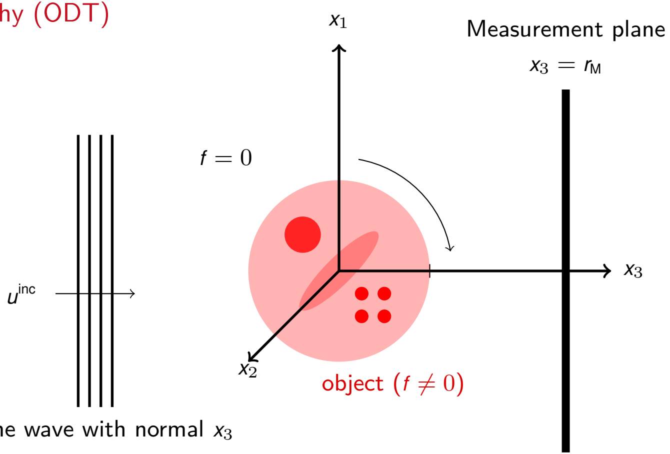



# Motion Detection in Diffraction Tomography

Michael Quellmalz | TU Berlin | DMV Meeting, Section on Inverse Problems, Ilmenau, 28 September 2023
joint work with Robert Beinert, Peter Elbau, Clemens Kirisits, Monika Ritsch-Marte, Otmar Scherzer, Eric Setterqvist, Gabriele Steidl

## Outline

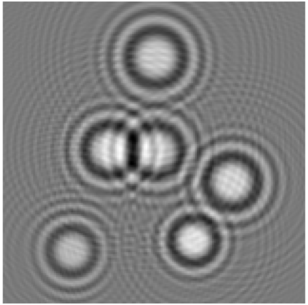
# Optical Diffraction Tomography (ODT)




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 ≈ the size of the object ($\mu m$ scale)



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

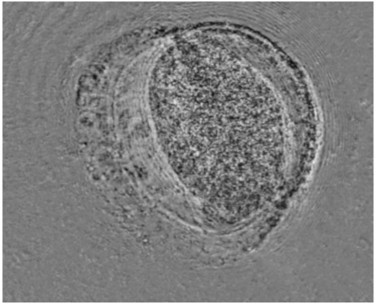


Image with diffraction
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# Model of Optical Diffraction Tomography (for one direction)

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

$$-\left(\Delta + f(\boldsymbol{x}) + k_0^2\right) u^{\mathrm{tot}}(\boldsymbol{x}) = 0$$

- Rearranging yields

$$-\left(\Delta + k_0^2\right) u^{\mathrm{sca}}(\boldsymbol{x}) - \underbrace{\left(\Delta + k_0^2\right) u^{\mathrm{inc}}(\boldsymbol{x})}_{=0} = f(\boldsymbol{x}) \left(u^{\mathrm{sca}}(\boldsymbol{x}) + u^{\mathrm{inc}}(\boldsymbol{x})\right)$$

## Born approximation

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

$$-\left(\Delta + k_0^2\right) u^{\mathrm{sca}}(\boldsymbol{x}) = f(\boldsymbol{x}) u^{\mathrm{inc}}(\boldsymbol{x})$$

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## Fourier diffraction theorem

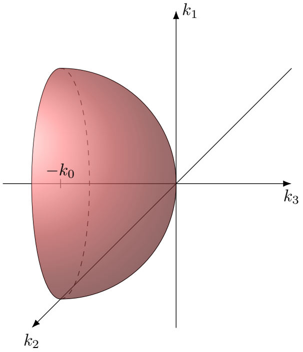
Let the previous assumptions hold, $f \in L^p(\mathbb{R}^3)$, $p > 1$, and $u^{\text{sca}}$ satisfy the Sommerfeld radiation condition ($u$ is an outgoing wave).

Then

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

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

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



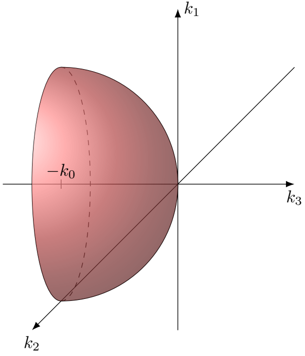

Semisphere $\boldsymbol{h}(\boldsymbol{k})$ of available data in Fourier space

# Comparison with Computerized Tomography

## Optical diffraction tomography (ODT)

diffraction of imaging wave

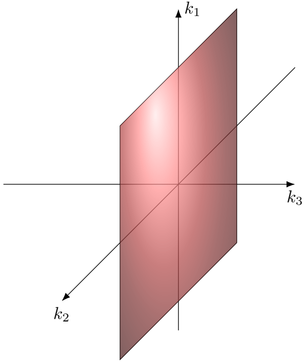
Data: Fourier transform on semispheres containing $\mathbf{0}$




## Computerized tomography (CT)

light travels along straight lines

Data: Fourier transform on planes containing $\mathbf{0}$



## Rigid Motion of the Object

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

**Fourier diffraction theorem (with motion)**

The quantity

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

depends only on the measurements.

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

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# Outline

# Discretization

- Object $f(\boldsymbol{x_k})$ with $\boldsymbol{x_k} = \boldsymbol{k}\frac{2L_\mathrm{s}}{K}$, $\boldsymbol{k} \in \mathcal{I}_K^3 := \{-K/2, \dots, K/2-1\}^3$
- Measurements $u_{t_m}^{\mathrm{tot}}(\boldsymbol{y_n}, r_\mathrm{M})$ with $\boldsymbol{y_n} = \boldsymbol{n}\frac{2L_\mathrm{M}}{N}$, $\boldsymbol{n} \in \mathcal{I}_N^2$
- discrete Fourier transform (DFT)

$$\left[\boldsymbol{F}_\mathrm{DFT}\, u_{t_m}^{\mathrm{sca}}\right]_{\boldsymbol{\ell}} := \sum_{\boldsymbol{n}\in\mathcal{I}_N^2} u_{t_m}^{\mathrm{sca}}(\boldsymbol{y_n}, r_\mathrm{M})\,\mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{n}\cdot\boldsymbol{\ell}/N}, \qquad \boldsymbol{\ell} \in \mathcal{I}_N^2,$$

- Non-uniform discrete Fourier transform (NDFT)

$$\left[\boldsymbol{F}_\mathrm{NDFT}\boldsymbol{f}\right]_{m,\boldsymbol{\ell}} := \sum_{\boldsymbol{k}\in\mathcal{I}_K^3} f_{\boldsymbol{k}}\,\mathrm{e}^{-\mathrm{i}\boldsymbol{x_k}\cdot\left(R_{t_m}\boldsymbol{h}(\boldsymbol{y_\ell})\right)}, \qquad m \in \mathcal{J}_M,\ \boldsymbol{\ell} \in \mathcal{I}_N^2$$

## Discretized forward operator

$$\boldsymbol{D}^{\mathrm{tot}}\boldsymbol{f} := \boldsymbol{F}_\mathrm{DFT}^{-1}(\boldsymbol{c} \odot \boldsymbol{F}_\mathrm{NDFT}\boldsymbol{f}) + \mathrm{e}^{\mathrm{i}k_0 r_\mathrm{M}}, \qquad \boldsymbol{f} \in \mathbb{R}^{K^d},$$

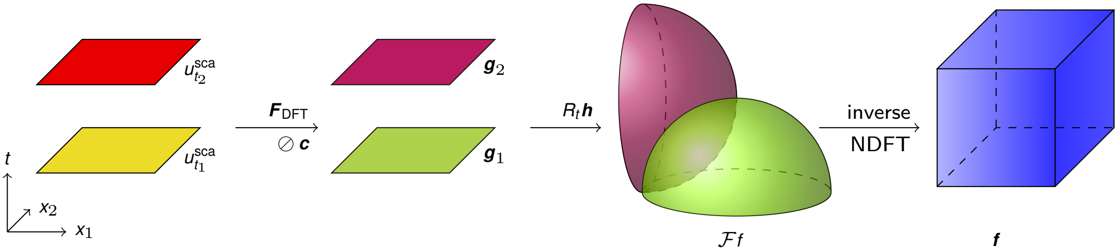
where $\boldsymbol{c} = \left[\frac{\mathrm{i}}{\kappa(\boldsymbol{y_\ell})}\,\mathrm{e}^{\mathrm{i}\,\kappa(\boldsymbol{y_\ell})\,r_\mathrm{M}}\left(\frac{N}{L_\mathrm{M}}\right)^{d-1}\left(\frac{L_\mathrm{s}}{K}\right)^{d}\right]_{\boldsymbol{\ell}\in\mathcal{I}_N^2}$

# Reconstruction of $f$

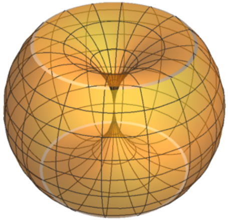
## Inverse

$$\boldsymbol{f} \approx \boldsymbol{F}_{\mathrm{NDFT}}^{-1}\left(\left(\boldsymbol{F}_{\mathrm{DFT}}\boldsymbol{u}^{\mathrm{tot}} - \mathrm{e}^{ik_0 r_{\mathrm{M}}}\right) \oslash \boldsymbol{c}\right)$$

Crucial part: inversion of NDFT $\boldsymbol{F}_{\mathrm{NDFT}}^{-1}$



## Approach 1: Filtered Backpropagation



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

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

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

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

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

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

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

Previously known only for constant axis $\boldsymbol{a}$ [Devaney 1982]

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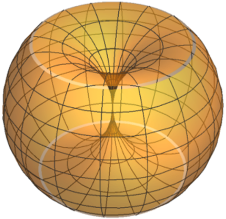

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## Approach 2: Conjugate Gradient (CG) Method

- Conjugate Gradients (CG) on the normal equations

$$\operatorname*{arg\,min}_{\boldsymbol{f}\in\mathbb{R}^{K^3}} \quad \|\boldsymbol{F}_{\text{NDFT}}(\boldsymbol{f}) - \boldsymbol{g}\|_2^2$$

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

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

## Approach 3: TV (Total Variation) Regularization

- Regularized inverse

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

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

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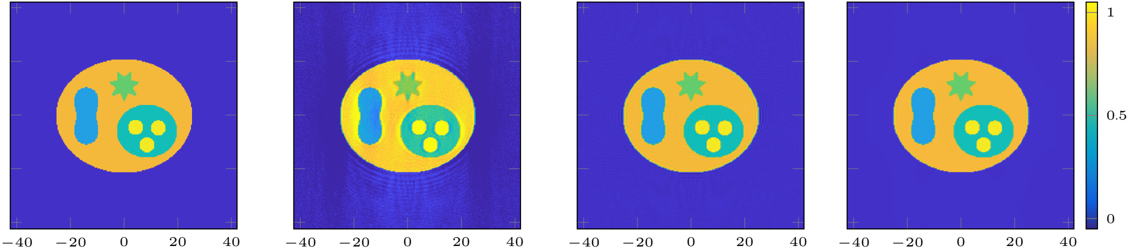
# Reconstruction: Moving Axis




Ground truth $\boldsymbol{f}$
($240 \times 240 \times 240$ grid)

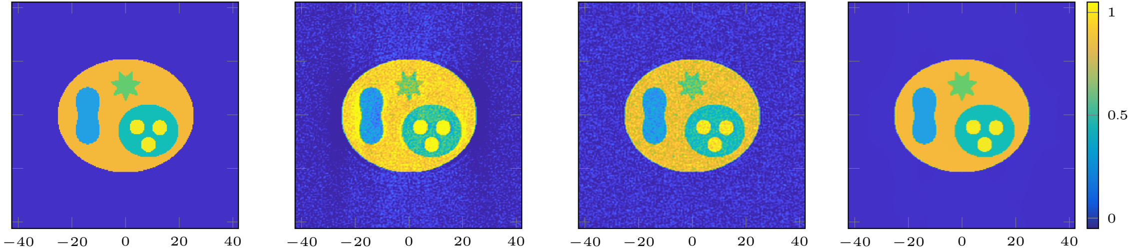
Backpropagation
PSNR 24.17, SSIM 0.171

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

# Reconstruction: Moving Axis and 5 % Gaussian Noise




Ground truth $\boldsymbol{f}$

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

# Outline

# 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 $\boldsymbol{d}_t$ be restricted to a known plane,
- the rotations $R_t$ cover $\mathrm{SO}(3)$.

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

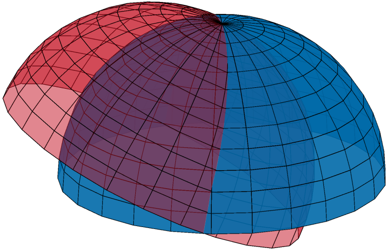
We find an algorithm to recover the rotations and translations

# Detection of the Rotation

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

Common circle approach:

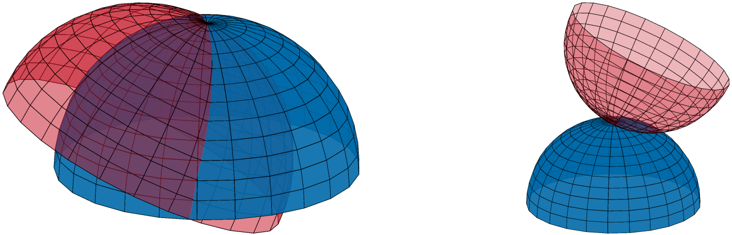
- For each $t$ we have the Fourier data $\mathcal{F}f$ on one semisphere
- Two semispheres intersect in a circle (arc), where $\mathcal{F}f$ must agree
- Find the common circle of two semispheres



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 $\mathcal{F}f(\boldsymbol{y}) = \overline{\mathcal{F}f(-\boldsymbol{y})}$
- 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

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

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

**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

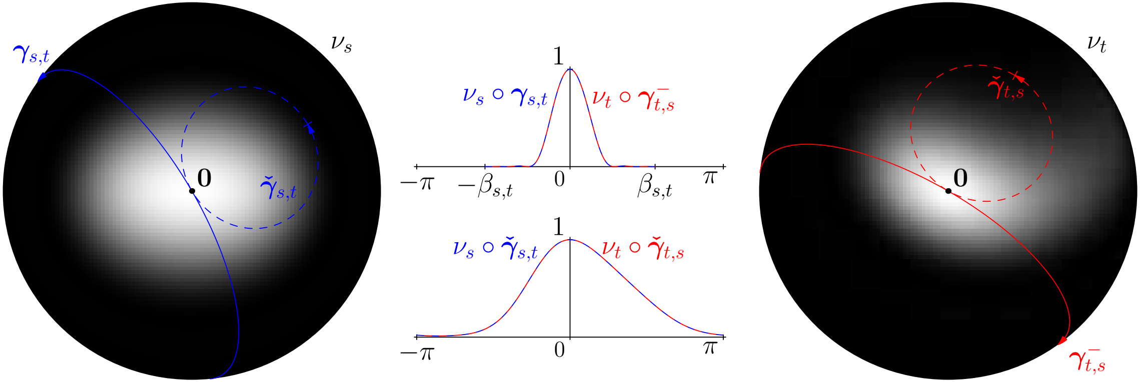
$$\nu_s(\gamma^{\varphi,\theta}(\beta)) = \nu_t(\gamma^{\pi-\psi,\theta}(-\beta)) \quad \forall \beta \in [-\tfrac{\pi}{2}, \tfrac{\pi}{2}] \quad \text{and}$$
$$\nu_s(\check{\gamma}^{\varphi,\theta}(\beta)) = \nu_t(\check{\gamma}^{\pi-\psi,\theta}(\beta)) \quad \forall \beta \in [-\tfrac{\pi}{2}, \tfrac{\pi}{2}].$$

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 $\alpha$.

# 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 2023]

Let the rotation $R \in C^1([0, T] \to \mathrm{SO}(3))$ and $t \in (0, T)$.
We define the associated **angular velocity** as the vector $\boldsymbol{\omega}_t \in \mathbb{R}^3$ satisfying

$$R_t^\top R_t' \boldsymbol{y} = \boldsymbol{\omega}_t \times \boldsymbol{y}, \qquad \boldsymbol{y} \in \mathbb{R}^3,$$

and write it in cylindrical coordinates

$$\boldsymbol{\omega}_t = \begin{pmatrix} \rho \cos \varphi \\ \rho \sin \varphi \\ \zeta \end{pmatrix}.$$

Then

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

## Reconstructing the Translation

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

**Theorem** [Q. Elbau Scherzer Steidl 2023]

Let $s,t \in [0,T]$ be such that $R_s\boldsymbol{e}^3 \neq \pm R_t\boldsymbol{e}^3$ and let $f \geq 0$ with $f \not\equiv 0$.
If $\boldsymbol{d}_0 = \mathbf{0}$, then $\boldsymbol{d}_t$ can be uniquely reconstructed from the two equations:

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

and

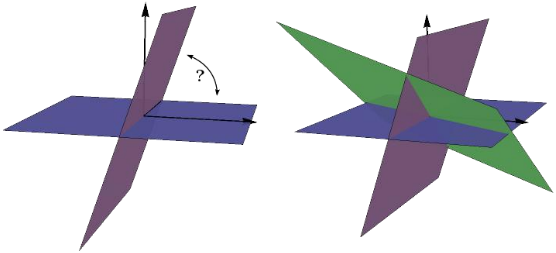
$$\mathrm{e}^{\mathrm{i}\left\langle R_t\boldsymbol{d}_t - R_s\boldsymbol{d}_s, R_s\boldsymbol{h}(\check{\gamma}_{s,t}(\beta))\right\rangle} = \frac{\mu_s(\check{\gamma}_{s,t}(\beta))}{\overline{\mu_t(\check{\gamma}_{t,s}(\beta))}}, \qquad \beta \in [-\pi,\pi],\ \mu_s(\check{\gamma}_{s,t}(\beta)) \neq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

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

# Comparision with CT

Method of common lines in Cryo-EM [Crowther DeRosier Klug 70] [van Heel 87] [Goncharov 88] [Wang Singer Zen 13]

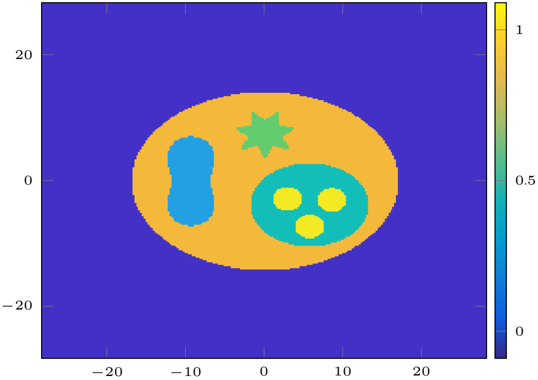
- Based on different model (ray transform)
- Requires 3 common planes (instead of 2 semi-spheres)
- Ambiguities (mirroring, translation along imaging direction)



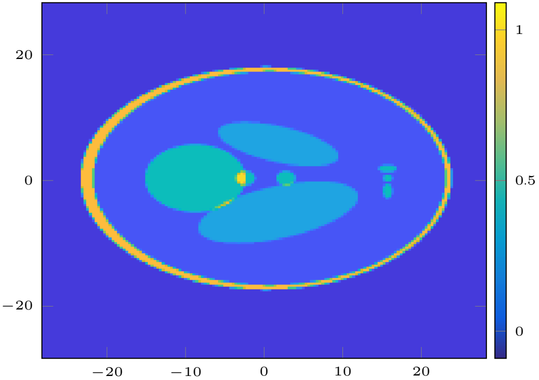

Images by [Schmutz 17]

# Numerical Simulation: Test Functions (3D)

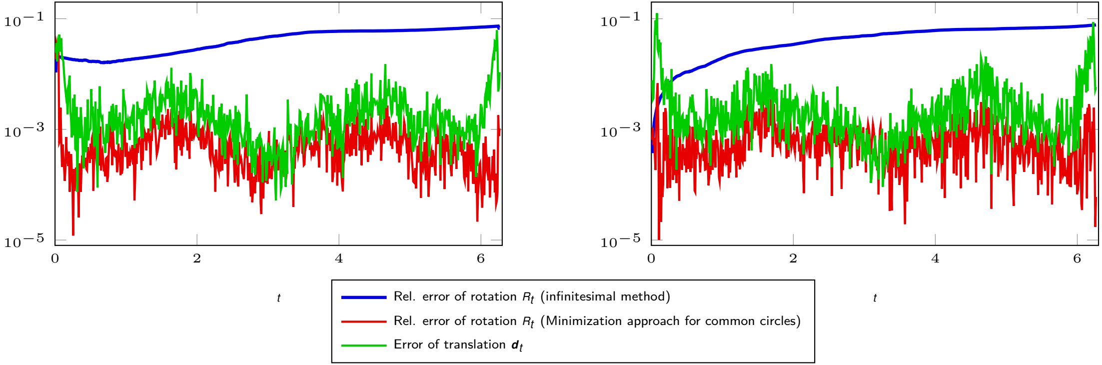
## Cell phantom




## Shepp-Logan phantom

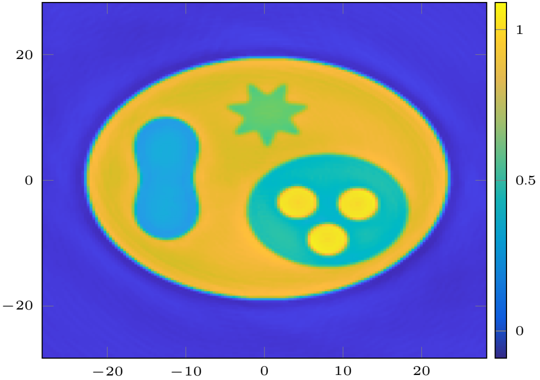


# Numerical Simulation: Results

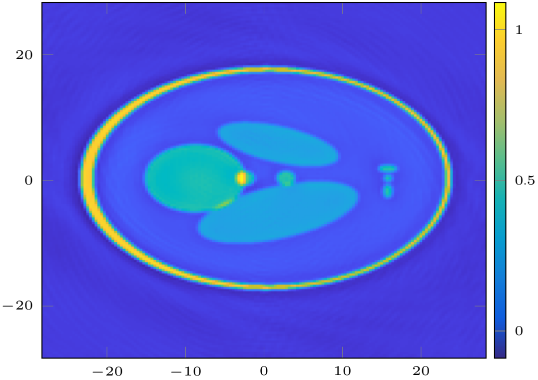



The rotation is around the moving axis $(\sqrt{1-a^2}\cos(b\sin(t/2)), \sqrt{1-a^2}\sin(b\sin(t/2)), a) \in \mathbb{S}^2$ for $a = 0.28$ and $b = 0.5$. The translation is $\boldsymbol{d}_t = 2(\sin t, \sin t, \sin t)$.
Left: cell phantom. Right: Shepp–Logan phantom.

# Reconstructed Scattering Potential $f$

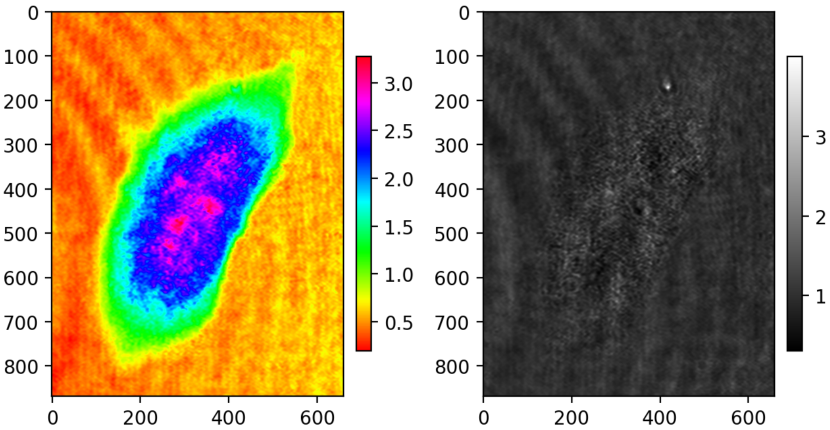



Cell phantom (PSNR 32.21, SSIM 0.754)




Shepp–Logan (PSNR 30.85, SSIM 0.772)

# Next Step: Real-World Data




Images courtesy of Franziska Strasser and Monika Ritsch-Marta (Medical University of Innsbruck)

## 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

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# Thank you for your attention!