



Diffraction Tomography for Generalized Incident Fields

joint work with Otmar Scherzer and Clemens Kirisits

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Figure: Conceptual setup, tomographic data acquisition. ¹

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¹from P. Müller, M. Schürrmann, and J. Guck. "The Theory of Diffraction Tomography", 2016

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Inverse scattering problem

- $n : \mathbb{R}^3 \to \mathbb{C}$ refractive index, $n(\mathbf{r}) = 1$ outside of $\mathcal{B}_{r_s}(\mathbf{0})$
- $k_0 = \omega/c_0$ wave number
- Consider the system
 - $$\begin{split} \Delta u^{\text{inc}} + k_0^2 u^{\text{inc}} &= 0\\ \Delta u^{\text{tot}} + k_0^2 n^2 u^{\text{tot}} &= 0\\ u^{\text{tot}} &= u^{\text{sca}} + u^{\text{inc}} \end{split}$$
- $f(\mathbf{r}) := k_0^2[n(\mathbf{r})^2 1]$ scattering potential
- $\{\mathbf{r} \in \mathbb{R}^3 \mid r_3 = \pm r_M\}$ detector plane

about amplitudes and phase.

²from C. Kirisits, M. Quellmalz, M. Ritsch-Marte, O. Scherzer, E. Setterqvist, and G. Steidl. "Fourier reconstruction for diffraction tomography of an object rotated into arbitrary orientations", 2021.

• Measurement data $\mathcal{M}(r_1, r_2, \pm r_M) := [u^{\text{tot}} - u^{\text{inc}}](r_1, r_2, \pm r_M)$ include information

Reconstruct the scattering potential $f(\mathbf{r})$ from the received information $\mathcal{M}(r_1, r_2, \pm r_M)$.



Figure: Reflection and transmission imaging ²



 $r_3 = r_M$



Diffraction tomography provides under Born approximation an analytical solution to the inverse scattering problem.

It is valid if...

- ... *n* differs only weakly from the homogeneous background (small contrast)
- ...scattering is sufficiently weak such that multiple scattering can be neglected

and highly efficient with respect to computational time!

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We combine the system and obtain

$$\begin{array}{c} \Delta u^{\rm inc} + k_0^2 u^{\rm inc} = 0 \\ \Delta u^{\rm tot} + k_0^2 n^2 u^{\rm tot} = 0 \\ u^{\rm tot} = u^{\rm sca} + u^{\rm inc} \end{array} \right\} \qquad \longrightarrow \qquad \Delta u^{\rm sca} + k_0^2 u^{\rm sca} = -f(u^{\rm inc} + u^{\rm sca}).$$

Assuming $u^{\rm sca} \ll u^{\rm inc}$ we obtain the Born approximation u, that satisfies

$$\Delta u + k_0^2 u = -f u^{\rm inc}$$

and a convolution with the fundamental solution $x \to {\it G}(x) = \frac{e^{ik_0 \|x\|}}{4\pi \|x\|}$, $x \neq 0$ gives

$$u(\mathbf{r}) = \int_{\mathbb{R}^3} G(\mathbf{r} - \mathbf{r}') f(\mathbf{r}') u^{\text{inc}}(\mathbf{r}') d\mathbf{r}', \quad \mathbf{r} \in \mathbb{R}^3$$

The incident field



In conventional diffraction tomography $u^{\rm inc}$ is assumed to be a monochromatic plane wave

$$u^{\mathrm{inc}}(\mathbf{r}) = e^{ik_0\mathbf{s}_0\cdot\mathbf{r}}$$

arriving from the direction $\mathbf{s}_0 \in \mathbb{S}^2$.

For this case there are reconstruction algorithms of back-propagation type:

- A. C. Kak and M. Slaney. "Principles of Computerized Tomographic Imaging", 2001.
- A. Devaney. "A filtered backpropagation algorithm for diffraction tomography", 1982.
- C. Kirisits, M. Quellmalz, M. Ritsch-Marte, O. Scherzer, E. Setterqvist, and G. Steidl. "Fourier reconstruction for diffraction tomography of an object rotated into arbitrary orientations", 2021.

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What if the plane wave assumption is not compatible with the emitting device used in practice?

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What if the plane wave assumption is not compatible with the emitting device used in practice?

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Novel ultrasound devices allow to control the shape of the incident wave:



- Limited width of the plane wave
- Focused imaging
- → Make diffraction tomography applicable to these setups.



Figure: beam focusing³

³from https://radiologykey.com/ultrasound-12/



We extend the incident wave to be a superposition of plane waves interacting with different propagation directions:

$$u^{\mathrm{inc}}(\mathbf{r}) = \int_{\mathbb{S}^2} a(\mathbf{s}) e^{ik_0 \mathbf{s} \cdot \mathbf{r}} d\mathbf{s},$$

where $a \in L^2(\mathbb{S}^2)$.

Then, the resulting scattered wave reads as

$$u(\mathbf{r}) = \int_{\mathbb{S}^2} \mathsf{a}(\mathbf{s}) \int_{\mathbb{R}^3} \frac{e^{ik_0(\|\mathbf{r}-\mathbf{r}'\|+\mathbf{r}'\cdot\mathbf{s})}}{4\pi\|\mathbf{r}-\mathbf{r}'\|} f(\mathbf{r}') d\mathbf{r}' d\mathbf{s}, \qquad \mathbf{r} \in \mathbb{R}^3$$

and is evaluated at the measurement plane.



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Fourier diffraction result



We define

$$\begin{split} \mathbf{\bar{k}} &:= (k_1, k_2) \in \mathbb{R}^2 \\ \mathbf{\bar{k}} &= \mathbf{k}^{\pm} (\mathbf{\bar{k}}) := (\mathbf{\bar{k}}, \pm \kappa)^{\mathsf{T}} \\ \mathbf{\bar{k}} &= \kappa (\mathbf{\bar{k}}) := \begin{cases} \sqrt{k_0^2 - |\mathbf{\bar{k}}|^2}, & |\mathbf{\bar{k}}| \le k_0 \\ i\sqrt{|\mathbf{\bar{k}}|^2 - k_0^2}, & \mathbf{\bar{k}} > k_0 \end{cases} \\ \mathbf{\bar{k}} &= G_1^{\kappa}(r_M) = \sqrt{\frac{\pi}{2}} \frac{i}{\kappa} e^{i\kappa |r_M|} \end{split}$$

and perform the two-dimensional Fourier transform, such that

$$\mathcal{F}_{1,2}u(\overline{\mathbf{k}},\pm r_M) = G_1^{\kappa}(r_M) \int_{\mathbb{S}^2} a(\mathbf{s}) \mathcal{F}f(\mathbf{k}^{\pm}-k_0\mathbf{s}) d\mathbf{s}, \quad \overline{\mathbf{k}} \in \mathbb{R}^2, \ |\overline{\mathbf{k}}| < k_0$$

gives the relation between the recorded scattered wave and the scattering potential.⁴

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⁴follows from Theorem 3.1 in C. Kirisits, M. Quellmalz, M. Ritsch-Marte, O. Scherzer, E. Setterqvist, and G. Steidl. "Fourier reconstruction for diffraction tomography of an object rotated into arbitrary orientations", 2021.

Measurement setup



For 3D tomographic reconstruction:

• rotate the direction of incidence by $\mathcal{R} \in SO(3)$

•
$$u^{\text{inc}}(\mathbf{r}, \mathcal{R}) = \int_{\mathbb{S}^2} a(\mathbf{s}) e^{ik_0 \mathcal{R}^{\mathsf{T}} \mathbf{s} \cdot \mathbf{r}} d\mathbf{s}$$

resulting scattered wave $u(\mathbf{r}, \mathcal{R})$ satisfies

$$(\Delta + k_0^2)u(\mathbf{r}, \mathcal{R}) = -f(\mathbf{r})u^{\text{inc}}(\mathbf{r}, \mathcal{R})$$

• measurements given by $\mathcal{M}(\bar{\mathbf{k}}, \pm r_M, \mathcal{R}) = \mathcal{F}_{1,2}u(\bar{\mathbf{k}}, \pm r_M, \mathcal{R})$

We propose the following setups:

Rotation of incidence direction and fixed measurement plane

Rotation of the object

The measurements are related to the scattering potential via

$$\mathcal{M}(\overline{k}, \pm r_M, \mathcal{R}) = G_1^{\kappa}(r_M) \int_{\mathbb{R}^2} a(\mathcal{R}^{\intercal-1}s) \mathcal{F}f(k^{\pm} - k_0 s) ds,$$

for all $\overline{\mathbf{k}} \in \mathbb{R}^2$ and all $\mathcal{R} \in SO(3)$.



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We propose the following setups:

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The measurements are related to the scattering potential via

$$\mathcal{M}(\overline{\mathbf{k}},\pm r_M,\mathcal{R})=G_1^\kappa(r_M)\int_{\mathbb{R}^2}a(\mathcal{R}^{\intercal-1}\mathbf{s})\mathcal{F}f(\mathbf{k}^{\pm}-k_0\mathbf{s})d\mathbf{s},$$

for all $\overline{\mathbf{k}} \in \mathbb{R}^2$ and all $\mathcal{R} \in SO(3)$.





We rewrite the equation to

$$\mathcal{M}(\mathcal{R}) = G_1^{\kappa}(r_M) \int_{\mathbb{S}^2} a(\mathcal{R}^{\intercal-1}\mathbf{s})g(\mathbf{s})d\mathbf{s},$$

where $g(\mathbf{s}) = \mathcal{F}f(\mathbf{k}^{\pm} - k_0\mathbf{s})$ for fixed $\overline{\mathbf{k}} \in \mathbb{R}^2$.

• $g \in L^2(\mathbb{S}^2)$ has a expansion in spherical Fourier series

$$g(s) = \sum_{n\geq 0} \sum_{k=-n}^{n} g_n^k Y_n^k(s),$$

where the basis elements Y_n^k are spherical harmonics (Basis of $L^2(\mathbb{S}^2)$)

The rotated function $a \in L^2(\mathbb{S}^2)$ has the expansion

$$a(\mathcal{R}^{\top-1}\mathbf{s}) = \sum_{n\geq 0} \sum_{k=-n}^{n} a_n^k Y_n^k(\mathcal{R}^{\top-1}\mathbf{s}) = \sum_{n\geq 0} \sum_{k=-n}^{n} a_n^k \sum_{j=-n}^{n} D_n^{j,k}(\mathcal{R}^{\top}) Y_n^j(\mathbf{s})$$

where $a_n^k = \langle a, Y_n^k \rangle_{L^2(\mathbb{S}^2)}$ and $D_n^{j,k}$ are Wigner D-matrices.

⁵P. Kostelec, D. N. Rockmore. "FFTs on the Rotation Group", 2003.

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$$\mathcal{M}(\mathcal{R}) = G_1^\kappa(r_M) \int_{\mathbb{S}^2} a(\mathcal{R}^{\intercal-1} \mathbf{s}) g(\mathbf{s}) d\mathbf{s}, \quad ext{for all } \mathcal{R} \in SO(3)$$

Using

- the basis representations of $a, g \in L^2(\mathbb{S}^2)$ and
- calculating the rotational Fourier coefficients $\mathcal{M}_n^{j,k} = \langle \mathcal{M}, D_n^{j,k} \rangle_{L^2(SO(3))}$
- the orthogonality properties

$$\begin{split} \langle Y_{n}^{k}, Y_{n'}^{k'} \rangle_{L^{2}(\mathbb{S}^{2})} &= \delta_{n,n'} \delta_{k,k'} \\ \langle D_{n}^{j,k}, D_{n'}^{j',k'} \rangle_{L^{2}(SO(3))} &= \frac{8\pi^{2}}{2n+1} \delta_{n,n'} \delta_{j,j'} \delta_{k,k'} \end{split}$$

gives the spherical Fourier coefficients

$$g_n^j = \frac{2n+1}{8\pi^2 G_1^\kappa(r_M)} \frac{\mathcal{M}_n^{j,k}}{a_n^k}, \quad \text{for all } n \in \mathbb{N}_0, \ j,k = -n \dots, n$$

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Let $\mathcal{M} \in L^2(SO(3))$ and $a \in L^2(\mathbb{S}^2)$ be given. Find $g \in L^2(\mathbb{S}^2)$ from

$$\mathcal{M}(\mathcal{R}) = G_1^{\kappa}(\mathbf{r}_M) \int_{\mathbb{S}^2} \mathsf{a}(\mathcal{R}^{\intercal-1}\mathbf{s}) \mathbf{g}(\mathbf{s}) d\mathbf{s},$$

for all $\mathcal{R} \in SO(3)$.

Calculate

$$a_n^k = \langle a, Y_n^k \rangle_{L^2(\mathbb{S}^2)}, \text{ for all } n \in \mathbb{N}_0, \ k = -n \dots, n,$$

$$\mathcal{M}_n^{j,k} = \langle \mathcal{M}, D_n^{j,k} \rangle_{L^2(SO(3))}, \text{ for all } n \in \mathbb{N}_0, \ j, k = -n \dots, n,$$

$$g_n^j = \frac{2n+1}{8\pi^2 G_1^{\kappa}(r_M)} \frac{\mathcal{M}_n^{j,k}}{a_n^k}, \text{ for all } n \in \mathbb{N}_0, \ j, k = -n \dots, n,$$

then we reconstruct

$$g(\mathbf{s}) = \sum_{n \ge 0} \sum_{j=-n}^{n} g_n^j Y_n^j(\mathbf{s}).$$

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Finally, we obtain the relation

$$\sum_{n\geq 0}\sum_{j=-n}^{n}\frac{2n+1}{8\pi^{2}G_{1}^{\kappa}(r_{M})}\frac{\mathcal{M}_{n}^{j,k}(\overline{\mathbf{k}})}{a_{n}^{k}}Y_{n}^{j}(\mathbf{s})=\mathcal{F}f(\mathbf{k}^{\pm}-k_{0}\mathbf{s}),$$

for all $\overline{\mathbf{k}} \in \mathbb{R}^2$, $|\overline{\mathbf{k}}| < k_0$, $\mathbf{s} \in \mathbb{S}^2$ and $n \in \mathbb{N}_0$, $j, k = -n \dots, n$.

• scattering potential f can be obtained via the inverse Fourier transformation

measurements provide access to f on a volume

$$\left\{ (\mathbf{k}^{\pm} - k_0 \mathbf{s}): \ \overline{\mathbf{k}} \in \mathbb{R}^2, |\overline{\mathbf{k}}| < k_0, \ \mathbf{s} \in \mathbb{S}^2 \right\}$$

in k-space.

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3D frequency coverage for reflection imaging according to a parametrization ${\bf s}(\theta,\varphi)\in\mathbb{S}^2$ reads as

$$\left\{ \begin{pmatrix} k_1 - k_0 \sin\theta\cos\varphi \\ k_2 - k_0 \sin\theta\sin\varphi \\ -\kappa(\overline{\mathbf{k}}) - k_0 \cos\theta \end{pmatrix} : \ \overline{\mathbf{k}} \in \mathbb{R}^2, |\overline{\mathbf{k}}| < k_0, \ \theta \in [0, \pi], \ \varphi \in [0, 2\pi) \right\}$$

and we illustrate for $k_0 = 0.5$:



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- Currently, we work on implementation and numerical tests
- Limited view: Reconstructing f from a few rotation angles, i.e. if the available measurement data are limited.

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Thank you!

Noemi Naujoks

Diffraction Tomography for Generalized Incident Fields

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