



Motion Detection in Diffraction Tomography

Michael Quellmalz | TU Berlin | AIP Conference, Göttingen, 5 September 2023

joint work with Robert Beinert, Peter Elbau, Clemens Kirisits, Monika Ritsch-Marte, Otmar Scherzer, Eric Setterqvist, Gabriele Steidl



Outline

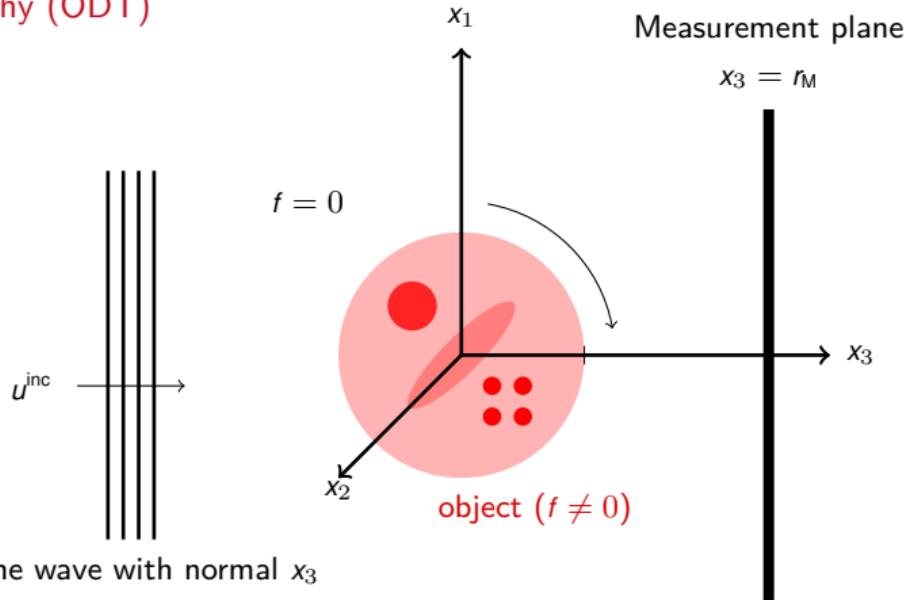
① Introduction

② Reconstruction of the object

③ Reconstructing the motion



Optical Diffraction Tomography (ODT)

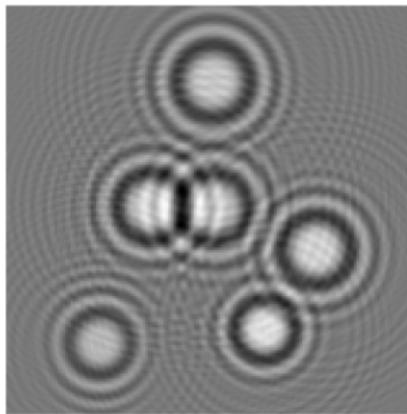


C Kirisits, M Quellmalz, M Ritsch-Marte, O Scherzer, E Setterqvist, G Steidl.
Fourier reconstruction for diffraction tomography of an object rotated into arbitrary orientations.
Inverse Problems 37, 2021.



Optical Diffraction

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



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

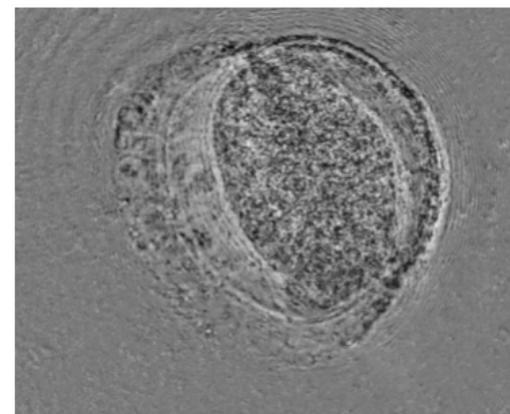


Image with diffraction
© Medizinische Universität Innsbruck



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

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

- Rearranging yields

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

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

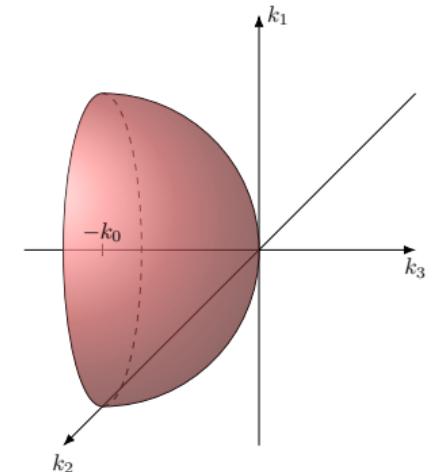
Let the previous assumptions hold, $f \in L^p(\mathbb{R}^3)$, $p > 1$, and u^{sca} satisfy the Sommerfeld radiation condition (u is an outgoing wave).

Then

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

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

based on [Wolf 1969] [Natterer Wuebbeling 2001] [Kak Slaney 2001]
 this L^p version from [Kirisits Q. Ritsch-Marte Scherzer Setterqvist Steidl 2021]



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

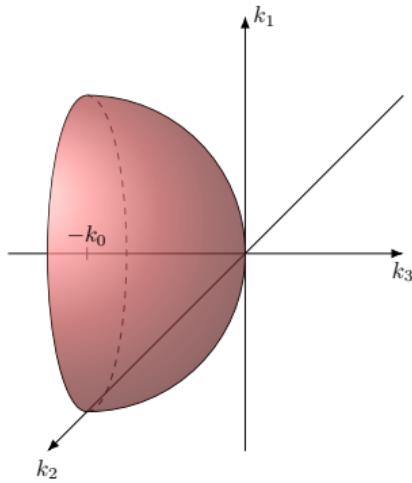


Comparison with Computerized Tomography

Optical diffraction tomography (ODT)

diffraction of imaging wave

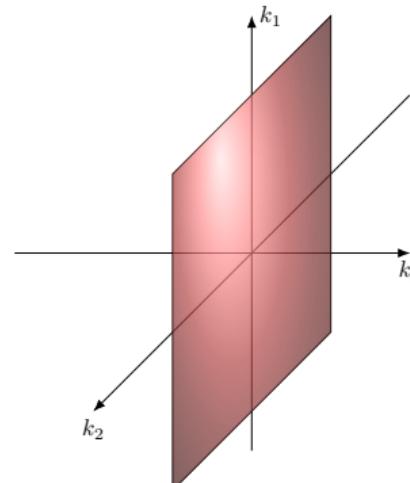
Data: Fourier transform on **semispheres** containing **0**



Computerized tomography (CT)

light travels along straight 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

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

depends only on the measurements.

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



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Discretization

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

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

- Non-uniform discrete Fourier transform (NDFT)

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

Discretized forward operator

$$\mathbf{D}^{\text{tot}} \mathbf{f} := \mathbf{F}_{\text{DFT}}^{-1} (\mathbf{c} \odot \mathbf{F}_{\text{NDFT}} \mathbf{f}) + e^{ik_0 r_M}, \quad \mathbf{f} \in \mathbb{R}^{K^d},$$

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

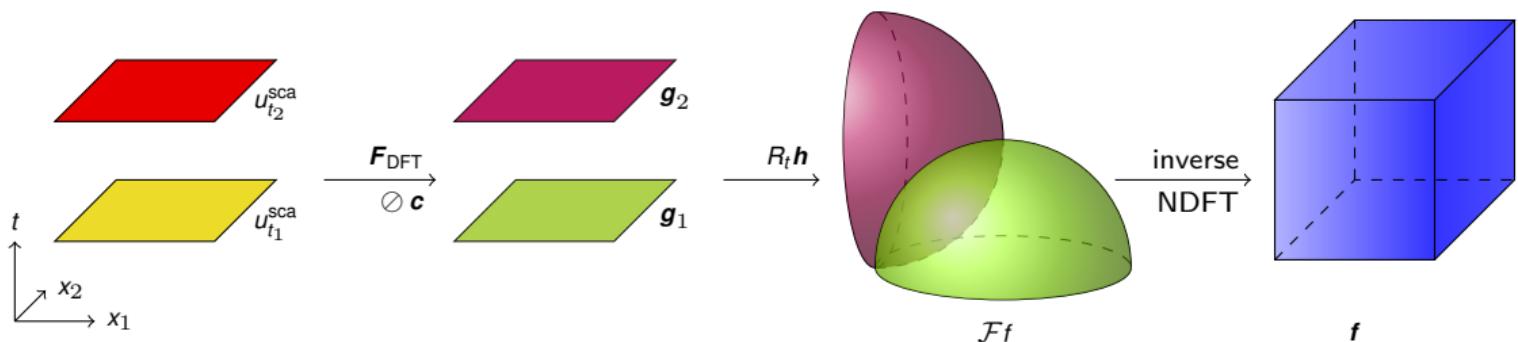


Reconstruction of f

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 $\mathbf{F}_{\text{NDFT}}^{-1}$

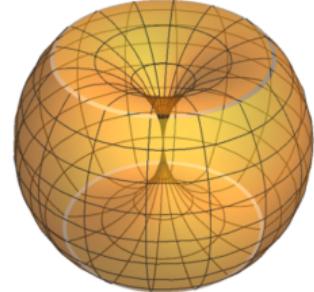




Approach 1: Filtered Backpropagation

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 $a(t)$ with angle $\alpha(t)$ in $C^1[0, T]$. Then

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

where $T(k_1, k_2, t) := R_t h(k_1, k_2)$ 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 a

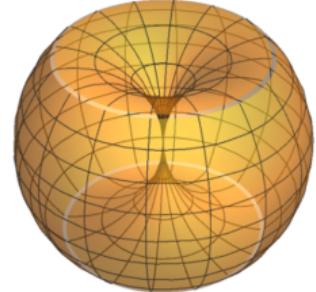
[Devaney 1982]



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Previously known only for constant axis \mathbf{a}

[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

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

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



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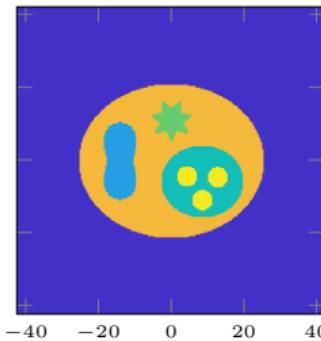
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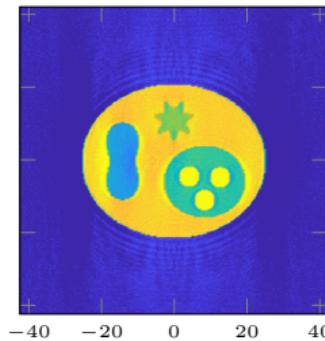
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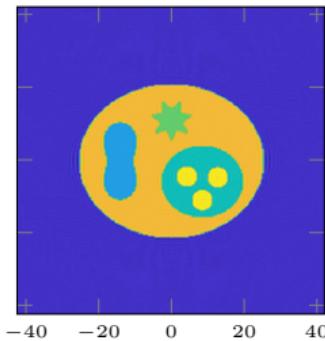
Reconstruction: Moving Axis



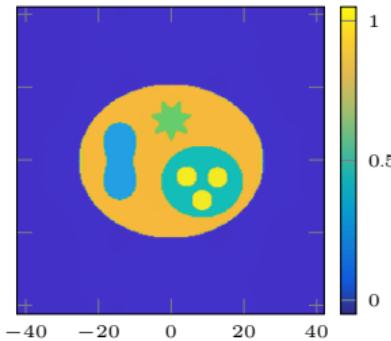
Ground truth f
($240 \times 240 \times 240$ grid)



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



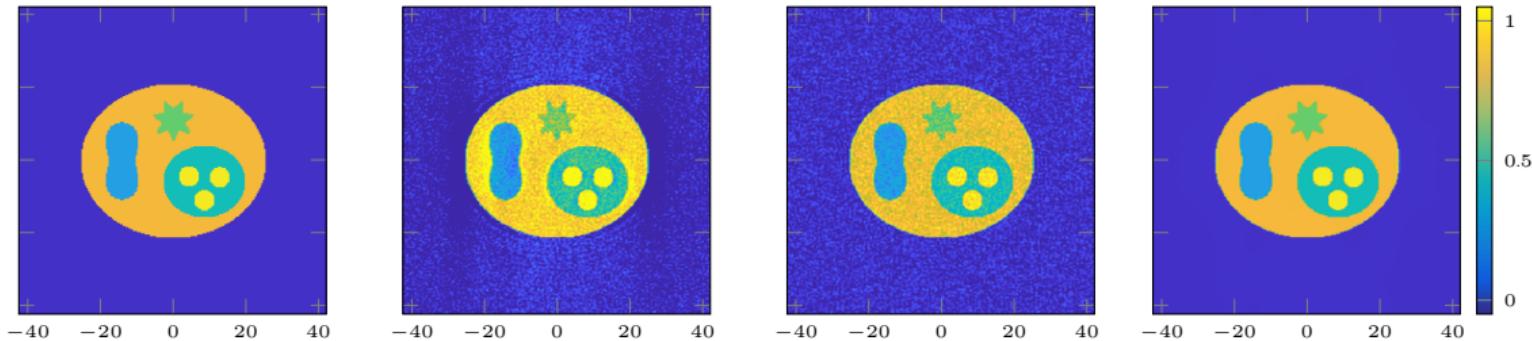
R Beinert, M Quellmalz.

Total Variation-Based Reconstruction and Phase Retrieval for Diffraction Tomography with an Arbitrarily Moving Object.

[Arxiv preprint 2210.03495](https://arxiv.org/abs/2210.03495)



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



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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 $\text{SO}(3)$.

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

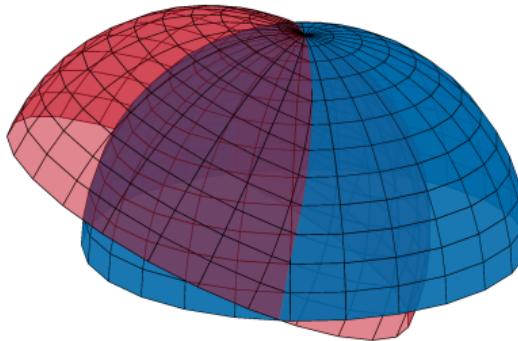


Detection of the Rotation

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.

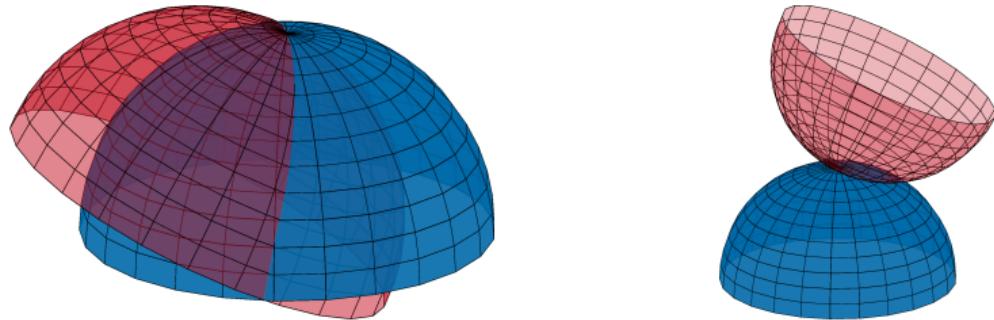
Motion detection in diffraction tomography with common circle methods.

Math Comp. (in press) doi:10.1090/mcom/3869



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

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

Theorem (unique reconstruction)

[Q. Elbau Scherzer Steidl 2023]

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

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

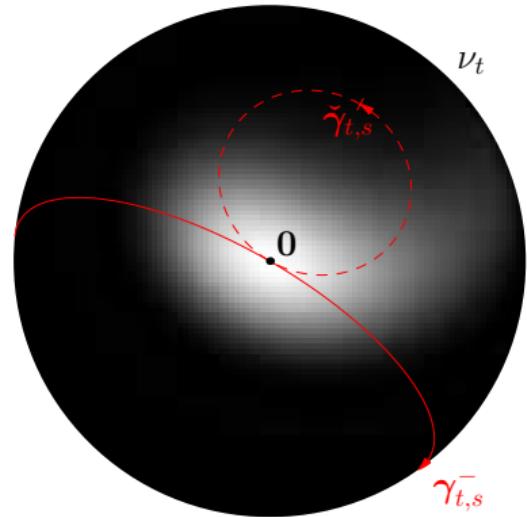
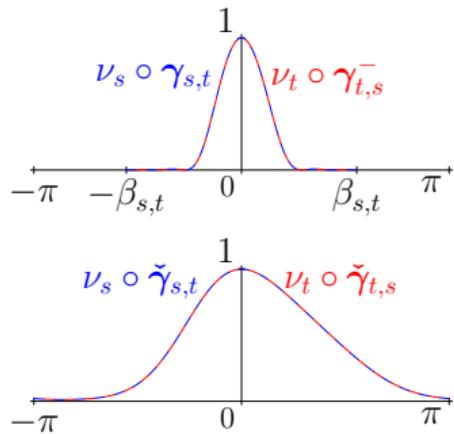
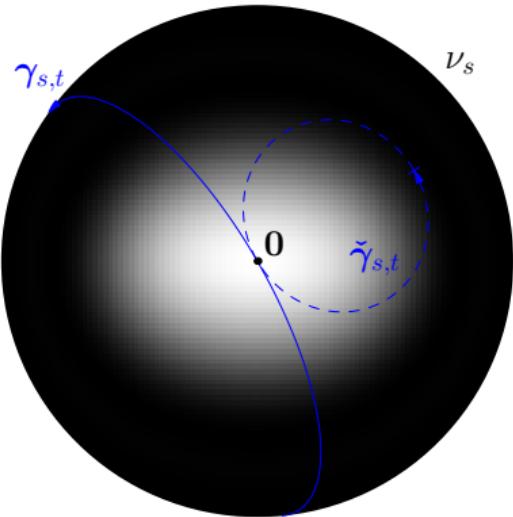
Then the relative rotation $R_s^\top R_t$ is uniquely determined by the Euler angles

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

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



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 2023]

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 cylindrical coordinates

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

Then

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



Reconstructing the Translation

Recall: 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 2023]

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:

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

and

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

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

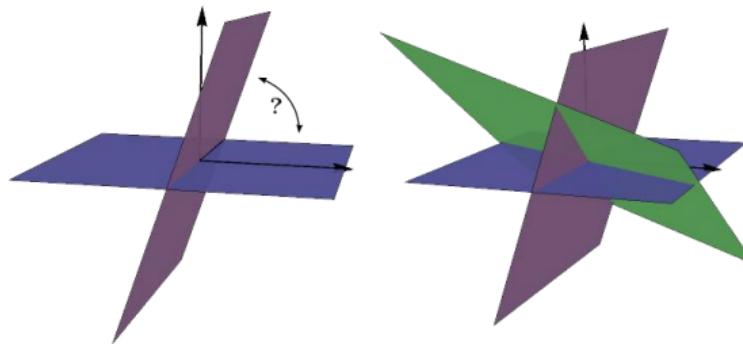


Comparision with CT

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)

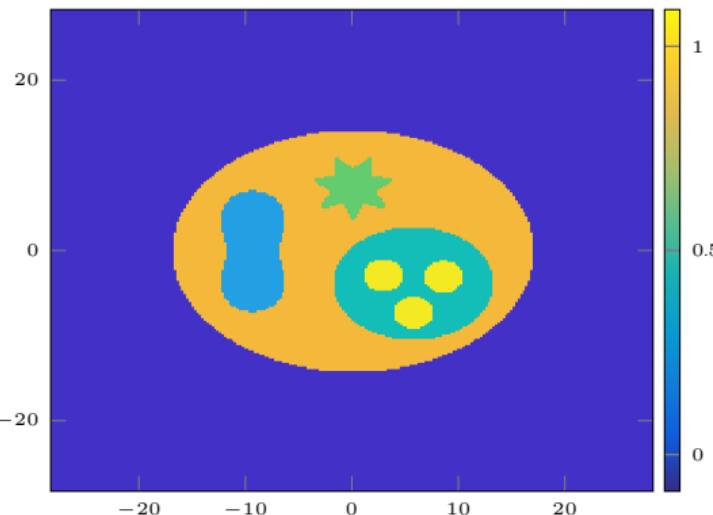


Images by [Schmutz 17]

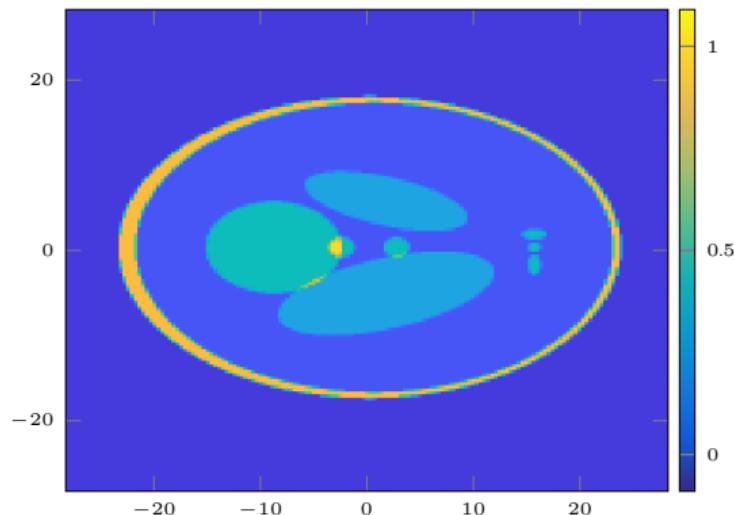


Numerical Simulation: Test Functions (3D)

Cell phantom

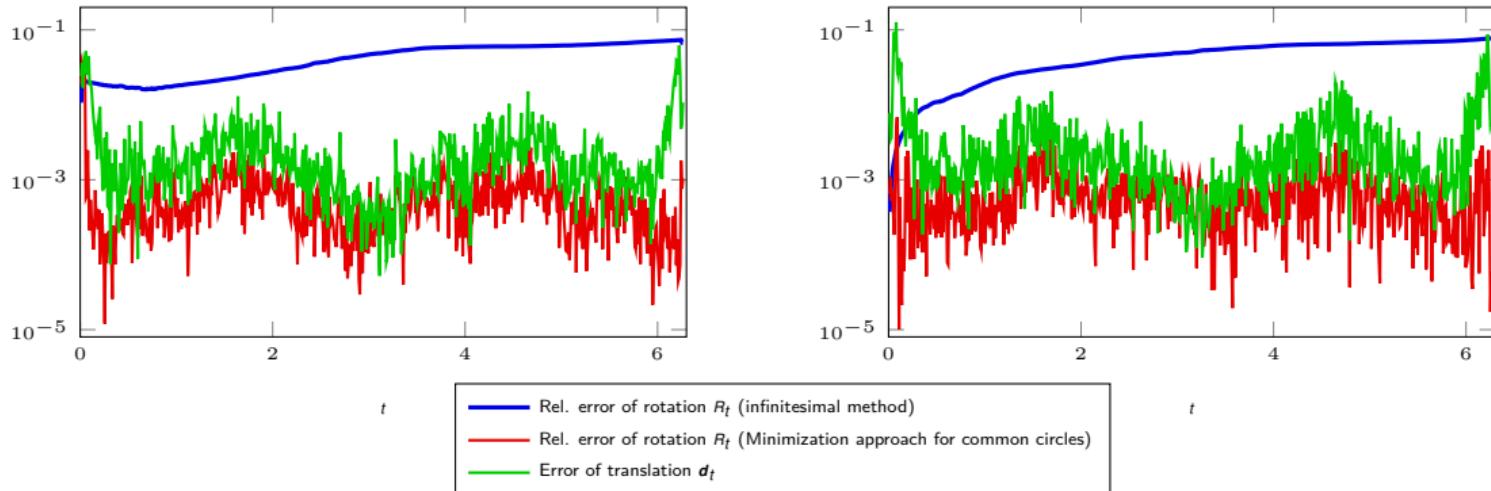


Shepp-Logan phantom





Numerical Simulation: Results

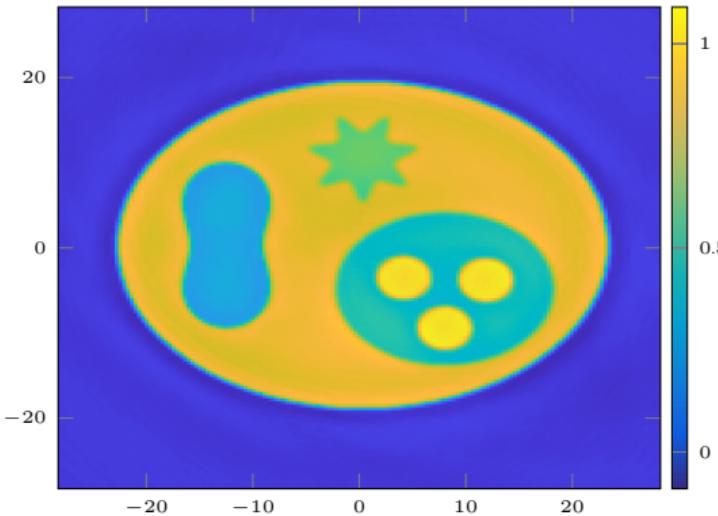


The rotation is around the moving axis $(\sqrt{1 - a^2} \cos(b \sin(t/2)), \sqrt{1 - a^2} \sin(b \sin(t/2)), a) \in \mathbb{S}^2$ for $a = 0.28$ and $b = 0.5$. The translation is $\mathbf{d}_t = 2(\sin t, \sin t, \sin t)$.

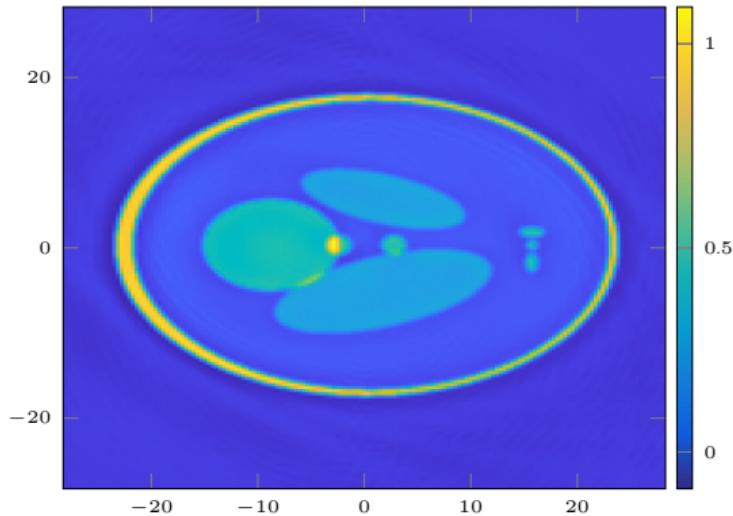
Left: cell phantom. Right: Shepp–Logan phantom.



Reconstructed Scattering Potential f



Cell phantom (PSNR 32.21, SSIM 0.754)



Shepp–Logan (PSNR 30.85, SSIM 0.772)

Thank you for your attention!