

SFB F68  
Tomography Across the Scales



## Motion Detection in Diffraction Tomography

Michael Quellmalz | TU Berlin | Chemnitz Summer School on Applied Analysis, 16 September 2024  
joint work with Robert Beinert, Peter Elbau, Clemens Kirisits, Monika Ritsch-Martens, Otmar Scherzer, Eric Setterqvist, Gabriele Steidl

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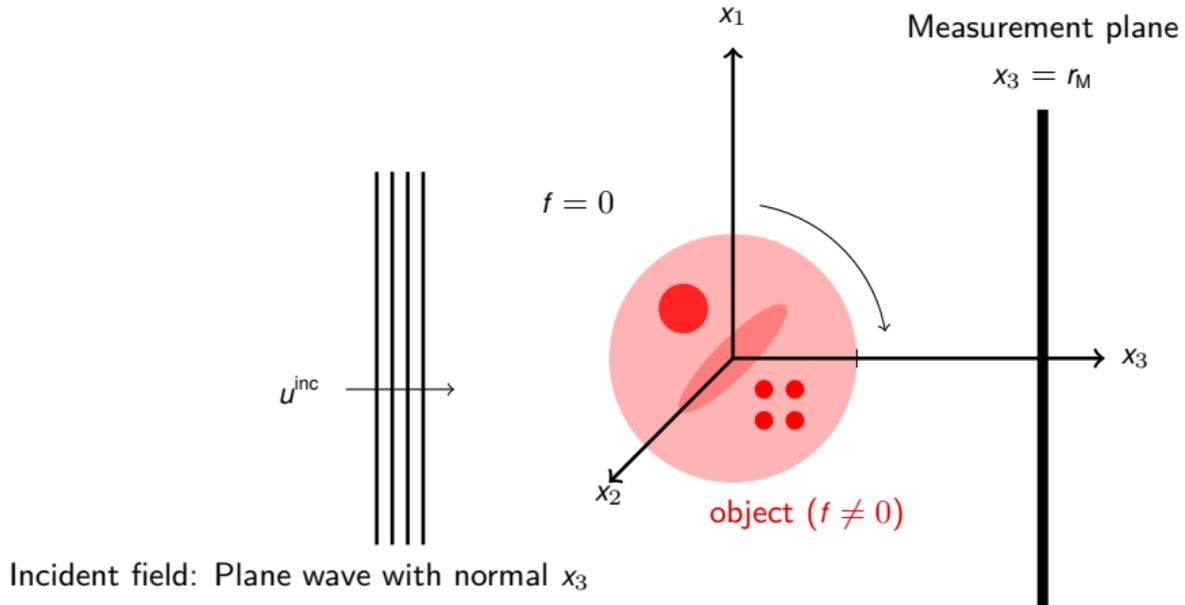
## Outline

### 1 Introduction

### 2 Reconstruction of the object

### 3 Reconstructing the motion

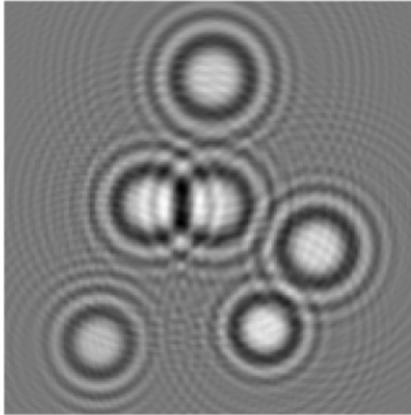
## Optical Diffraction Tomography (ODT)





## 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)

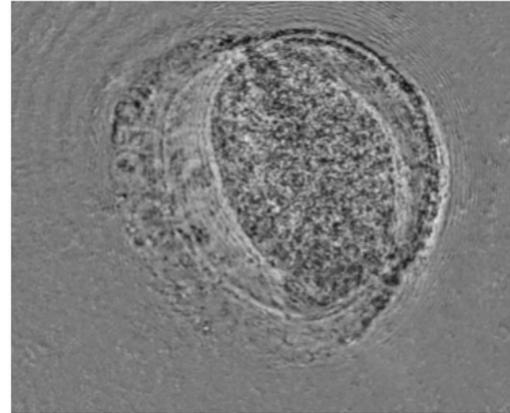


Image with diffraction  
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## Model of Optical Diffraction Tomography (for one direction)

- **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

$$-(\Delta + k_0^2) u(\mathbf{x}) = f(\mathbf{x}) u^{\text{inc}}(\mathbf{x}) \quad (1)$$

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## Fourier diffraction theorem

Let

- $u$  be the outgoing solution of the Helmholtz equation (1),
- $f \in L^1(\mathbb{R}^d)$  have compact support,
- the incident field  $u^{\text{inc}}(\mathbf{x}) = e^{ik_0 \mathbf{x} \cdot \mathbf{s}}$ , and
- the measurement plane  $x_d = r_M$  not intersect  $\text{supp } f$ .

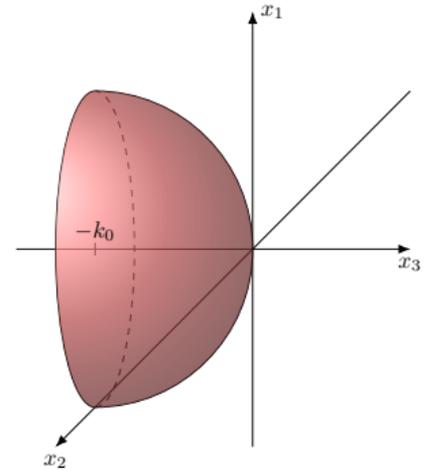
Then

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

where  $\tilde{\mathcal{F}}$  is the Fourier transform in  $d - 1$  coordinates,  $\mathbf{h}(\tilde{\mathbf{x}}) := \begin{pmatrix} \tilde{\mathbf{x}} \\ \kappa \end{pmatrix}$  and

$$\kappa := \sqrt{k_0^2 - |\tilde{\mathbf{x}}|^2}.$$

based on [Wolf 1969] [Natterer Wuebbeling 2001] [Kak Slaney 2001]  
this  $L^1$  version from [Kirisits Q. Setterqvist 2024]



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



## Rigid Motion of the Object

- Scattering potential of the **moved object**:  $f(R_t(\mathbf{x} - \mathbf{d}_t))$
- 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  $\mathbf{s}_t \in \mathbb{S}^{d-1}$

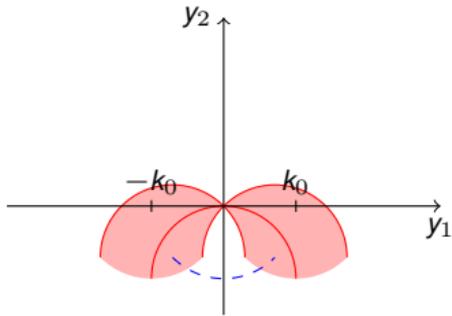
## Fourier diffraction theorem (with motion)

The quantity

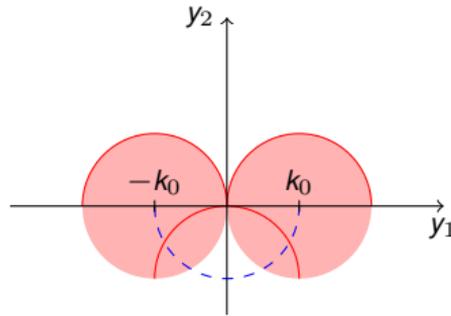
$$\mu_t(\mathbf{x}) := \sqrt{\frac{2}{\pi}} \kappa i e^{-i\kappa r_M} \tilde{\mathcal{F}}u(\mathbf{k}, r_M) = \mathcal{F}f(\underbrace{R_t \mathbf{h}(\mathbf{x}) - k_0 \mathbf{s}_t}_{\text{Fourier cover}}) e^{-i\langle \mathbf{d}_t, \mathbf{h}(\mathbf{x}) \rangle}, \quad \|\mathbf{x}\| < k_0,$$

depends only on the measurements of  $u$ .

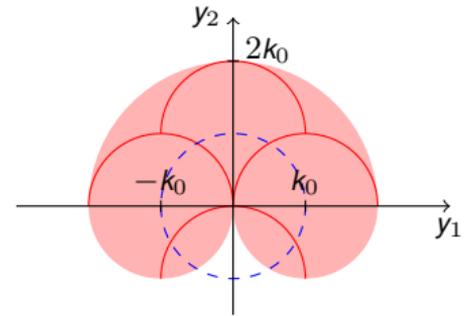
## Fourier cover: Angle scan



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



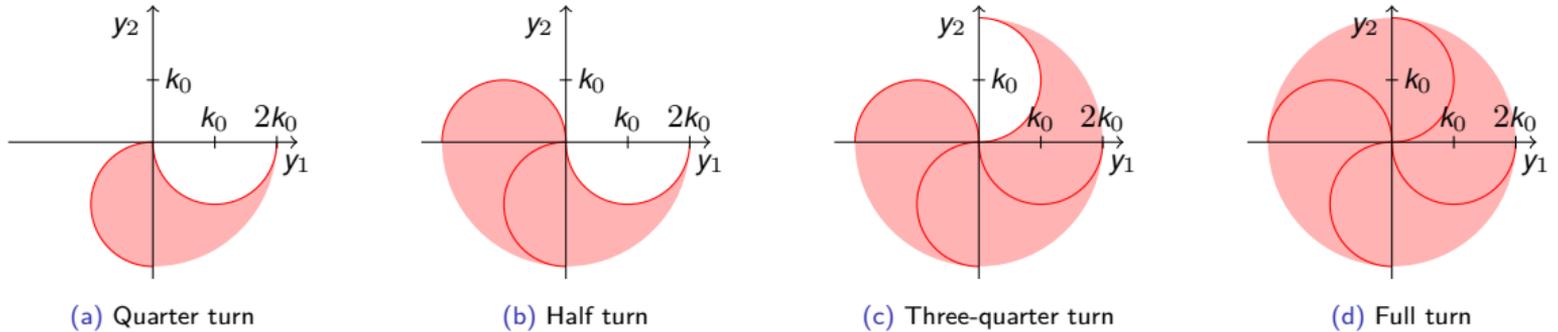
Half turn  $t \in [0, \pi]$



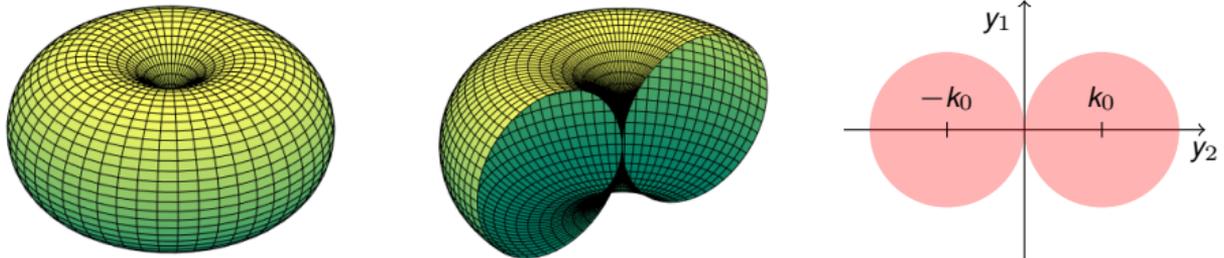
Full turn  $t \in [0, 2\pi]$

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 cover: Object rotation



**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  $\mathbf{s} = (0, 1, 0)$ .



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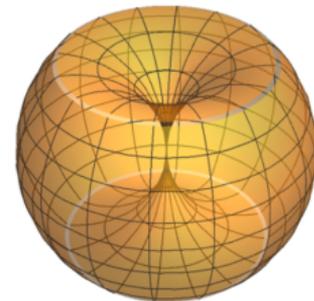


## Approach 1: Filtered Backpropagation

**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).

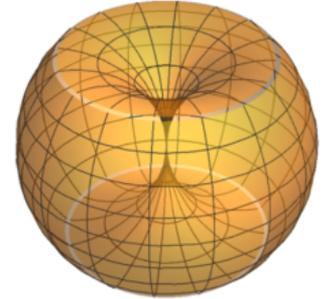
Well-known for rotation around coordinate axis [Devaney 1982]

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## 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

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

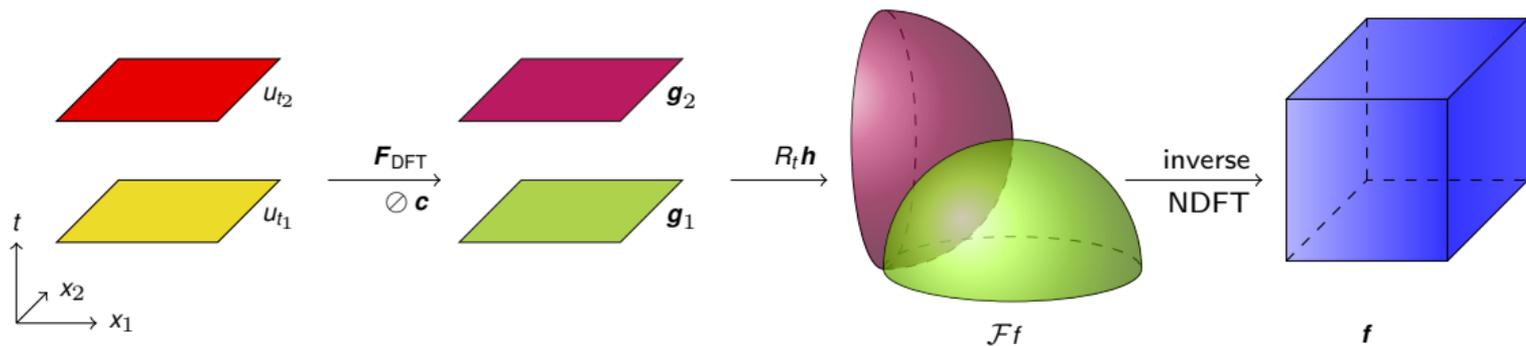
where  $\mathbf{c} = \left[ \frac{i}{\kappa(\mathbf{y}_{\boldsymbol{\ell}})} e^{i \kappa(\mathbf{y}_{\boldsymbol{\ell}}) r_M} \left(\frac{N}{L_M}\right)^{d-1} \left(\frac{L_S}{K}\right)^d \right]_{\boldsymbol{\ell} \in \mathcal{I}_N^{d-1}}$

## 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]

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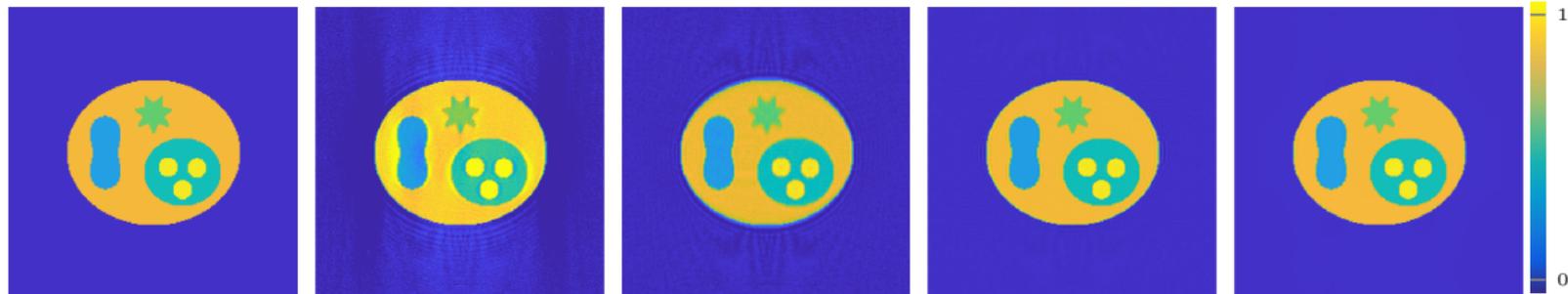
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## 3D Reconstruction: Moving Rotation Axis



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

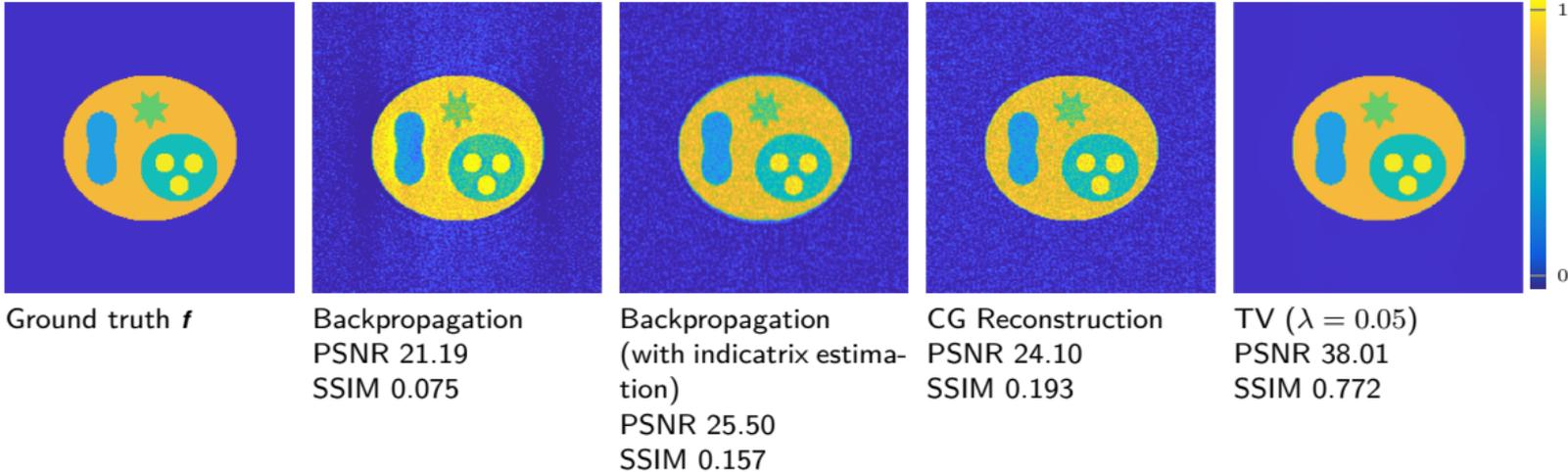
Backpropagation  
PSNR 24.17  
SSIM 0.171  
5 s

Backpropagation  
(with intermatrix estima-  
tion)  
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





## Outline

① Introduction

② Reconstruction of the object

③ **Reconstructing the motion**

## Formal Uniqueness Result

### Theorem

[Kurlberg Zickert 2021]

Let

- the matrix of second-order moments of  $f$  have distinct, real eigenvalues,
- certain third-order moments do not vanish,
- the translation  $\mathbf{d}_t$  be restricted to a known plane,
- the rotations  $R_t$  cover  $SO(3)$ .

Then  $f$  is uniquely determined given the diffraction images  $u_t$  for all (unknown) motions.

We find an algorithm to recover the rotations and translations

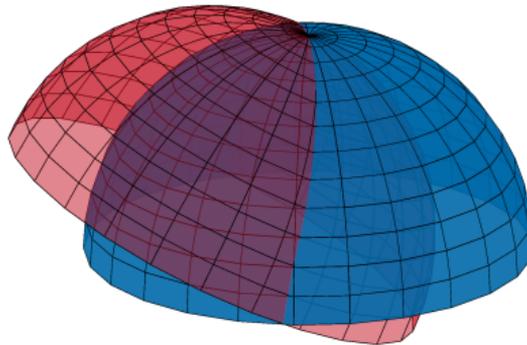


## Detection of the Rotation in 3D

**Goal:** Estimate the rotation  $R_t$  from the transformed measurements  $\nu_t(\mathbf{k}) = |\mathcal{F}f(R_t\mathbf{h}(\mathbf{k}))|^2$

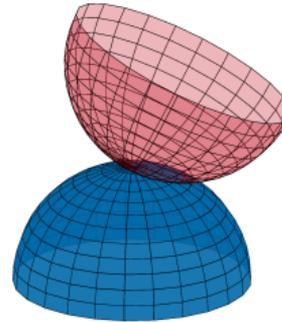
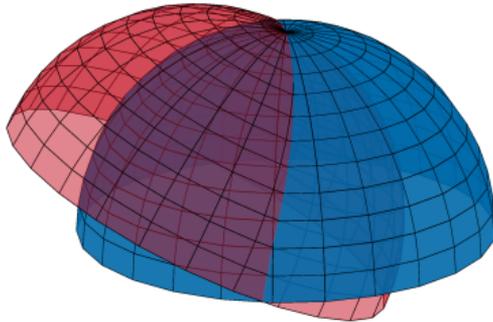
**Common circle approach:**

- For each  $t$  we have the Fourier data  $\mathcal{F}f$  on one hemisphere
- Two hemispheres intersect in a circle (arc), where  $\mathcal{F}f$  must agree
- Find the common circle of two hemispheres



## Dual Common Circles

- $f$  real-valued (no absorption)
- Additional symmetry  $\mathcal{F}f(\mathbf{y}) = \overline{\mathcal{F}f(-\mathbf{y})}$
- Additional pair of “dual” common circles



For  $\varphi \in [0, 2\pi)$ ,  $\theta \in [0, \pi]$ , we can parameterize the common circles in the 2D data by

$$\begin{aligned}\gamma^{\varphi, \theta}(\beta) &:= \frac{k_0}{2} \sin(\theta)(\cos(\beta) - 1) \begin{pmatrix} \cos(\varphi) \\ \sin(\varphi) \end{pmatrix} + k_0 \cos(\frac{\theta}{2}) \sin(\beta) \begin{pmatrix} -\sin(\varphi) \\ \cos(\varphi) \end{pmatrix}, \quad \beta \in \mathbb{R}, \\ \check{\gamma}^{\varphi, \theta}(\beta) &:= -\frac{k_0}{2} \sin(\theta)(\cos(\beta) - 1) \begin{pmatrix} \cos(\varphi) \\ \sin(\varphi) \end{pmatrix} - k_0 \sin(\frac{\theta}{2}) \sin(\beta) \begin{pmatrix} -\sin(\varphi) \\ \cos(\varphi) \end{pmatrix}, \quad \beta \in \mathbb{R}.\end{aligned}$$

### Theorem (unique reconstruction)

[Q. Elbau Scherzer Steidl 2024]

Let  $s, t \in [0, T]$ . Assume that there exist unique angles  $\varphi, \psi \in \mathbb{R}/(2\pi\mathbb{Z})$  and  $\theta \in [0, \pi]$  such that

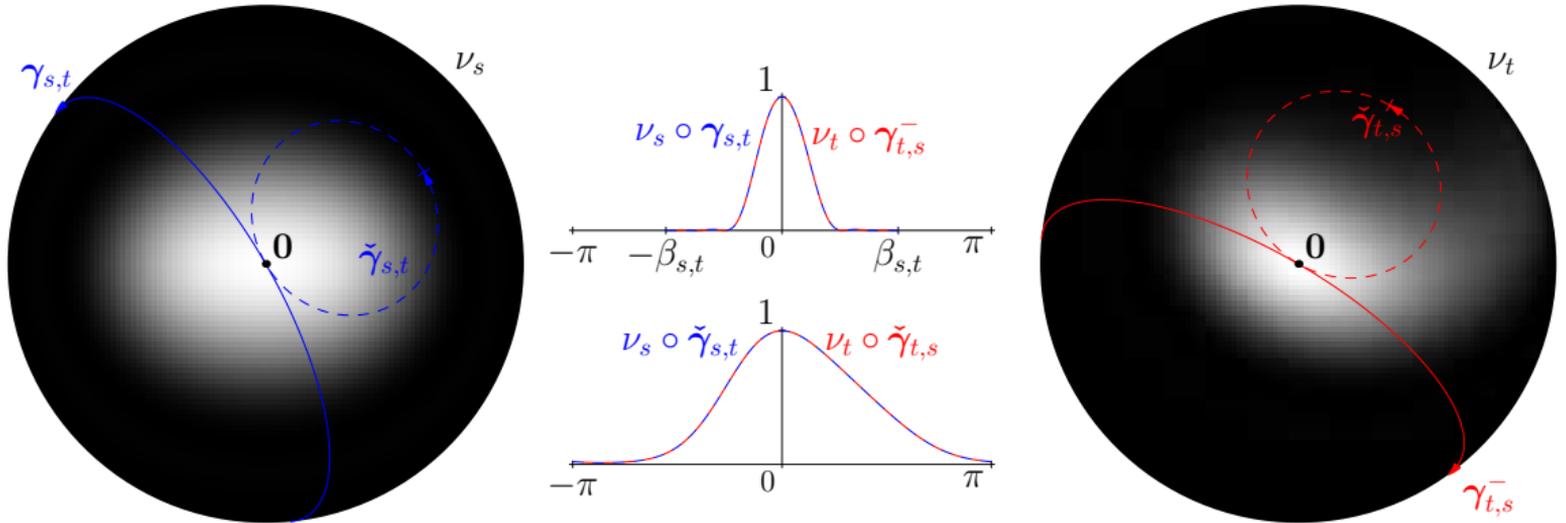
$$\begin{aligned}\nu_s(\gamma^{\varphi, \theta}(\beta)) &= \nu_t(\gamma^{\pi - \psi, \theta}(-\beta)) \quad \forall \beta \in [-\frac{\pi}{2}, \frac{\pi}{2}] \quad \text{and} \\ \nu_s(\check{\gamma}^{\varphi, \theta}(\beta)) &= \nu_t(\check{\gamma}^{\pi - \psi, \theta}(\beta)) \quad \forall \beta \in [-\frac{\pi}{2}, \frac{\pi}{2}].\end{aligned}$$

Then the relative rotation  $R_s^\top R_t$  is uniquely determined by the Euler angles

$$R_s^\top R_t = Q^{(3)}(\varphi) Q^{(2)}(\theta) Q^{(3)}(\psi),$$

where  $Q^{(i)}(\alpha)$  denotes the rotation around the  $i$ -th coordinate with angle  $\alpha$ .

## Visualization of the Common Arcs



Here  $\gamma_{s,t} := \gamma^{\varphi,\theta}$  and  $\gamma_{t,s} := \gamma^{\pi-\psi,\theta}$  for  $R_s^\top R_t = Q^{(3)}(\varphi) Q^{(2)}(\theta) Q^{(3)}(\psi)$

## Infinitesimal Common Circles Method

### Theorem

[Q. Elbau Scherzer Steidl 2024]

Let the rotation  $R \in C^1([0, T] \rightarrow SO(3))$  and  $t \in (0, T)$ .

We define the associated **angular velocity** as the vector  $\omega_t \in \mathbb{R}^3$  satisfying

$$R_t^\top R_t' \mathbf{y} = \omega_t \times \mathbf{y}, \quad \mathbf{y} \in \mathbb{R}^3,$$

and write it in cylindrical coordinates

$$\omega_t = \begin{pmatrix} \rho \cos \varphi \\ \rho \sin \varphi \\ \zeta \end{pmatrix}.$$

Then

$$-r \partial_t \nu_t(r\varphi) = \left( \left( \sqrt{k_0^2 - r^2} - k_0 \right) \rho + r\zeta \right) \partial_\varphi \nabla \nu_t \begin{pmatrix} r \cos \varphi \\ r \sin \varphi \end{pmatrix} \quad \forall r \in (-k_0, k_0).$$

## Reconstructing the Translation

Recall: Data  $\mu_t(\mathbf{x}) = \mathcal{F}f(R_t\mathbf{h}(\mathbf{x})) e^{-i\langle \mathbf{d}_t, \mathbf{h}(\mathbf{x}) \rangle}$

### Theorem

[Q. Elbau Scherzer Steidl 2024]

Let  $s, t \in [0, T]$  be such that  $R_s\mathbf{e}^3 \neq \pm R_t\mathbf{e}^3$ . Assume  $f \geq 0$ ,  $f \neq 0$  and  $\mathbf{d}_0 = \mathbf{0}$ .

Then  $\mathbf{d}_t$  can be uniquely reconstructed from the two equations:

$$e^{i\langle R_t\mathbf{d}_t - R_s\mathbf{d}_s, R_s\mathbf{h}(\gamma_{s,t}(\beta)) \rangle} = \frac{\mu_s(\gamma_{s,t}(\beta))}{\mu_t(\gamma_{t,s}(-\beta))}, \quad \beta \in [-\pi, \pi], \mu_s(\gamma_{s,t}(\beta)) \neq 0,$$

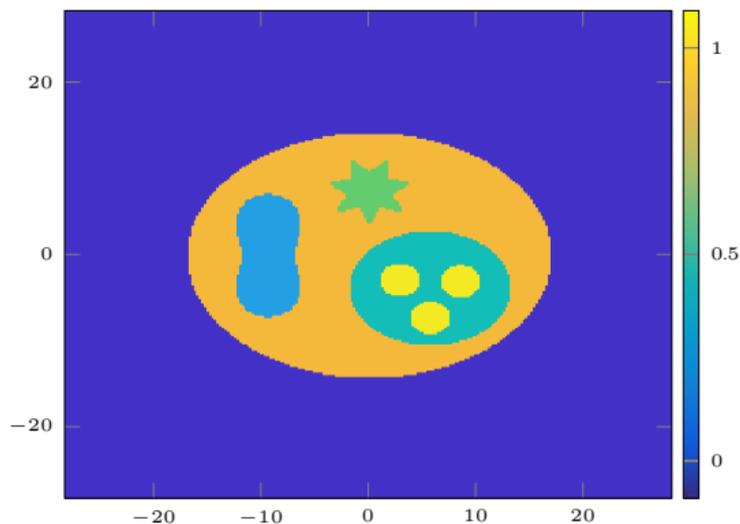
$$e^{i\langle R_t\mathbf{d}_t - R_s\mathbf{d}_s, R_s\mathbf{h}(\check{\gamma}_{s,t}(\beta)) \rangle} = \frac{\mu_s(\check{\gamma}_{s,t}(\beta))}{\mu_t(\check{\gamma}_{t,s}(\beta))}, \quad \beta \in [-\pi, \pi], \mu_s(\check{\gamma}_{s,t}(\beta)) \neq 0.$$

Similar reconstruction result for  $R_s\mathbf{e}^3 = \pm R_t\mathbf{e}^3$

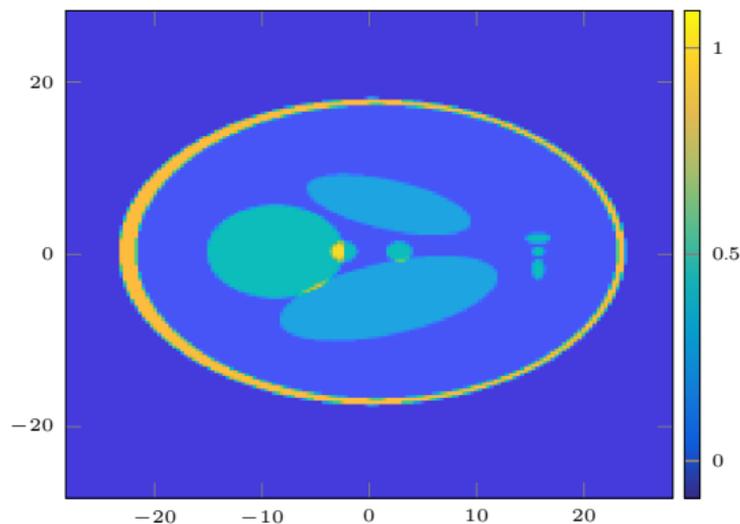


## Numerical Simulation: Test Functions (3D)

Cell phantom



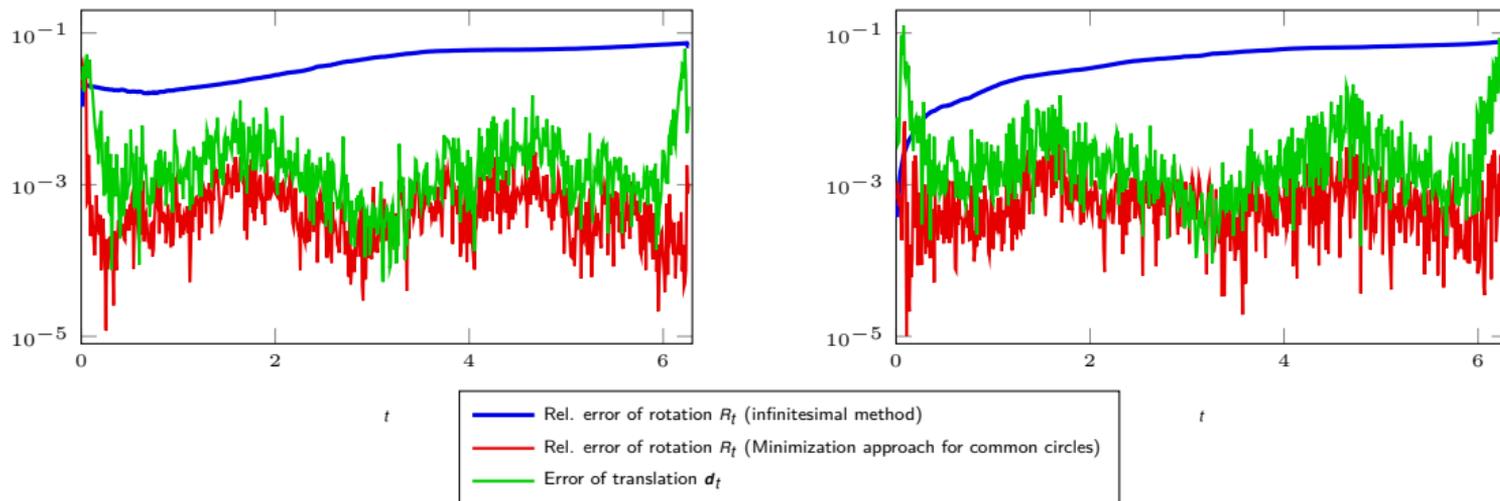
Shepp-Logan phantom



2D slices of test functions  $f$



## Numerical Simulation: Results

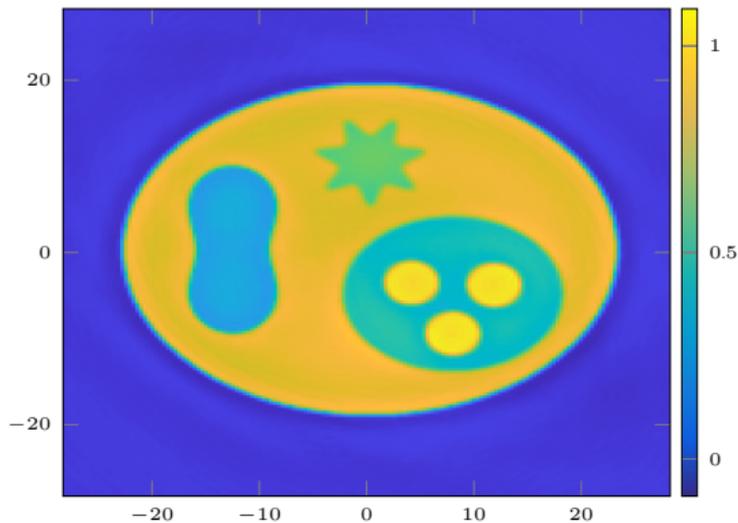


The rotation is around the moving axis  $(\sqrt{1-a^2} \cos(b \sin(t/2)), \sqrt{1-a^2} \sin(b \sin(t/2)), a) \in \mathbb{S}^2$  for  $a = 0.28$  and  $b = 0.5$ . The translation is  $d_t = 2(\sin t, \sin t, \sin t)$ .

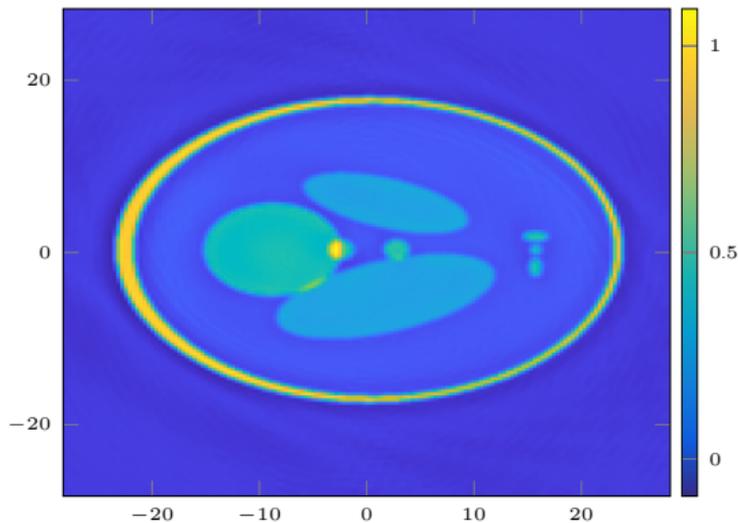
Left: cell phantom. Right: Shepp-Logan phantom.



## Reconstructed Scattering Potential $f$



Cell phantom (PSNR 32.21, SSIM 0.754)



Shepp-Logan (PSNR 30.85, SSIM 0.772)



## Conclusions

- Fourier diffraction theorem on  $L^1(\mathbb{R}^d)$
- Filtered backpropagation formula for a wide range of experimental setups
- Detection of rotation is mostly possible
- Detection of translation is possible

## Future research

- Application to real-world data
- Combining motion detection with phase retrieval



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Thank you for your attention!

## References



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