Propagation-based phase contrast imaging with X-rays – from uniqueness theory to nano-scale reconstructions

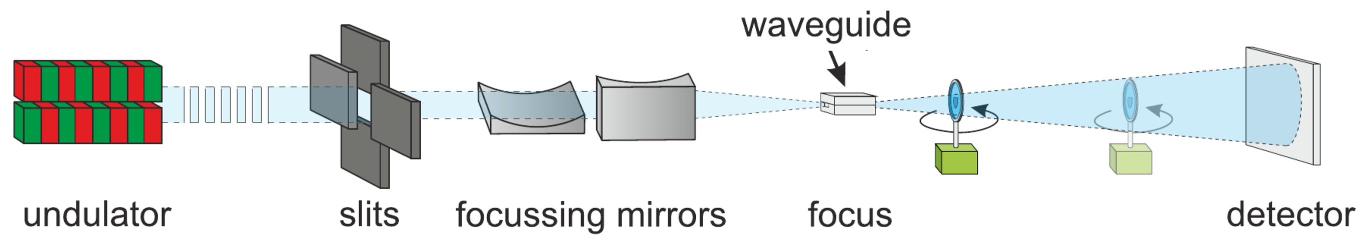
Simon Maretzke

1. Introduction

Motivation: Imaging with X-rays permits nano-scale resolution owing to small wavelengths $\lesssim 1$ nm but suffers from weak absorption for microscopic light-element samples.

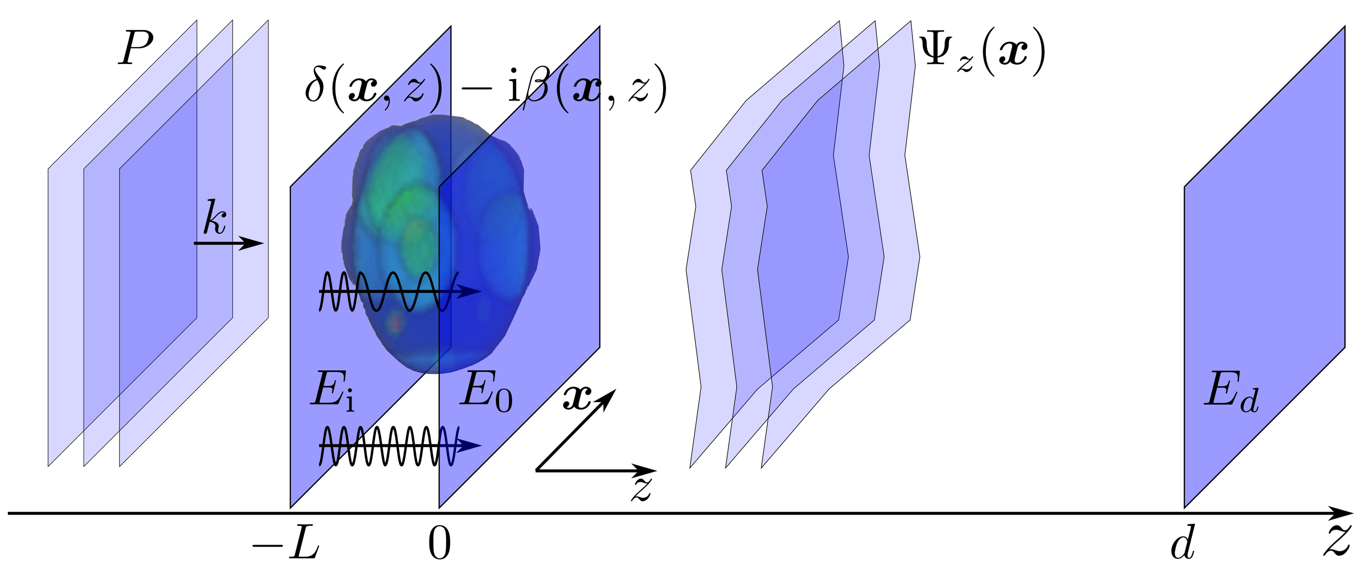
$\rightsquigarrow$ **Need for *refraction*-based imaging techniques** $\rightsquigarrow$ ***phase contrast***

Imaging Setup: A specimen is illuminated by coherent X-rays (e.g. from synchrotrons, FELs), resulting diffraction patterns are recorded downstream at propagation distance d:



Physical Model:

- Sample characterized by spatially varying refractive index $n = 1 - \delta + \mathrm{i}\beta$ $(\delta, \beta \geq 0)$
- δ, β induce phase shifts + absorption to incident probe wave field P (*ray approximation*)
- Free-space propagation in $z \in [0; d]$ encodes phase into detectable intensities $I = |\Psi_d|^2$



Forward Operator: (paraxial Helmholtz + ray optics in sample → valid for X-rays [2])

$$F_{\mathrm{image}}(\boldsymbol{n}) := I = \Big| \underbrace{\mathcal{D}}_{\text{Fresnel propagator}} \underbrace{(P \cdot \exp(-\mathrm{i}k\boldsymbol{n}))}_{\text{exit wave field } \Psi_0 = P \cdot O} \Big|^2, \quad \boldsymbol{n} = \int_{-L}^{0} \underbrace{(\delta - \mathrm{i}\beta)}_{\text{Refraction (+absorption)}} \, \mathrm{d}z \qquad (1)$$

Inverse Problem 1 (Propagation-based Phase Contrast Imaging):
Reconstruct the object transmission function (OTF) O from intensity data I given by (1).

Phase Contrast Tomography: Illuminate the sample at different incident angles θ ⇒ resulting OTFs $\{O_\theta\}$ given by ensemble of rotated line integrals ⇒ 2D *Radon transform*:

$$F_{\mathrm{tomo}}(\delta - \mathrm{i}\beta) := \{I_\theta\} = \left|\mathcal{D}\left(P \cdot \exp\left(-\mathrm{i}k\mathcal{R}(\delta - \mathrm{i}\beta)\right)\right)\right|^2 \qquad (2)$$

Inverse Problem 2 (Propagation-based Phase Contrast Tomography):
From tomographic intensity data $\{I_\theta\}$ given by (2), reconstruct the sample structure $\delta - \mathrm{i}\beta$.

2. Uniqueness Results

Phase Retrieval Problem: Solving **IP1** and **IP2** requires inversion of $|\cdot|^2$, i.e. *phase recovery*, due to the physical restriction of detector measurements to wave *intensities*

$\rightsquigarrow$ **Can we uniquely reconstruct the phase + absorption image?**

Theorem (Uniqueness of Phase Contrast Imaging and Tomography [6]): *Let P be a known plane wave or Gaussian beam and let $\delta - \mathrm{i}\beta$ be compactly supported. Then*

- **IP1** *is uniquely solvable from intensity data $I_{|U}$ on an arbitrary open set $U \subset \mathbb{R}^m$*
- **IP2** *is uniquely solvable from data $\{I_{\theta|U}\}_{\theta \in V}$ on $U \subset \mathbb{R}^m, \theta \subset \mathbb{S}^1$ open if $k\mathcal{R}(\delta) \in [0; 2\pi)$*

Basic ideas: If $\delta_j - \mathrm{i}\beta_j$ compactly supported, so are the wave disturbances $h_j := P \cdot (O_j - 1)$:

$$F_{\mathrm{image}}(O_1) - F_{\mathrm{image}}(O_2) = \underbrace{\mathcal{D}(h_1 - h_2)}_{\text{(A)}} + \underbrace{\overline{\mathcal{D}(h_1 - h_2)}}_{\text{(B)}} + \underbrace{|\mathcal{D}(h_1)|^2 - |\mathcal{D}(h_2)|^2}_{\text{(C)}} \qquad (\text{case } P = 1)$$

- $\mathcal{D} = \gamma \exp(\mathrm{i}\boldsymbol{\xi}^2) \cdot \mathcal{F}(\exp(\mathrm{i}\boldsymbol{x}^2) \cdot h_j)$ related to the Fourier transform $\mathcal{F}$
- $\exp(-\mathrm{i}\boldsymbol{\xi}^2) \cdot \mathcal{D}(h_j) \propto \mathcal{F}(\exp(\mathrm{i}\boldsymbol{x}^2) \cdot h_j)$ *entire function* of exponential type by Paley-Wiener
- **(A)**, **(B)**, **(C)** grow *superexponentially* in disjoints subsets of $\mathbb{C}^m$ if $h_1 \neq h_2 \Rightarrow h_1 = h_2$

3. Reconstructions and Stability for 2D-Imaging

Numerical approach: Solve **IP1** by iteratively regularized Gauss-Newton method:

$$\boldsymbol{n}_{k+1} = \underset{\boldsymbol{n}}{\operatorname{argmin}} \left\| F_{\mathrm{image}}(\boldsymbol{n}_k) + F'_{\mathrm{image}}[\boldsymbol{n}_k](\boldsymbol{n} - \boldsymbol{n}_k) - I \right\|_{L^2}^2 + \alpha_k \left\| \boldsymbol{n} - \boldsymbol{n}_0 \right\|_{H^s}^2$$

- *Non-absorbing samples* ($\beta = 0$): Favorable robustness and improved accuracy compared to commonly used (approximate) direct inversion formulas [4]
- *General samples* ($\delta, \beta \neq 0$): Faithful reconstructions up to characteristic *halo artifacts*:

(a) Intensity data (GINIX/DESY [3]) **(b)** Reconstructed refraction $\int_{-L}^{0} \delta \, \mathrm{d}z$ **(c)** Reconstructed absorption $\int_{-L}^{0} \beta \, \mathrm{d}z$

Stability analysis: For $P = 1$ and $h = O - 1$ s.t. $|h| \ll 1$, $\mathrm{supp}(h) \subset \Omega$ compact:

$$\mathcal{D}(F_{\mathrm{image}}(\boldsymbol{n}) - 1) = \underbrace{\mathcal{D}^2(h)}_{\neq 0 \text{ a.e.}} + \underbrace{\overline{h}}_{= 0 \text{ in } \mathbb{R}^m \setminus \Omega} + \mathcal{O}(|h|^2)$$

$$\overset{\mathcal{D} \text{ unitary}}{\Rightarrow} \tfrac{1}{2}\left\|F_{\mathrm{image}}(\boldsymbol{n}) - 1\right\|_{L^2}^2 \geq \left\|\mathcal{D}^2(h)_{|\mathbb{R}^m \setminus \Omega}\right\|_{L^2}^2 = \left\|\mathcal{F}(\exp(\mathrm{i}\boldsymbol{x}^2/2) \cdot h)_{|\mathbb{R}^m \setminus \Omega}\right\|_{L^2}^2 \geq (1 - \sigma_0^2)\|h\|_{L^2}^2$$

- $\sigma_0 < 1$: maximum singular value of $\mathcal{F}_\Omega : L^2(\Omega) \to L^2(\Omega)$; $f \mapsto \mathcal{F}(f)_{|\Omega}$
- Worst-case-signals given by principal singular modes $\rightsquigarrow$ *low-frequency halos*

4. Newton-Kaczmarz Method for Phase Contrast Tomography

Standard method in phase contrast tomography:

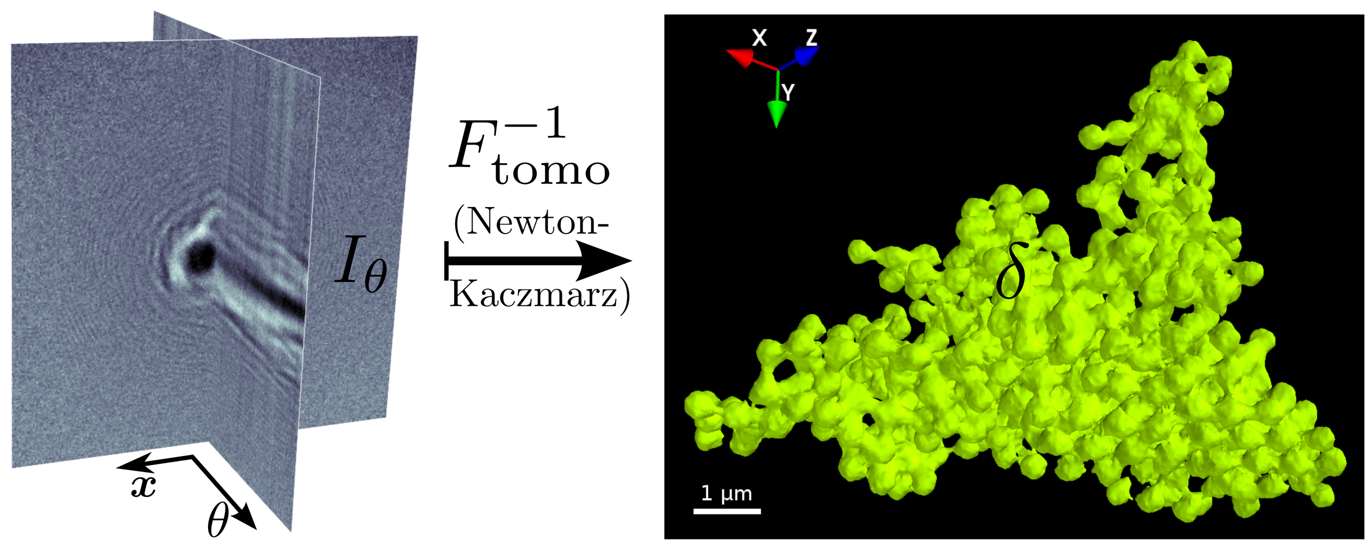
1. *Independent* phase retrieval for all incident angles: $F_{\mathrm{tomo}}(\delta - \mathrm{i}\beta) \mapsto \mathcal{R}(\delta - \mathrm{i}\beta)$
2. *Subsequent* tomographic reconstruction by Radon inversion: $\mathcal{R}(\delta - \mathrm{i}\beta) \mapsto \delta - \mathrm{i}\beta$

Simultaneous approach: *All-at-once* inversion of F_{tomo} by regularized Newton methods

- *Benefit:* Stabilization of reconstruction by exploitation of tomographic correlations [5]
- *Drawback:* Computationally expensive as $F, F'[\boldsymbol{n}_k], F'[\boldsymbol{n}_k]^*$ map large 3D data sets
- *Remedy:* Process small subsets of incident angles per iteration → *Newton-Kaczmarz* [1]:

$$n_{k+1} = \underset{n}{\operatorname{argmin}} \underbrace{\left\| \mathcal{P}_k \left(F_{\mathrm{tomo}}(n_k) + F'_{\mathrm{tomo}}[n_k](n - n_k) - I\right) \right\|_{L^2}^2}_{\text{restriction to small wedges of incident angles}} + \underbrace{\alpha_k \left\|n - n_0\right\|_{X_k}^2}_{\text{approximate } L^p\text{, TV, positivity, …}} + \underbrace{\alpha_0 \left\|n - n_k\right\|_{L^2}^2}_{\text{strong regularization} \Rightarrow \text{well-conditioned}}$$

$\rightsquigarrow$ **Efficient + accurate combination of phase retrieval and tomography**



5. References

[1] Burger M and Kaltenbacher B. Regularizing Newton–Kaczmarz methods for nonlinear ill-posed problems. *SIAM Journal on Numerical Analysis*, 44(1):153–182, 2006.

[2] Jonas P and Louis A. Phase contrast tomography using holographic measurements. *Inverse Problems*, 20(1):75, 2004.

[3] Kalbfleisch S, Neubauer H, Krüger S, Bartels M, Osterhoff M, Giewekemeyer K, Hartmann B, Sprung M, and Salditt T. The Göttingen holography endstation of beamline P10 at PETRA III/DESY. *AIP Conference Proceedings*, 1365(1):96–99, 2011.

[4] Krenkel M, Töpperwien M, Bartels M, Lingor P, Schild D, and Salditt T. X-ray phase contrast tomography from whole organ down to single cells. *SPIE Proceedings*, (9210):92120R, 2014.

[5] Maretzke S. Regularized Newton methods for simultaneous Radon inversion and phase retrieval in phase contrast tomography. *arXiv preprint*, page arXiv:1502.05073, 2015.

[6] Maretzke S. A uniqueness result for propagation-based phase contrast imaging from a single measurement. *Inverse Problems*, 31:065003, 2015.

Acknowledgements: Support by the German Research Foundation DFG through the Collaborative Research Center 755 – Nanoscale Photonic Imaging is gratefully acknowledged.

Any questions?
Just ask me:

Simon Maretzke
Institute for Numerical and Applied Mathematics /
SFB 755 - Nanoscale Photonic Imaging
University of Goettingen
E-mail: s.maretzke@math.uni-goettingen.de

joint work with:
Thorsten Hohage
Tim Salditt