



Optical Diffraction Tomography with an Object Rotated into Arbitrary Orientations

Michael Quellmalz | TU Berlin | Symposium on Inverse Problems: From experimental data to models and back,
University of Potsdam, 21 September 2022
joint work with Robert Beinert, Peter Elbau, Clemens Kirisits, Monika Ritsch-Marte, Otmar Scherzer, Eric Setterqvist,
Gabriele Steidl



Content

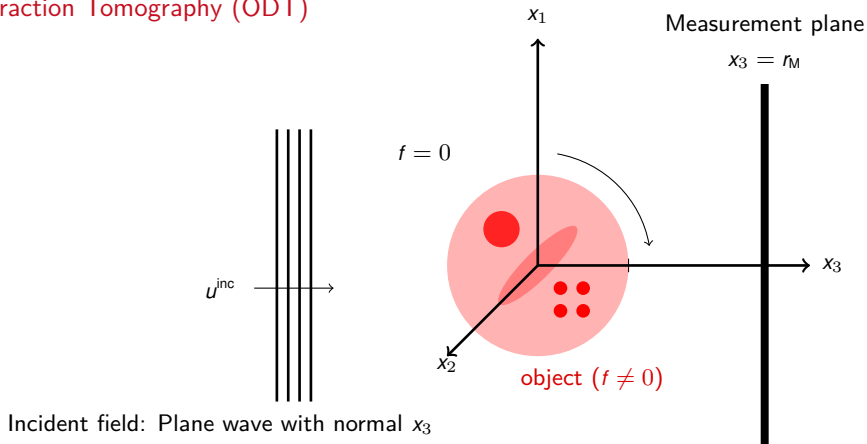
1 Introduction

2 Reconstruction of the object

3 Reconstructing the motion



Optical Diffraction Tomography (ODT)



C Kirisits, M Quellmalz, M Ritsch-Martel, O Scherzer, E Setterqvist, G Steidl.

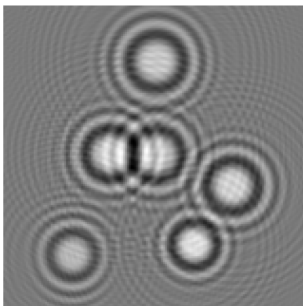
Fourier reconstruction for diffraction tomography of an object rotated into arbitrary orientations.

Inverse Problems 37, 2021.



Optical Diffraction

Optical diffraction occurs when the wavelength of the imaging beam is large
 \approx the size of the object (μm scale)



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

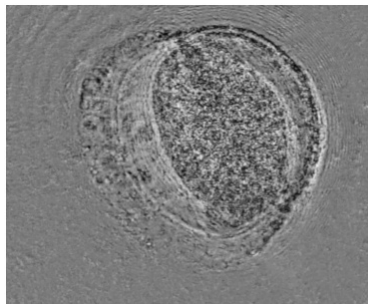


Image with diffraction
© Medizinische Universität Innsbruck



Model of Optical Diffraction Tomography (for one direction)

- **We have:** field $u^{\text{tot}}(x_1, x_2, r_M)$ at measurement plane $x_3 = r_M$
- **We want:** scattering potential $f(\mathbf{x})$ with $\text{supp } f \subset \mathcal{B}_{r_M} \subset \mathbb{R}^3$
- Object illuminated by plane wave $u^{\text{inc}}(\mathbf{x}) = e^{ik_0 x_3}$
- Total field $u^{\text{tot}}(\mathbf{x}) = u^{\text{sca}}(\mathbf{x}) + u^{\text{inc}}(\mathbf{x})$ solves the **wave equation**

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

Born approximation

Assuming $|u^{\text{sca}}| \ll |u^{\text{inc}}|$, we obtain

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



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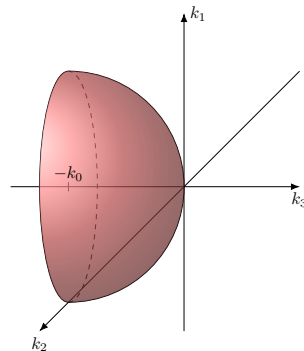
Fourier diffraction theorem [Kirisits Q. Ritsch-Marte Scherzer Setterqvist Steidl 2021]

Let the previous assumptions hold, $f \in L^p(\mathbb{R}^3)$, $p > 1$, and u^{sca} satisfy the Sommerfeld radiation condition (u is an outgoing wave) and.

Then

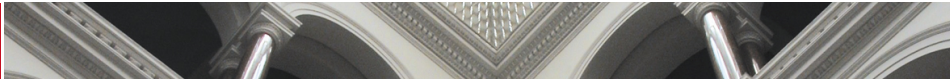
$$\sqrt{\frac{2}{\pi}} \kappa e^{-i\kappa r_M} \mathcal{F}_{1,2} \underbrace{u^{\text{sca}}(k_1, k_2, r_M)}_{\text{measurements}} = \mathcal{F}f(\mathbf{h}(k_1, k_2)), \quad (k_1, k_2) \in \mathbb{R}^2,$$

where $\mathbf{h}(k_1, k_2) := \begin{pmatrix} k_1 \\ k_2 \\ \kappa - k_0 \end{pmatrix}$ and $\kappa := \sqrt{k_0^2 - k_1^2 - k_2^2}$.



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

based on [Wolf 1969] [Natterer Wuebbeling 2001] [Kak Slaney 2001]

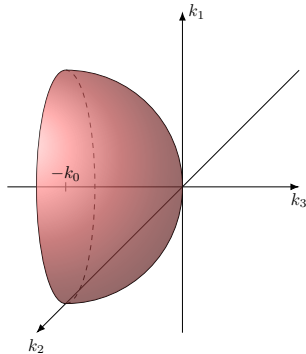


Comparison with Computerized Tomography

Optical diffraction tomography (ODT)

diffraction of imaging beam

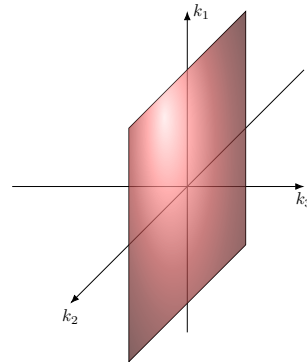
Data: Fourier transform on semispheres containing 0



Computerized tomography (CT)

light travels on lines

Data: Fourier transform on planes containing 0





Rigid Motion of the Object

- Scattering potential of the **moved object**: $f(R_t(\mathbf{x} - \mathbf{d}_t))$
- Rotation $R_t \in \text{SO}(3)$ (with $R_0 := \text{id}$)
- Translation $\mathbf{d}_t \in \mathbb{R}^3$ (with $\mathbf{d}_0 := \mathbf{0}$)

Fourier diffraction theorem (with motion)

The quantity

$$\mu_t(k_1, k_2) := \sqrt{\frac{2}{\pi}} \kappa i e^{-i\kappa r_M} \mathcal{F}_{1,2} \underbrace{u^{\text{sca}}(k_1, k_2, r_M)}_{\text{measurements}} = \mathcal{F}f(R_t \mathbf{h}(k_1, k_2)) e^{-i\langle \mathbf{d}_t, \mathbf{h}(k_1, k_2) \rangle}, \quad \|(k_1, k_2)\| < k_0,$$

depends only on the measurements.

- 1 Reconstruct the rotation using $\nu_t(k_1, k_2) := |\mu_t(k_1, k_2)|^2 = |\mathcal{F}f(R_t \mathbf{h}(k_1, k_2))|^2$.
- 2 Reconstruct the translation \mathbf{d}_t
- 3 Reconstruct f



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Fourier diffraction theorem (with motion)

The quantity

$$\mu_t(k_1, k_2) := \sqrt{\frac{2}{\pi}} \kappa i e^{-i\kappa r_M} \underbrace{\mathcal{F}_{1,2}^{\text{sca}}(k_1, k_2, r_M)}_{\text{measurements}} = \mathcal{F}f(R_t \mathbf{h}(k_1, k_2)) e^{-i\langle \mathbf{d}_t, \mathbf{h}(k_1, k_2) \rangle}, \quad \|(k_1, k_2)\| < k_0,$$

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Discretization

- Object $f(\mathbf{x}_k)$ with $\mathbf{x}_k = \mathbf{k} \frac{2L_S}{K}$, $\mathbf{k} \in \mathcal{I}_K^3 := \{-K/2, \dots, K/2 - 1\}^3$
- Measurements $u_{l_m}^{\text{tot}}(\mathbf{y}_n, r_M)$ with $\mathbf{y}_n = \mathbf{n} \frac{2L_M}{N}$, $\mathbf{n} \in \mathcal{I}_N^2$
- discrete Fourier transform (DFT)

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

- Non-uniform discrete Fourier transform (NDFT)

$$[\mathbf{F}_{\text{NDFT}} \mathbf{f}]_{m, \ell} := \sum_{\mathbf{k} \in \mathcal{I}_K^3} f_{\mathbf{k}} e^{-i \mathbf{x}_{\mathbf{k}} \cdot (R_{l_m} h(\mathbf{y}_{\ell}))}, \quad m \in \mathcal{J}_M, \ell \in \mathcal{I}_N^2$$

Discretized forward operator

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

$$\text{where } \mathbf{c} = \left[\frac{i}{\kappa(\mathbf{y}_{\ell})} e^{i \kappa(\mathbf{y}_{\ell}) r_M} \left(\frac{N}{L_M} \right)^{d-1} \left(\frac{L_S}{K} \right)^d \right]_{\ell \in \mathcal{I}_N^2}$$

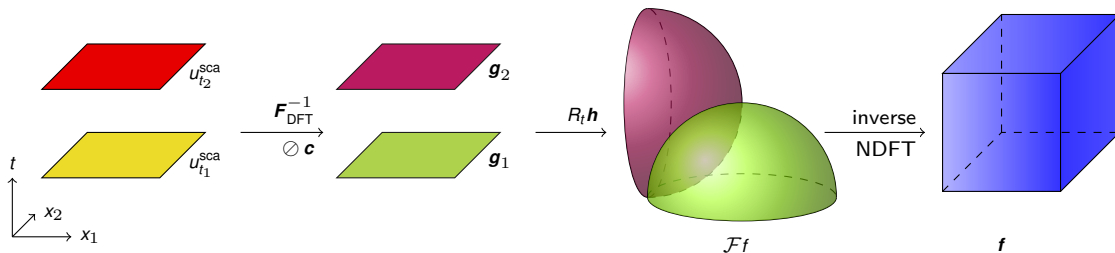


Reconstruction of f

Inverse

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

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

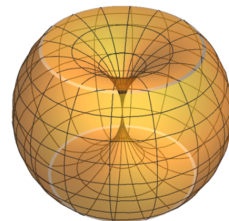




Approach 1: Backpropagation

Idea: Compute inverse Fourier transform of $\mathcal{F}f$ restricted to the set of available data \mathcal{Y} :

$$f_{\text{bp}}(\mathbf{x}) := (2\pi)^{-\frac{3}{2}} \int_{\mathcal{Y}} \mathcal{F}f(\mathbf{y}) e^{i\mathbf{y} \cdot \mathbf{x}} d\mathbf{y}.$$



Theorem

[Kirisits, Q, Ritsch-Marte, Scherzer, Setterqvist, Steidl 2021]

Consider the rotation R_t round axis $\mathbf{a}(t)$ with angle $\alpha(t)$ in $C^1[0, T]$. Then

$$f_{\text{bp}}(\mathbf{x}) = (2\pi)^{-\frac{3}{2}} \int_0^T \int_{\mathcal{B}_{k_0}} \mathcal{F}f(R_t \mathbf{h}(k_1, k_2)) e^{i R_t \mathbf{h}(k_1, k_2) \cdot \mathbf{x}} \frac{|\det \nabla T(k_1, k_2, t)|}{\text{Card } T^{-1}(T(k_1, k_2, t))} d(k_1, k_2) dt,$$

where $T(k_1, k_2, t) := R_t \mathbf{h}(k_1, k_2)$ and

$$|\det \nabla T(k_1, k_2, t)| = \frac{k_0}{\kappa} \left| \left((1 - \cos \alpha)(a_3 \mathbf{a}' \cdot \mathbf{h} - a'_3 \mathbf{a} \cdot \mathbf{h}) - a_3 \mathbf{a} \cdot (\mathbf{a}' \times \mathbf{h}) \sin \alpha \right) - \alpha' (a_1 k_2 - a_2 k_1) + (\mathbf{a} \cdot \mathbf{h})(a_1 a'_2 - a_2 a'_1) \sin \alpha \right|.$$

Previously known only for constant axis \mathbf{a}

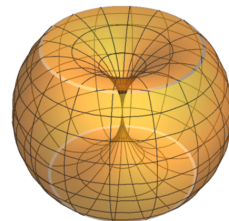
[Devaney 1982]



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[Devaney 1982]



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

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

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



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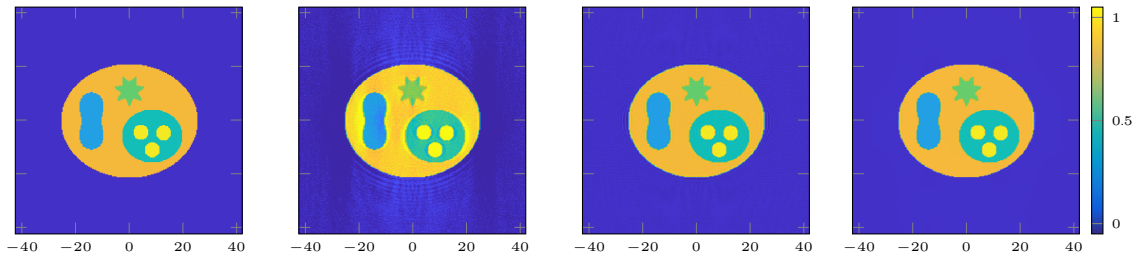
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Reconstruction: Moving Axis



Ground truth f

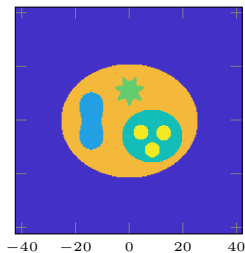
Backpropagation
PSNR 24.17, SSIM 0.171

CG Reconstruction
PSNR 35.84, SSIM 0.962

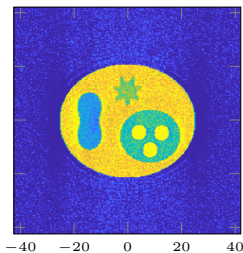
PD with TV ($\lambda = 0.02$)
PSNR 40.95, SSIM 0.972



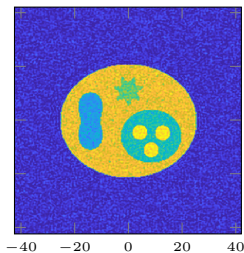
Reconstruction: Moving Axis and 5 % Gaussian Noise



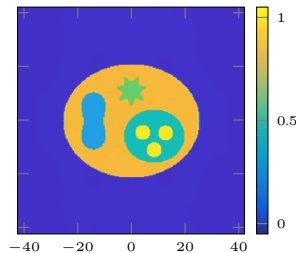
Ground truth f



Backpropagation
PSNR 21.19, SSIM 0.075



CG Reconstruction
PSNR 24.10, SSIM 0.193



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



Content

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Formal Uniqueness Result

Theorem

[Kurlberg Zickert 2021]

Let

- the second order moments of f have distinct, real eigenvalues,
- the translation \mathbf{d}_t be restricted to a known plane,
- the rotations R_t cover $SO(3)$.

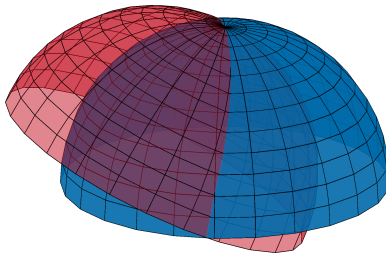
Then f is uniquely determined given the diffraction images u_t for all (unknown) motions.

Detection of the Rotation

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 semisphere
- Two semispheres intersect in a circle (arc), where $\mathcal{F}f$ must agree
- Find the common circle of two semispheres



P Elbau, M Quellmalz, O Scherzer, G Steidl.

Motion detection in diffraction tomography with common circle methods.

[Arxiv preprint 2209.08086](https://arxiv.org/abs/2209.08086)



Common Circles

Theorem

[Q. Elbau Scherzer Steidl 2022]

Let $t, s \in [0, T]$ such that there uniquely exist two curves

$$\begin{aligned}\gamma_{s,t}(\beta) &= \frac{k_0}{2} \sin \theta (\cos \beta - 1) \begin{pmatrix} \cos \varphi \\ \sin \varphi \end{pmatrix} + k_0 \cos \frac{\theta}{2} \sin \beta \begin{pmatrix} -\sin \varphi \\ \cos \varphi \end{pmatrix} \\ \gamma_{t,s}(\beta) &= \frac{k_0}{2} \sin \theta (\cos \beta - 1) \begin{pmatrix} -\cos \psi \\ \sin \psi \end{pmatrix} + k_0 \cos \frac{\theta}{2} \sin \beta \begin{pmatrix} -\sin \varphi \\ -\cos \varphi \end{pmatrix}\end{aligned}$$

with some parameters $\varphi, \psi \in \mathbb{R}/(2\pi\mathbb{Z})$, $\theta \in [0, \pi]$ such that

$$\nu_s \circ \gamma_{s,t}(\beta) = \nu_t \circ \gamma_{t,s}(-\beta), \quad |\beta| < \pi.$$

Then the rotation $R_s^\top R_t$ has the Euler angles φ, θ, ψ .

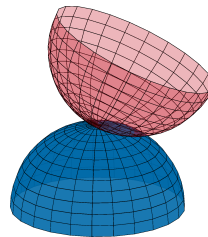
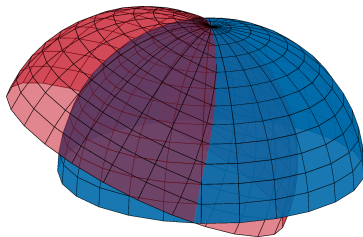


Dual Common Circles

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

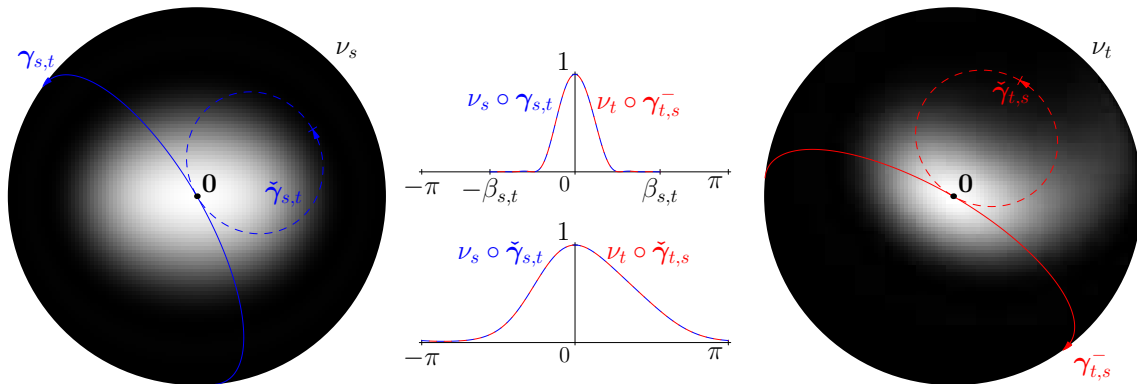
$$\check{\gamma}_{s,t}(\beta) = -\frac{k_0}{2} \sin \theta (\cos \beta - 1) \begin{pmatrix} \cos \varphi \\ \sin \varphi \end{pmatrix} + k_0 \sin \frac{\theta}{2} \sin \beta \begin{pmatrix} -\sin \varphi \\ \cos \varphi \end{pmatrix}$$

$$\check{\gamma}_{t,s}(\beta) = -\frac{k_0}{2} \sin \theta (\cos \beta - 1) \begin{pmatrix} -\cos \psi \\ \sin \psi \end{pmatrix} + k_0 \sin \frac{\theta}{2} \sin \beta \begin{pmatrix} -\sin \varphi \\ -\cos \varphi \end{pmatrix}$$





Visualization of the Arcs





Infinitesimal Common Circles Method

Theorem

[Q. Elbau Scherzer Steidl 2022]

Let the rotation $R \in C^1([0, T] \rightarrow \text{SO}(3))$ 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 cylinder coordinates

$$\omega_t = \begin{pmatrix} \rho_t \varphi_t \\ \zeta_t \end{pmatrix}, \quad \varphi_t = \begin{pmatrix} \cos \varphi_t \\ \sin \varphi_t \end{pmatrix} \in \mathbb{S}^1,$$

Then, for all $r \in (-k_0, k_0)$, it holds that

$$- \partial_t \nu_t(r \varphi_t) = \left(\rho(t) \left(\sqrt{k_0^2 - r^2} - k_0 \right) + r \zeta_t \right) \left\langle \nabla \nu_t(r \varphi_t), \begin{pmatrix} -\sin \varphi_t \\ \cos \varphi_t \end{pmatrix} \right\rangle.$$



Reconstructing the Translation

Reminder: Data $\mu_t(k_1, k_2) := \mathcal{F}f(R_t \mathbf{h}(k_1, k_2)) e^{-i\langle \mathbf{d}_t, \mathbf{h}(k_1, k_2) \rangle}$

Theorem

[Q. Elbau Scherzer Steidl 2022]

Let $s, t \in [0, T]$ be such that $R_s \mathbf{e}^3 \neq \pm R_t \mathbf{e}^3$ and let $f \geq 0$ with $f \not\equiv 0$.

If $\mathbf{d}_0 = \mathbf{0}$, then \mathbf{d}_t can be uniquely reconstructed from the two equations:

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

and

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

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

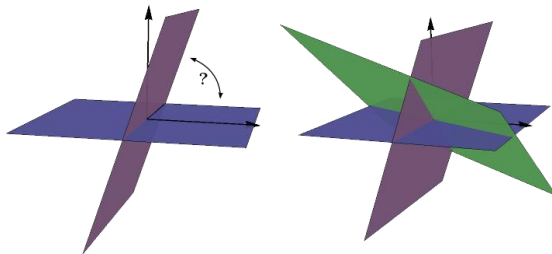


Comparison with CT

Method of common lines in Cryo-EM

[Crowther DeRosier Klug 70] [van Heel 87] [Goncharov 88] [Wang Singer Zen 13]

- Based on different model (ray transform)
- Requires 3 common planes (instead of 2 semi-spheres)
- Ambiguities (mirroring, translation along imaging direction)

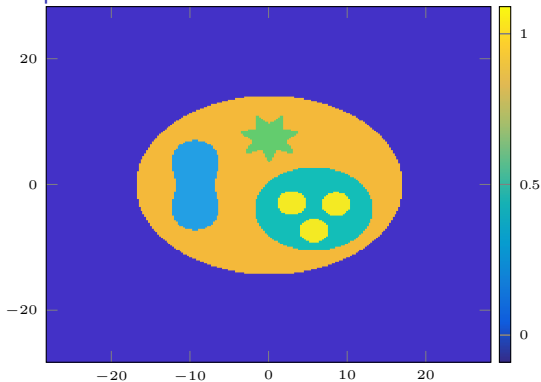


Images by [Schmutz 17]

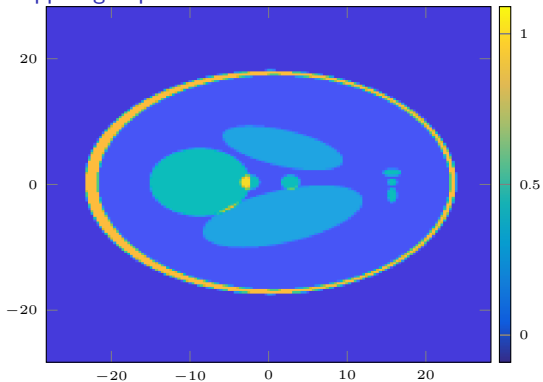


Numerical Simulation: Test Functions (3D)

Cell phantom

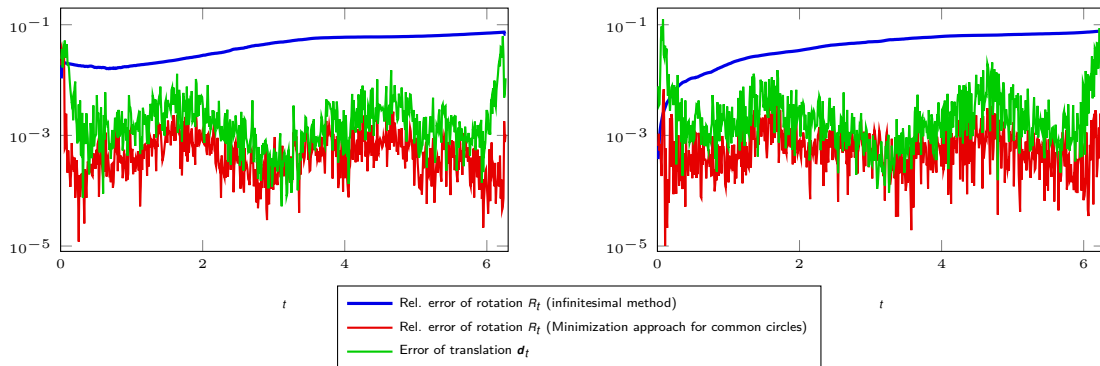


Shepp-Logan phantom





Numerical Simulation: Results

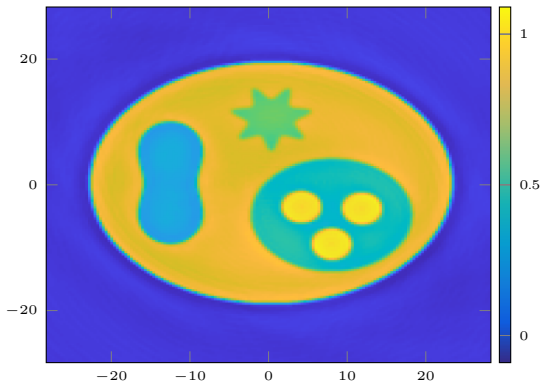


The rotation is around the moving axis $(\sqrt{1 - a^2} \cos(b \sin(t/2)), \sqrt{1 - a^2} \sin(b \sin(t/2)), a) \in \mathbb{S}^2$ for $a = 0.28$ and $b = 0.5$. The translation is $d_t = 2(\sin t, \sin t, \sin t)$.

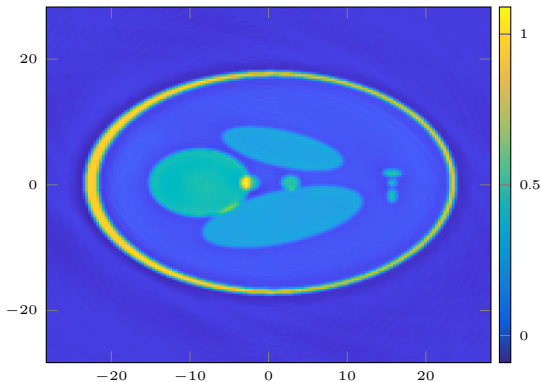
Left: cell phantom. Right: Shepp-Logan phantom.



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 $L^p(\mathcal{B}_{r_s})$, $p > 1$
- Backpropagation formula for arbitrary rotations
- Compared image reconstruction methods
 - Backpropagation is faster
 - Conjugate Gradients and Primal-Dual show better results
- Detection of rotation is usually possible
- Detection of translation is possible

Future research

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

Thank you for your attention!



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