdot R_t\mathbf{e}^d > -k_0(t)\mathbf{s}_t \cdot \mathbf{e}^d\},$$

which moves continuously with  $t$ .

- Idea: a point  $\mathbf{y}$  is hit by  $T_+$  between the time steps  $t_{n-1}$  and  $t_n$ , if the sign of  $\|\mathbf{y} - R_t\mathbf{s}_t\| - k_0(t)$  changes between these time steps. We use the approximation

$$\text{Card}(T_+^{-1}(\mathbf{y})) \approx \sum_{n=1}^N \frac{\chi(n)}{2} |\text{sgn}(\|\mathbf{y} + k_0(t_{n-1})R_{t_{n-1}}\mathbf{s}_{t_{n-1}}\| - k_0(t_{n-1})) - \text{sgn}(\|\mathbf{y} + k_0(t_n)R_{t_n}\mathbf{s}_{t_n}\| - k_0(t_n))|,$$

where

$$\chi(n) := \begin{cases} 1, & \text{if } \mathbf{y} \cdot (R_t\mathbf{e}^d) > -k_0(t)\mathbf{s}_{t_n} \cdot \mathbf{e}^d, \\ 0, & \text{otherwise.} \end{cases}$$

with the sign function  $\text{sgn}(x) := \frac{x}{|x|}$  for  $x \neq 0$  and  $\text{sgn}(0) := 0$ .