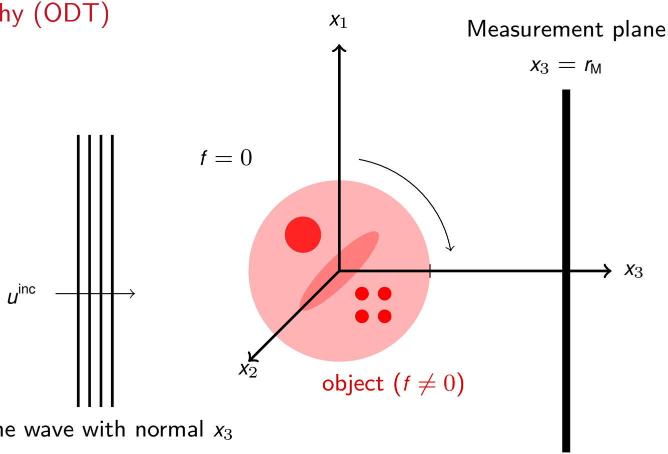
Technische Universität Berlin

Fourier Reconstruction in Diffraction Tomography of an Irregularly Moving Object

Michael Quellmalz | TU Berlin | IPMS Conference, Malta, 23 May 2022
joint work with Robert Beinert, Florian Faucher, Clemens Kirisits, Monika Ritsch-Marte, Otmar Scherzer, Eric Setterqvist, Gabriele Steidl

Optical Diffraction Tomography (ODT)

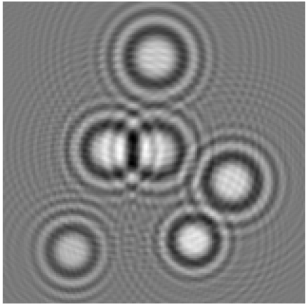


Incident field: Plane wave with normal x_3

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 imaging beam is large $\approx$ the size of the object (μm scale)



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

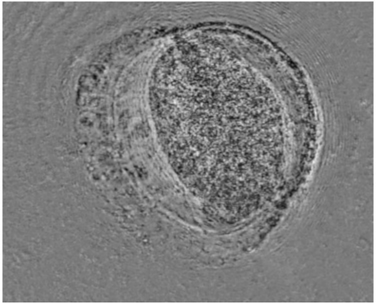


Image with diffraction

Model of Optical Diffraction Tomography (for one illumination)

- We have: field $u^{\text{tot}}(x_1, x_2, r_M)$ 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 $u^{\text{inc}}(\boldsymbol{x}) = e^{ik_0 x_3}$
- Total field $u^{\text{tot}}(\boldsymbol{x}) = u^{\text{sca}}(\boldsymbol{x}) + u^{\text{inc}}(\boldsymbol{x})$ solves the wave equation

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

- Rearranging yields

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

Born approximation

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

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

Model of Optical Diffraction Tomography (for one illumination)

- We have: field $u^{\mathrm{tot}}(x_1, x_2, r_{\mathrm{M}})$ at measurement plane $x_3 = r_{\mathrm{M}}$
- We want: scattering potential $f(\boldsymbol{x})$ with $\operatorname{supp} f \subset \mathcal{B}_{r_{\mathrm{M}}} \subset \mathbb{R}^3$
- Object illuminated by plane wave $u^{\mathrm{inc}}(\boldsymbol{x}) = \mathrm{e}^{\mathrm{i}k_0 x_3}$
- 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

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

Model of Optical Diffraction Tomography (for one illumination)

- We have: field $u^{\text{tot}}(x_1, x_2, r_{\text{M}})$ at measurement plane $x_3 = r_{\text{M}}$
- We want: scattering potential $f(\boldsymbol{x})$ with $\operatorname{supp} f \subset \mathcal{B}_{r_{\text{M}}} \subset \mathbb{R}^3$
- Object illuminated by plane wave $u^{\text{inc}}(\boldsymbol{x}) = \mathrm{e}^{\mathrm{i}k_0 x_3}$
- Total field $u^{\text{tot}}(\boldsymbol{x}) = u^{\text{sca}}(\boldsymbol{x}) + u^{\text{inc}}(\boldsymbol{x})$ solves the wave equation

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

- Rearranging yields

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

Born approximation

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

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

Model of Optical Diffraction Tomography (for one illumination)

- We have: field $u^{\mathrm{tot}}(x_1, x_2, r_\mathrm{M})$ at measurement plane $x_3 = r_\mathrm{M}$
- We want: scattering potential $f(\boldsymbol{x})$ with $\operatorname{supp} f \subset \mathcal{B}_{r_\mathrm{M}} \subset \mathbb{R}^3$
- Object illuminated by plane wave $u^{\mathrm{inc}}(\boldsymbol{x}) = \mathrm{e}^{\mathrm{i}k_0 x_3}$
- 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 $\left|u^{\mathrm{sca}}\right| \ll \left|u^{\mathrm{inc}}\right|$, we obtain

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

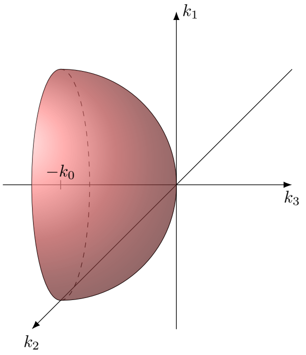
Fourier diffraction theorem [Kirisits Q. Ritsch-Marte Scherzer Setterqvist Steidl 2021]

1. scattering potential $f \in L^p$, $p > 1$, where $\operatorname{supp}(f) \subset \mathcal{B}_{r_M}$, $0 < r_M$,
2. incident field is plane wave $u^{\text{inc}}(\boldsymbol{x}) = \mathrm{e}^{\mathrm{i}k_0 x_3}$,
3. Born approximation is valid and u^{sca} satisfies the Sommerfeld condition (u^{sca} is an outgoing wave),
4. scattered field u^{sca} measured at the plane $x_3 = r_M$.

Then

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

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



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

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

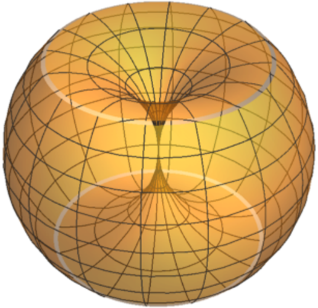
Fourier diffraction theorem (with rotation)

1. scattering potential $f \in L^p$, $p > 1$, where $\operatorname{supp}(f) \subset \mathcal{B}_{r_M}$, $0 < r_M$,
2. incident field is plane wave $u^{\mathrm{inc}}(\boldsymbol{x}) = \mathrm{e}^{\mathrm{i}k_0 x_3}$,
3. Born approximation is valid and u^{sca} satisfies the Sommerfeld condition (u^{sca} is an outgoing wave),
4. scattered field u^{sca} measured at the plane $x_3 = r_M$.

Then

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

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



Set of available Fourier space data for full rotation

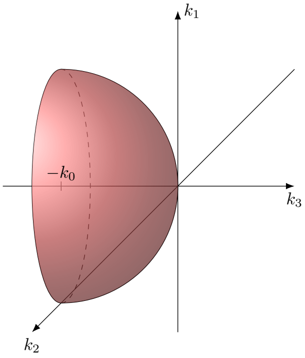
Rotation $R_t \in \mathrm{SO}(3)$ at time $t \in [0, T]$

Comparison with Computerized Tomography

Optical diffraction tomography (ODT)

diffraction of imaging beam

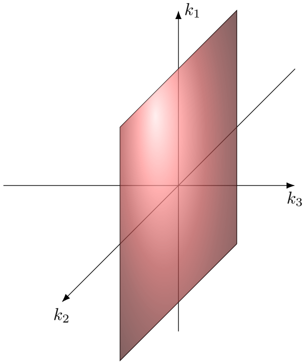
Data: Fourier transform on semispheres containing $\mathbf{0}$



Computerized tomography (CT)

light travels on lines

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



Discretization

- Uniform sampling of $f(\boldsymbol{x_k} = \boldsymbol{k}\frac{2L_\mathrm{s}}{K})$, $\boldsymbol{k} \in \mathcal{I}_K^3 := \{-K/2, \dots, K/2-1\}^3$
- Uniform sampling of measurements $u_{t_m}^{\mathrm{tot}}(\boldsymbol{y_n}, r_\mathrm{M})$, $\boldsymbol{y_n} = \boldsymbol{n}\frac{2L_\mathrm{M}}{N}$, $m = 1, \dots, M$, $\boldsymbol{n} \in \mathcal{I}_N^2$
- 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

Input: Scattered wave $\boldsymbol{v}^{\mathrm{sca}}_{m,\boldsymbol{n}} := u^{\mathrm{tot}}_{t_m}\left(\boldsymbol{n}\frac{2L_{\mathrm{M}}}{N}, r_{\mathrm{M}}\right) - \mathrm{e}^{\mathrm{i}k_0 r_{\mathrm{M}}}$, $m \in \mathcal{J}_M$, $\boldsymbol{n} \in \mathcal{I}_N^{d-1}$.

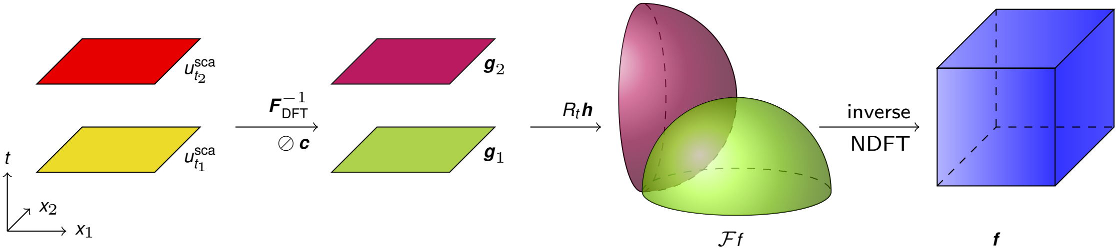
for $m = 1, \dots, M$

$\tilde{\boldsymbol{g}}_m := \boldsymbol{F}_{\mathrm{DFT}} \boldsymbol{v}^{\mathrm{sca}}_m$

$\boldsymbol{g}_m := \tilde{\boldsymbol{g}}_m \oslash \boldsymbol{c}$, where $\oslash$ is the Hadamard (entrywise) division

Solve $\boldsymbol{F}_{\mathrm{NDFT}} \boldsymbol{f} = \boldsymbol{g}$ for $\boldsymbol{f}$ (inverse NDFT)

Output: Scattering potential $\boldsymbol{f} \approx [f(\boldsymbol{x_k})]_{\boldsymbol{k} \in I_K^d}$.



Approach 1: 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

$$|\det \nabla T(k_1,k_2,t)| = \frac{k_0}{\kappa} \left| \left((1-\cos\alpha)(a_3\, \boldsymbol{a}'\cdot\boldsymbol{h} - a_3'\boldsymbol{a}\cdot\boldsymbol{h}) - a_3\, \boldsymbol{a}\cdot(\boldsymbol{a}'\times\boldsymbol{h})\sin\alpha\right) - \alpha'\,(a_1k_2 - a_2k_1) + (\boldsymbol{a}\cdot\boldsymbol{h})(a_1a_2' - a_2a_1')\sin\alpha \right|,$$

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

It is complicated to determine the Crofton symbol $\operatorname{Card}(T^{-1}(\boldsymbol{y}))$ algebraically (except for a constant $\boldsymbol{a}$).

Approach 1: 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

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

where

$$|\det \nabla T(k_1,k_2,t)| = \frac{k_0}{\kappa} \left| \left((1-\cos\alpha)(a_3\, \boldsymbol{a}'\cdot\boldsymbol{h} - a_3'\boldsymbol{a}\cdot\boldsymbol{h}) - a_3\, \boldsymbol{a}\cdot(\boldsymbol{a}'\times\boldsymbol{h})\sin\alpha \right) - \alpha'\,(a_1k_2 - a_2k_1) + (\boldsymbol{a}\cdot\boldsymbol{h})(a_1a_2' - a_2a_1')\sin\alpha \right|,$$

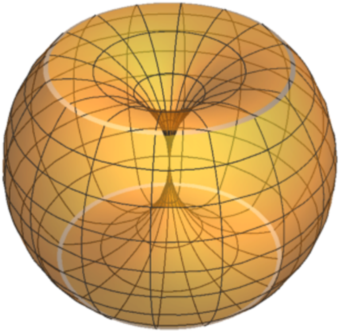
and $T(k_1,k_2,t) := R_t\boldsymbol{h}(k_1,k_2)$.

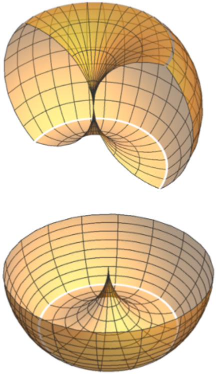
It is complicated to determine the Crofton symbol $\mathrm{Card}(T^{-1}(\boldsymbol{y}))$ algebraically (except for a constant $\boldsymbol{a}$).

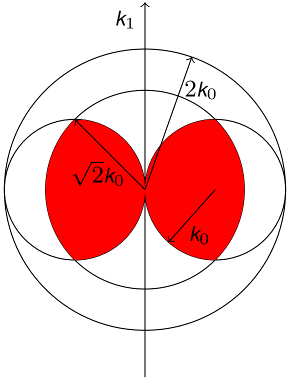
Example: Rotation Around the First Axis

[Devaney 1982]

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







Set $\mathcal{Y}$ of available data in Fourier space

Approach 2: Conjugate Gradient (CG) Method

- Inverse of the NDFT

- Find

$$\operatorname*{arg\,min}_{\boldsymbol{f}\in\mathbb{R}^{K^d}} \quad \left\|\boldsymbol{F}_{\mathrm{NDFT}}\boldsymbol{f}-\boldsymbol{g}\right\|_{2,\boldsymbol{w}}^2 = \sum_{\boldsymbol{x}} \left(\boldsymbol{F}_{\mathrm{NDFT}}\boldsymbol{f}(\boldsymbol{x}) - g(\boldsymbol{x})\right)^2 w(\boldsymbol{x})$$

- Use Conjugate Gradients (CG) on the normal equations

Approach 3: TV (Total Variation) Regularization

- Regularized inverse of the NDFT

- Find

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

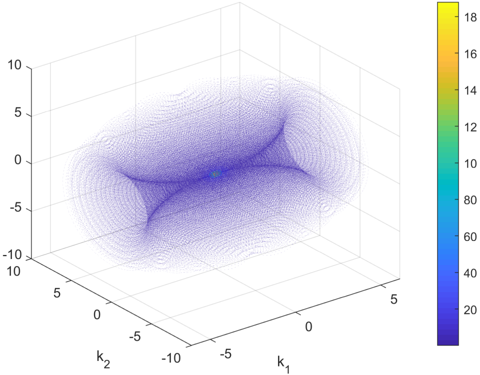
  with total variation

$$\mathrm{TV}(\boldsymbol{f}) := \sum_{\boldsymbol{k}\in\mathcal{I}_K^3} \|\operatorname{grad} \boldsymbol{f}(\boldsymbol{x_k})\|_2$$

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

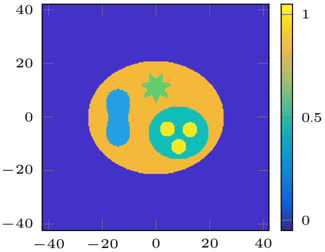
Test Setup

- Normalized wavelength $1 \Rightarrow k_0 = 2\pi$
- Test function f given analytically
- Simulate data via convolution with the Green function (also based on Born approximation) to avoid the "inverse crime"
- "missing cones" around the axis of rotation
- 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+]

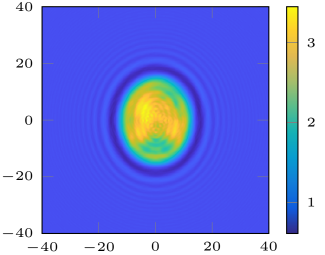


Simulated data: Fourier transform $|\mathcal{F}f|$ at 496944 nodes (constant rotation axis)

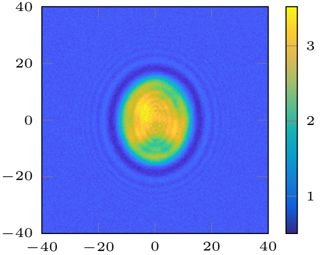
Test data



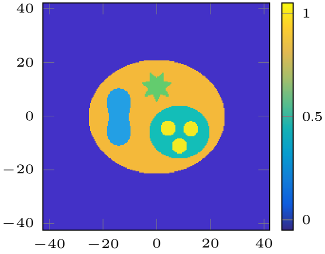
Ground truth f
($240 \times 240 \times 240$ grid)
Slice at $x_3 = 0.35$



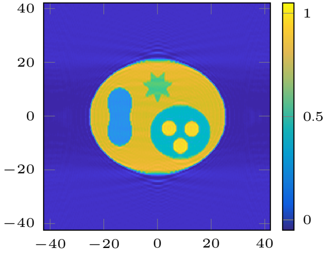
Exact data $\left|u_t^{\mathrm{tot}}(\cdot, r_{\mathrm{M}})\right|$
240×240 grid and 240 rotations



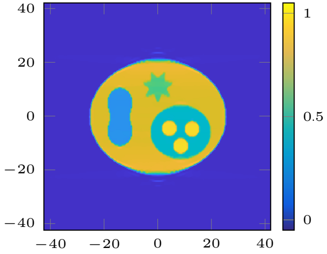
Data with 5 % Gaussian noise



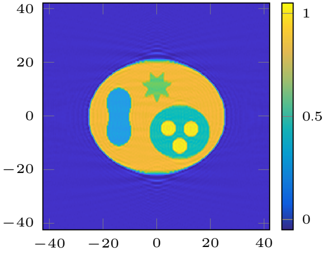
Ground truth $\boldsymbol{f}$



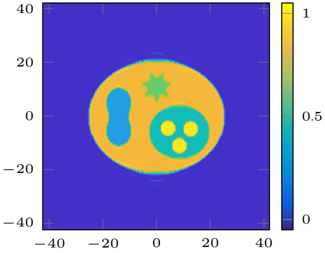
Backpropagation
PSNR 29.07, SSIM 0.614
4 sec



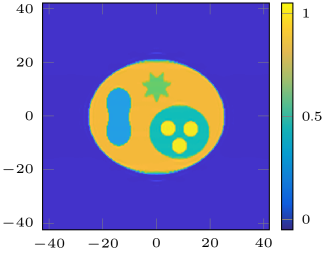
Backprop. and TVdenoise (λ=0.02)
PSNR 32.79, SSIM 0.987
37 sec



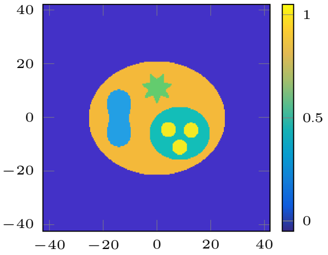
CG Reconstruction
PSNR 33.36, SSIM 0.955
79 sec



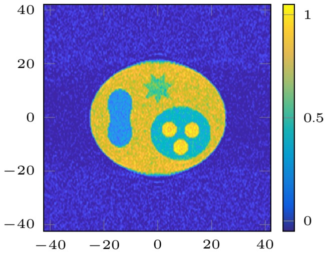
CG and TVdenoise ($\lambda = 0.02$)
PSNR 33.82, SSIM 0.988
31 sec



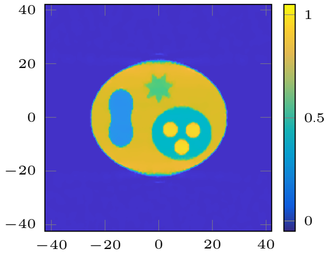
PD with TV ($\lambda = 0.02$)
PSNR 34.36, SSIM 0.957
21 min



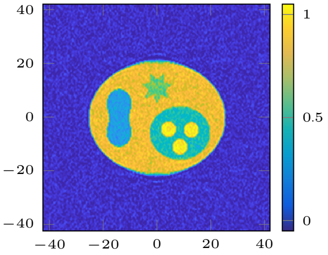
Ground truth ***f***



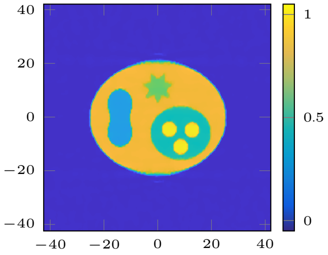
Backpropagation
PSNR 24.53, SSIM 0.178



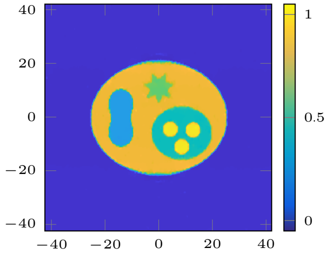
Backpropagation and TVdenoise (λ=0.05)
PSNR 32.51, SSIM 0.968



CG Reconstruction
PSNR 26.74, SSIM 0.309

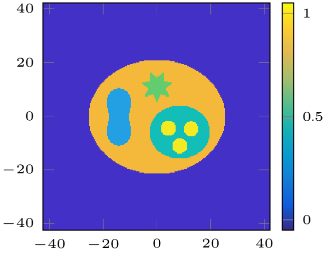


CG and TVdenoise ($\lambda = 0.02$)
PSNR 33.53, SSIM 0.965

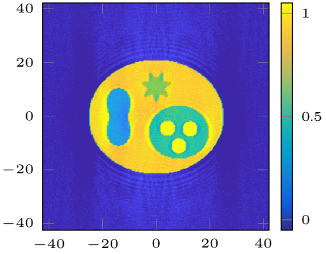


PD with TV ($\lambda = 0.02$)
PSNR 33.58, SSIM 0.736

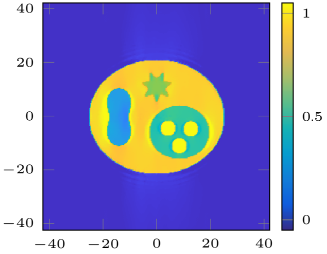
Noisy data



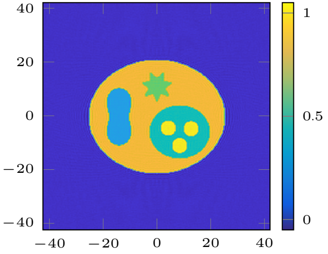
Ground truth $\boldsymbol{f}$



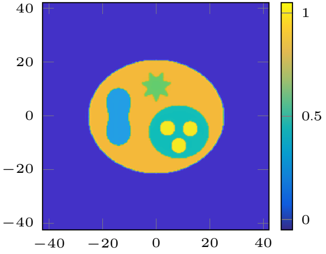
Backpropagation
PSNR 24.17, SSIM 0.171



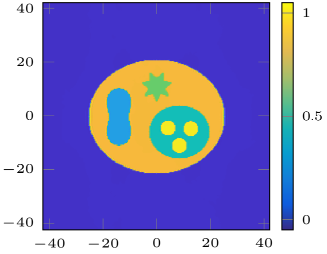
Backpropagation and TVdenoise (λ=0.02)
PSNR 29.17, SSIM 0.783



CG Reconstruction
PSNR 35.84, SSIM 0.962



CG and TVdenoise ($\lambda = 0.02$)
PSNR 36.88, SSIM 0.995



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

Moving rotation axis

Phase Retrieval

– In practice, one can often measure only the intensity

$$\left|u_t^{\mathrm{tot}}(\boldsymbol{y}, r_{\mathrm{M}})\right| = \left|u_t^{\mathrm{sca}}(\boldsymbol{y}, r_{\mathrm{M}}) + \mathrm{e}^{ik_0 r_{\mathrm{M}}}\right|, \qquad \boldsymbol{y} \in \mathbb{R}^2, t \in [0, T]$$

– Existing phase retrieval methods in diffraction tomography
  - require more measurements [Gbur & Wolf 2002] [Wedberg & Stamnes 1995]
  - use far zone approximations [Cheng & Han 2001] [Gureyev & Davis 2004]
  - Consider phase retrieval separate from reconstruction [Maleki & Devaney 1993]
  - Use techniques of ptychography [Horstmeyer Chung Ou Zheng & Yang 2016]

– We require additional information:
  - $f \geq 0$
  - f has bounded support
  - total variation of f

R Beinert, M Quellmalz.
Total Variation-Based Phase Retrieval for Diffraction Tomography.
ArXiv preprint 2201.11579, 2022.

All-at-Once Approach for Phase Retrieval

Forward operator $\boldsymbol{D}f(t, \boldsymbol{y}) = u_t^{\text{tot}}(\boldsymbol{y}, r_\text{M})$

Hybrid input-output (HIO) algorithm [Fienup 1982]

Input: Data $\boldsymbol{d} = |\boldsymbol{D}(\boldsymbol{f})| = |u^{\text{tot}}|$, parameter $\beta \in [0,1]$, support radius $r_\text{s} > 0$.

Initialize $\boldsymbol{g}^{(0)} := \boldsymbol{d}$

for $j = 0, 1, 2, \ldots$

$$\boldsymbol{f}^{(j)} := \boldsymbol{D}^{-1}\boldsymbol{g}^{(j)}$$

$$\tilde{f}_{\boldsymbol{k}}^{(j)} := \begin{cases} \max\{f^{(j)}(\boldsymbol{x_k}), 0\}, & \|\boldsymbol{x_k}\|_2 \le r_\text{s} \\ 0, & \|\boldsymbol{x_k}\|_2 > r_\text{s} \end{cases}$$

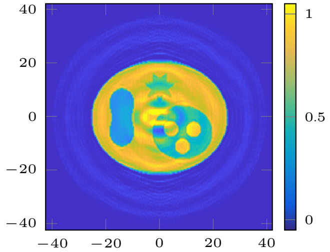
$$f^{(j+1/2)}(\boldsymbol{x_k}) := \begin{cases} f^{(j)}(\boldsymbol{x_k}), & \text{if } f^{(j)}(\boldsymbol{x_k}) = \tilde{f}^{(j)}(\boldsymbol{x_k}) \\ f^{(j-1/2)}(\boldsymbol{x_k}) - \beta(f^{(j)}(\boldsymbol{x_k}) - \tilde{f}^{(j)}(\boldsymbol{x_k})), & \text{otherwise} \end{cases}$$

$$\boldsymbol{g}^{(j+1/2)} := \boldsymbol{D}\boldsymbol{f}^{(j+1/2)}$$

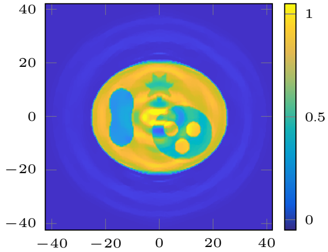
$$\boldsymbol{g}^{(j+1)} := \boldsymbol{d}\,\operatorname{sgn}(\boldsymbol{g}^{(j+1/2)})$$

Output: Approximate scattering potential $\boldsymbol{f}^{(j)}$.

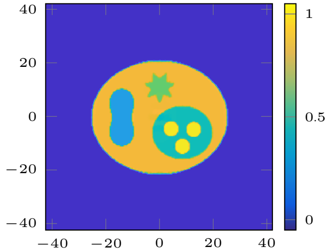
Numerical Phase Retrieval (Exact Data)



(a) HIO/CG reconstruction
$J_{\mathrm{IO}} = 10$, $J_{\mathrm{CG}} = 5$
PSNR 29.52, SSIM 0.713
5 min

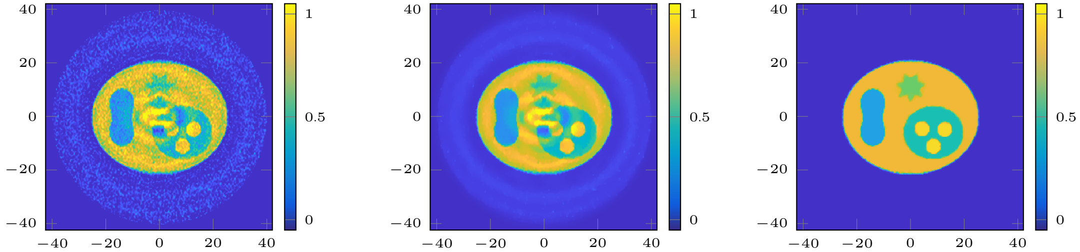


(b) HIO/CG and TVdenoise
$\lambda = 0.02$, $J_{\mathrm{TV}} = 20$
PSNR 29.88, SSIM 0.713
31 sec



(c) HIO/PD with TV
$\lambda{=}0.01$, $J_{\mathrm{IO}}{=}200$, $J_{\mathrm{PD}}{=}5$
PSNR 34.92, SSIM 0.994
3 h 48 min

Numerical Phase Retrieval (5 % Gaussian noise)



(a) HIO/CG reconstruction
$J_{\mathrm{IO}} = 10$, $J_{\mathrm{CG}} = 5$
PSNR 24.71, SSIM 0.589

(b) HIO/CG and TVdenoise
$\lambda = 0.05$, $J_{\mathrm{PD}} = 20$
PSNR 27.16, SSIM 0.623

(c) HIO/PD with TV
$\lambda{=}0.05$, $J_{\mathrm{IO}}{=}200$, $J_{\mathrm{PD}}{=}5$
PSNR 34.10, SSIM 0.993

Computational complexity

- Outer loop with HIO and inner loop with primal-dual (PD)

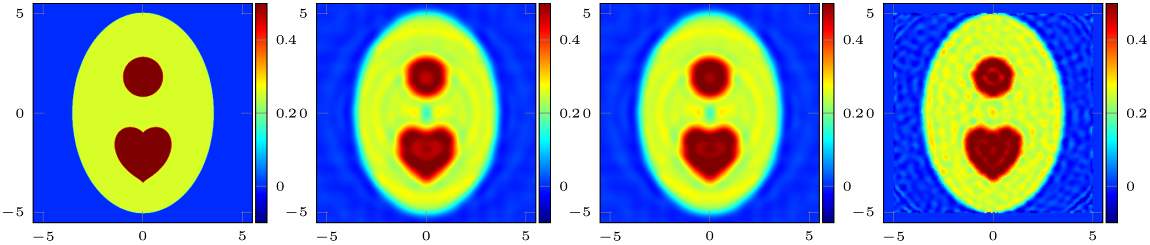
- Improvements:
- Restart primal-dual with the parameters dual variable from the previous outer step
- Use faster HIO/CG to obtain a starting solution for primal-dual
- Use fast FFT and NFFT algorithms
- Employ weights from the backpropagation to the minimization problem

Code available on `https://github.com/michaelquellmalz/FourierODT`

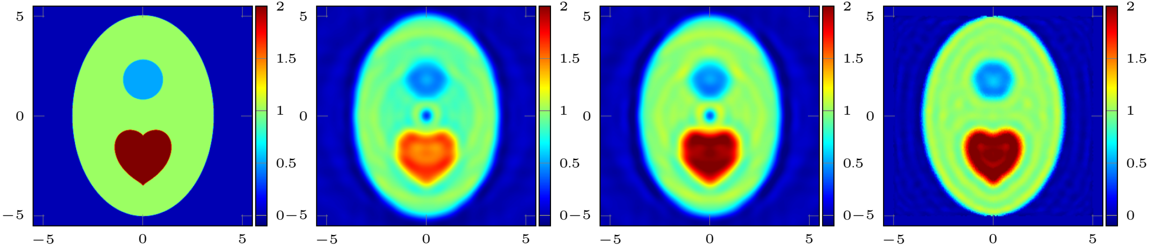
Validity of the Born approximation

- Compare Born approximation with solution of the wave equation by Full Waveform Inversion (FWI)
- Quality of Born approximation depends on object's contrast and size (in relation to k_0) [Slaney Kak Larsen 84]
- Rytov approximation is computed similarly to Born
- Numerical simulations in 2D, all using the same data

F Faucher, C Kirisits, M Quellmalz, O Scherzer, E Setterqvist.
Diffraction Tomography, Fourier Reconstruction, and Full Waveform Inversion.
Accepted for *Handbook of Mathematical Models and Algorithms in Computer Vision and Imaging*. ArXiv preprint 2110.07921, 2022.



(a) Ground truth $\boldsymbol{f}$ (b) Born reconstruction (c) Rytov Reconstruction (d) Full Waveform Inversion



(e) Ground truth $\boldsymbol{f}$ (f) Born reconstruction (g) Rytov Reconstruction (h) Full Waveform Inversion

Reconstructions for low/high contrast functions

Conclusion

- Fourier diffraction theorem on $L^p(\mathcal{B}_{r_s})$, $p > 1$
- Backpropagation formula for arbitrary rotations
- Compared reconstruction method
  - Backpropagation is faster
  - Inverse NFFT is always applicable and shows slightly better results
- Phase retrieval works well with all-at-once HIO and TV regularization

Future research

- Detection of rotation from data
- Application to real-world data

Thank you for your attention!

Conclusion

- Fourier diffraction theorem on $L^p(\mathcal{B}_{r_s})$, $p > 1$
- Backpropagation formula for arbitrary rotations
- Compared reconstruction method
  - Backpropagation is faster
  - Inverse NFFT is always applicable and shows slightly better results
- Phase retrieval works well with all-at-once HIO and TV regularization

Future research

- Detection of rotation from data
- Application to real-world data

Thank you for your attention!

Conclusion

- Fourier diffraction theorem on $L^p(\mathcal{B}_{r_s})$, $p > 1$
- Backpropagation formula for arbitrary rotations
- Compared reconstruction method
  - Backpropagation is faster
  - Inverse NFFT is always applicable and shows slightly better results
- Phase retrieval works well with all-at-once HIO and TV regularization

Future research

- Detection of rotation from data
- Application to real-world data

Thank you for your attention!