Propagation-based Phase Contrast X-ray Imaging – from Stability Estimates to 3D-Nanoscopy

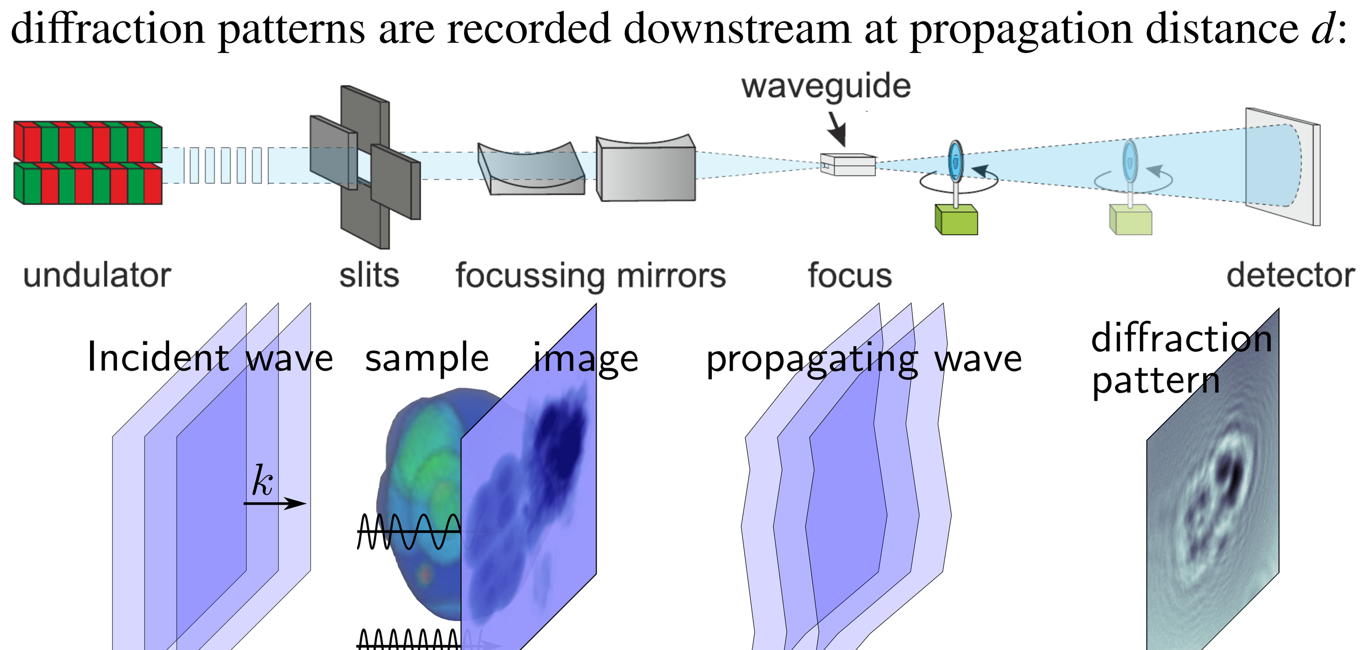
Project C02: Thorsten Hohage, Simon Maretzke

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 samples.

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

Imaging setup: Specimen is illuminated by coherent X-rays (e.g. from synchrotron [5]), resulting diffraction patterns are recorded downstream at propagation distance d:



Forward model: $F_{\mathrm{PCI}} : \boldsymbol{n} = \underbrace{\int_{-L}^{0} (\delta - \mathrm{i}\beta)\,\mathrm{d}z}_{\substack{\text{Phase shifts}\\ \text{(+absorption)}}} \mapsto I_{\mathrm{PCI}} = \Big| \underbrace{\mathcal{D}}_{\substack{\text{Fresnel}\\ \text{propagator}}} \underbrace{(\exp(-\mathrm{i}k\boldsymbol{n}))}_{\text{exit wave field}} \Big|^2$

unknown image $\mapsto$ **measurable intensity data**

- ▶ Model based on paraxial Helmholtz eq. + ray optics in sample → valid for X-rays [1]
- ▶ Images yield 2D-projections of the object's complex *refractive index* $n = 1 - \delta + \mathrm{i}\beta$

Phase contrast tomography: Image the refractive index *in 3D* by recording diffraction patterns under different incident angles θ (model: Radon transform $\mathcal{R}$)

$$F_{\mathrm{PCT}} : \ \tilde{n} = (\delta - \mathrm{i}\beta) \ \mapsto \ \{I_{\mathrm{PCI},\theta}\} = \left|\mathcal{D}\left(\exp\left(-\mathrm{i}k\mathcal{R}(\tilde{n})\right)\right)\right|^2$$

Inverse Problem: Reconstruct the 2D- or 3D-image $\boldsymbol{n}$ or $\tilde{n}$ from observed noisy data $I^{\varepsilon} = I_* + \boldsymbol{\varepsilon}$ and available *a priori* knowledge, i.e. *invert* the forward map F_*.

2. Phase Retrieval - an Unstable Procedure?

Phase retrieval: Image reconstruction requires inversion of $|\cdot|^2$, i.e. *phase recovery*, due to the physical restriction to measuring wave *intensities*

Is the image uniquely determined by the data? Yes! [3]

$\rightsquigarrow$ Is the reconstruction robust to measurement errors? ...

Weak object approximation: *Linearize* F_{PCI} in $h := -\mathrm{i}k\boldsymbol{n} = -\mu - \mathrm{i}\phi$ (valid if $\phi, \mu \ll 1$)

$$F_{\mathrm{PCI}}(\boldsymbol{n}) - 1 \approx \underbrace{\mathcal{D}(h)}_{\text{image}} + \underbrace{\mathcal{D}^{-1}(\overline{h})}_{\text{twin image}} =: T_{\mathrm{PCI}}h \qquad (\phi\text{: phase shifts, } \mu\text{: absorption})$$

Stability problem: Is there a constant $C_A > 0$ such that for all images $h_1, h_2 \in A \subset L^2(\mathbb{R}^2)$

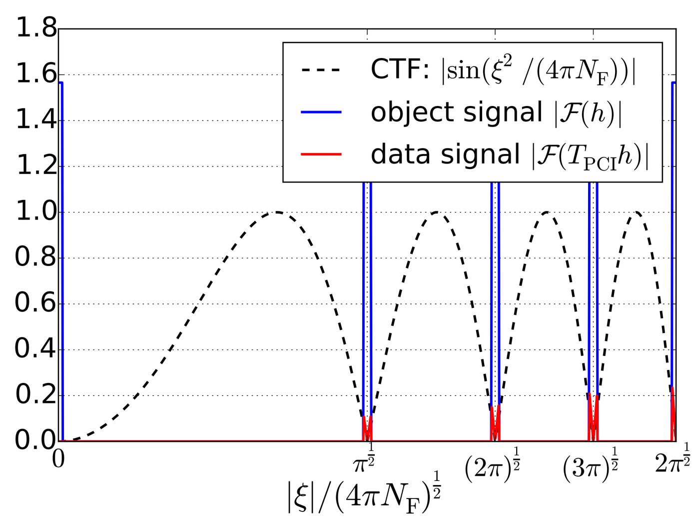
$$C_A \underbrace{\|h_1 - h_2\|}_{\text{object perturbation}} \leq \underbrace{\|T_{\mathrm{PCI}}(h_1 - h_2)\|}_{\text{increment in the data}} \ ? \quad \Leftrightarrow \quad \textbf{reconstruction error} \leq C_A^{-1}\|\varepsilon\|$$

Common a priori constraints – general instability:

- ▶ *Non-absorbing object*: $\mu = 0$ (biological tissue)
- ▶ *Single-material*: $\mu = \tan(\varphi_0)\phi$ (more general)

$$\Rightarrow \ T_{\mathrm{PCI}}h \propto 2\mathcal{F}^{-1}\Big(\underbrace{\sin\Big(\frac{\xi^2}{4\pi N_{\mathrm{F}}} + \varphi_0\Big)}_{\text{contrast transfer fct. (CTF)}} \underbrace{\mathcal{F}}_{\substack{\text{Fourier}\\ \text{transform}}}(h)\Big)$$

- ▶ Arbitrarily low contrast at CTF-zeros $\rightsquigarrow$ bad SNR
- ▶ Unstable reconstruction without further constraints



$\rightsquigarrow$ **How to choose the admissible objects A to ensure stability?**

References

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

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

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

[4] Maretzke S, Bartels M, Krenkel M, Salditt T, and Hohage T. Regularized Newton methods for X-ray phase contrast and general imaging problems. *Optics Express*, 2016. (accepted).

[5] Salditt T, Osterhoff M, Krenkel M, Wilke R N, Priebe M, Bartels M, Kalbfleisch S, and Sprung M. Compound focusing mirror and x-ray waveguide optics for coherent imaging and nano-diffraction. *Journal of synchrotron radiation*, 22(4):867–878, 2015.

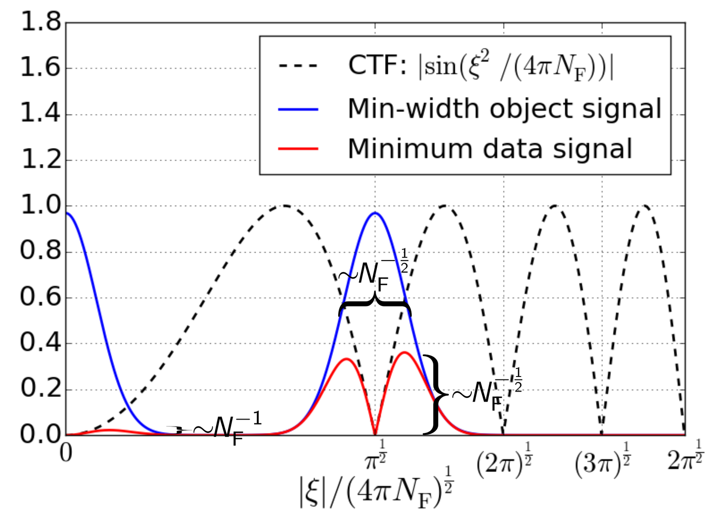
[6] Slepian D and Sonnenblick E. Eigenvalues associated with prolate spheroidal wave functions of zero order. *Bell System Technical Journal*, 44(8):1745–1759, 1965.

3. Stability Estimates for Single-Material Objects

Support constraint: Object h is contained in a known subdomain $\Omega \subset \mathbb{R}^2$ of the field of view.

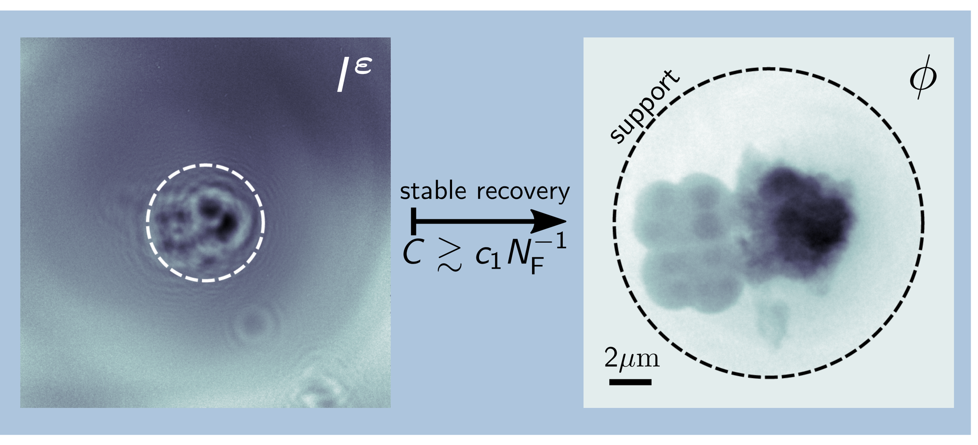
Uncertainty principle: Restriction $\mathrm{supp}(h) \subset \Omega$ in real-space induces a *minimum* lengthscale in Fourier space:

$$\underbrace{\sigma_{|h|^2}}_{\leq \mathrm{diam}(\Omega)} \cdot \ \sigma_{|\mathcal{F}(h)|^2} \gtrsim 1$$



Theorem 1: Let N_{F} the Fresnel number of the support diameter $\mathrm{diam}(\Omega)$. Then the recovery of *single-material objects* $h \propto \phi \in L^2(\Omega)$ is stable with

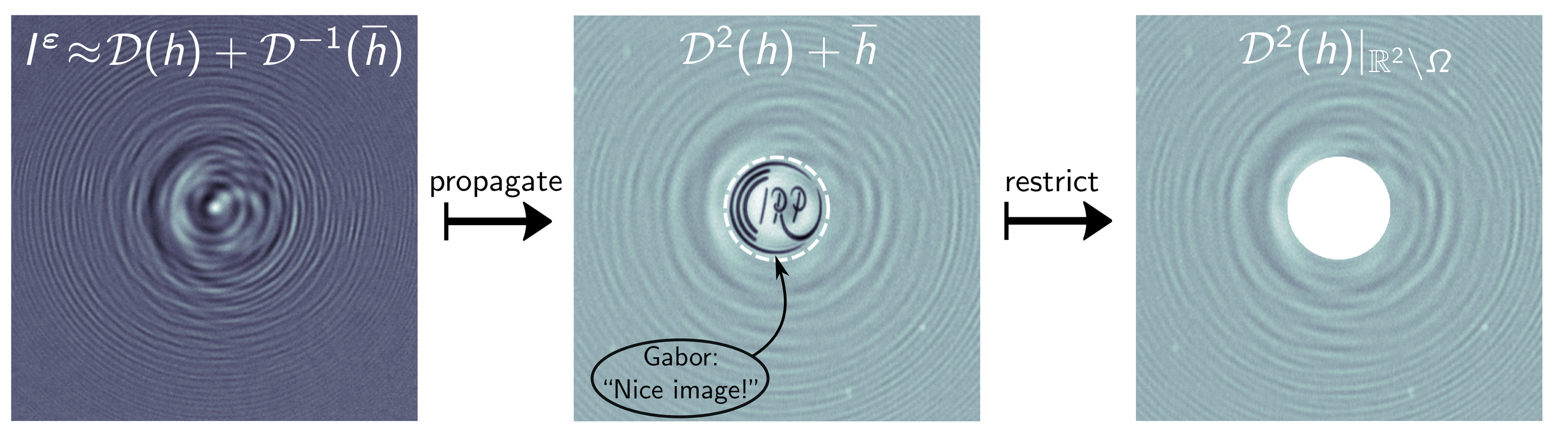
$$C_{\mathrm{single}}(N_{\mathrm{F}}) \geq \max\left\{ \min\{C_1, c_1 N_{\mathrm{F}}^{-1}\}, \ \min\{C_2\varphi_0^2, c_2 N_{\mathrm{F}}^{-\frac{1}{2}}\} \right\}$$



4. Stability Estimates for General Objects

$\rightsquigarrow$ **Can we simultaneously reconstruct phase shifts ϕ *and* absorption μ?**

Inverse Gabor holography: Propagate data and remove twin-image when in-focus



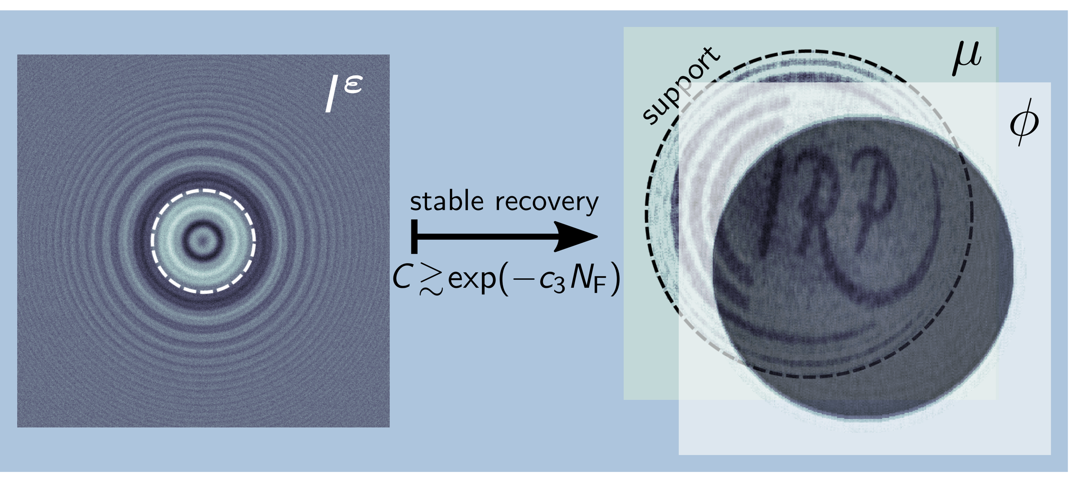
$$\|T_{\mathrm{PCI}}h\|_{L^2} = \|\mathcal{D}T_{\mathrm{PCI}}h\|_{L^2} = \|\mathcal{D}^2(h) + \overline{h}\|_{L^2} \geq \|\mathcal{D}^2(h)|_{\mathbb{R}^m\setminus\Omega}\|_{L^2} = \|\mathcal{F}(m_{\mathrm{F}} \cdot h)|_{\mathbb{R}^2\setminus(\pi N_{\mathrm{F}}\Omega)}\|_{L^2}$$

$$\Rightarrow C \geq \inf_{h \in L^2(\Omega), \|h\|=1} \|\mathcal{F}(h)|_{\mathbb{R}^2\setminus(\pi N_{\mathrm{F}}\Omega)}\| \qquad (N_{\mathrm{F}}\text{: Fresnel number of } \Omega)$$

- ▶ Image recovery *at least as stable as* inverting $\mathcal{F}_{\mathrm{F}} : L^2(\Omega) \to L^2(\mathbb{R}^2)$; $h \mapsto \mathcal{F}(h)|_{\mathbb{R}^2\setminus(\pi N_{\mathrm{F}}\Omega)}$
- ▶ Singular values of incomplete Fourier transform $\mathcal{F}_{\mathrm{F}}$ satisfy $\gtrsim \exp(-cN_{\mathrm{F}})$ [6] $\rightsquigarrow$ *stable*
- ▶ Simultaneous recovery of ϕ and μ is feasible for deeply holographic measurements [4]

Theorem 2: Let N_{F} the Fresnel number of the support diameter $\mathrm{diam}(\Omega)$. Then the recovery of *general objects* $h = -\mu - \mathrm{i}\phi \in L^2(\Omega)$ is stable with

$$C_{\mathrm{gen}}(N_{\mathrm{F}}) \geq C_3 \exp\left(-c_3 N_{\mathrm{F}}\right)$$



5. Newton-Kaczmarz Methods for Phase Contrast Tomography

Standard method in phase contrast tomography:

1. *Independent* phase retrieval for all incident angles: $I_{\mathrm{PCT}} = \{I_{\mathrm{PCI},\theta}\} \overset{F_{\mathrm{PCI}}^{-1}}{\mapsto} \{\boldsymbol{n}_\theta\} = \mathcal{R}(\delta - \mathrm{i}\beta)$
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_{PCT} by regularized Newton methods

- *Stabilizing*: exploitation of tomographic correlations in phase reconstruction [2]
- *Efficient*: Process small subsets of incident angles per iteration → *Newton-Kaczmarz* [4]
- *Flexible*: May account for non-ideal illumination, object motions, *misalignment*, etc.

$$\tilde{n}_{k+1} = \underset{\tilde{n}}{\mathrm{argmin}} \underbrace{\left\| \mathcal{P}_k\left(F_{\mathrm{PCT}}(\tilde{n}_k) + F'_{\mathrm{PCT}}[\tilde{n}_k](\tilde{n} - \tilde{n}_k) - I^{\varepsilon}\right)\right\|_{L^2}^2}_{\text{restriction to small wedges of incident angles}} + \underbrace{\alpha_k \left\|\tilde{n} - \tilde{n}_0\right\|_{X_k}^2}_{\substack{\text{approximate } L^p,\\ \text{TV, positivity, } \dots}} + \underbrace{\alpha_0 \left\|\tilde{n} - \tilde{n}_k\right\|_{L^2}^2}_{\substack{\text{strong regularization}\\ \Rightarrow \text{well-conditioned}}}$$

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