Pinhole-CDI: Unique and Deterministic Phase Retrieval via Beam-Confinement

Simon Maretzke, Thorsten Hohage

1. Motivation: Coherent Diffractive Imaging

Classical CDI:

- *Setup*: Lensless imaging from far-field diffraction patterns under coherent illumination
- *Benefit*: Diffraction-limited resolution and unsusceptible to vibrations of the sample
- *Drawback*: Requires *ab initio* phase retrieval from Fourier intensities $I = |\mathcal{F}(h)|^2 \mapsto h$

$\rightsquigarrow$ **Simple setup but non-convex + unstable image reconstruction**

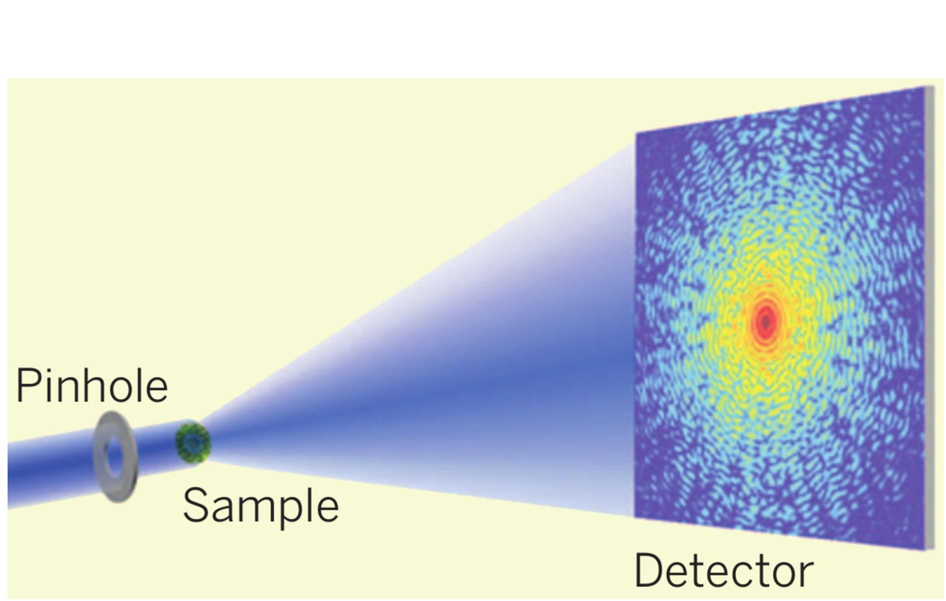


Figure 1: Classical CDI setup [5]

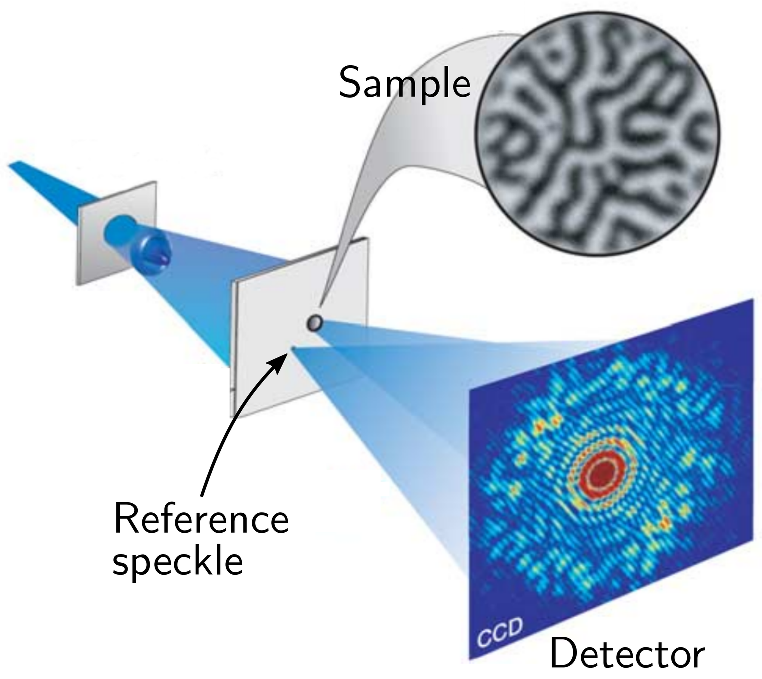


Figure 2: Fourier holography setup [1]

Fourier Holography:

- *Idea*: Superimpose *reference wave* $\mathcal{F}(r)$, generated by small speckle in object plane [4]:

  $\rightsquigarrow$ Holographic data: $I = |\mathcal{F}(r+h)|^2 = \underbrace{|\mathcal{F}(r)|^2}_{\text{known}} + \underbrace{2\Re(\overline{\mathcal{F}(r)}\mathcal{F}(h))}_{\text{interference term}} + \underbrace{|\mathcal{F}(h)|^2}_{\text{standard CDI}}$
- *Benefit*: Robust phase retrieval by support-separation of interference and CDI terms [6]
- *Drawback*: Less flexible setup, increased illumination- and oversampling requirements

$\rightsquigarrow$ **Can we exploit a holographic principle in a simple CDI setup?**

2. Holographic Reference by Beam-Confinement

Observation: CDI-data is superposition of *probe* p and *object transmission function* o:

$$I = \left|\mathcal{F}(p\cdot o)\right|^2 = |\mathcal{F}(p)|^2 + 2\Re(\overline{\mathcal{F}(p)}\mathcal{F}(h)) + |\mathcal{F}(h)|^2 \quad \text{with} \quad h = p(o-1)$$

$\rightsquigarrow$ **Probing beam profile p induces holographic reference wave**

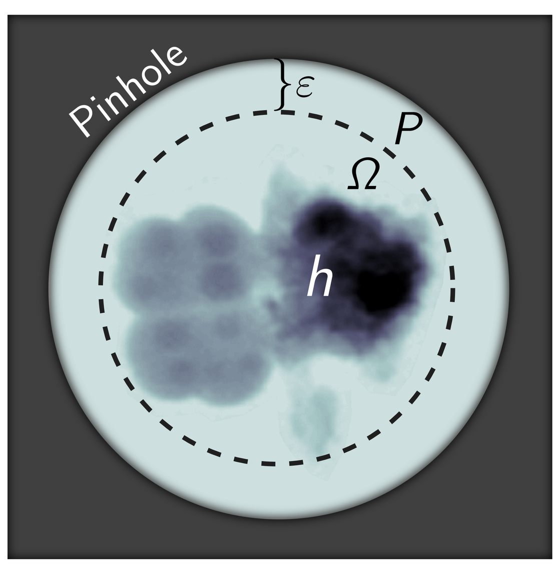
Proposed Pinhole-CDI	Classical CDI
Probe confined by circular pinhole: $p \approx \mathbf{1}_P$	*Probe* approximated as plane wave: $p \approx 1$
Reference wave: $\mathcal{F}(p) \approx$ airy disc	*No reference:* $\mathcal{F}(p) \approx 0$ outside beam stop
Support restricted by pinhole: $\mathrm{supp}(h) \subset P$	*No support*: $\mathrm{supp}(h)$ may be arbitrary

Mathematical framework:

- *Intensity data*: $I = |\mathcal{F}(p+h)|^2$ (and $I_0 = |\mathcal{F}(p)|^2$)
- *Auto-correlation* obtained by inverse FT:

$$\begin{aligned}\mathcal{F}^{-1}(I - I_0) &= (p+h)\star(p+h) - p\star p \\ &= \underbrace{2p * h^{\mathrm{h}}}_{\text{convolution}} + \underbrace{h^{\mathrm{h}} * h^{\mathrm{h}} - h^{\mathrm{a}} * h^{\mathrm{a}}}_{=h\star h \text{ (auto-correlation)}} \qquad (1)\end{aligned}$$

- Decomposition into (anti-)hermitean parts $h^{\mathrm{h}}(\boldsymbol{x}) := \frac{1}{2}(h(\boldsymbol{x}) + \overline{h(-\boldsymbol{x})})$ and $h^{\mathrm{a}}(\boldsymbol{x}) := \frac{1}{2}(h(\boldsymbol{x}) - \overline{h(-\boldsymbol{x})})$
- Support constraint: $\mathrm{supp}(h) \subset \Omega \subset (1-\varepsilon)P$



References

[1] Eisebitt S, Lüning J, Schlotter W, Lörgen M, Hellwig O, Eberhardt W, and Stöhr J. Lensless imaging of magnetic nanostructures by x-ray spectro-holography. *Nature*, 432(7019):885–888, 2004.

[2] Hohage T and Werner F. Iteratively regularized Newton-type methods for general data misfit functionals and applications to Poisson data. *Numerische Mathematik*, 123(4):745–779, 2013.

[3] Leshem B, Raz O, Jaffe A, and Nadler B. The discrete sign problem: uniqueness, recovery algorithms and phase retrieval applications. *arXiv preprint arXiv:1604.06933*, 2016.

[4] McNulty I, Kirz J, Jacobsen C, Anderson E H, Howells M R, and Kern D P. High-resolution imaging by fourier transform x-ray holography. *Science*, 256(5059):1009–1012, 1992.

[5] Miao J, Ishikawa T, Robinson I K, and Murnane M M. Beyond crystallography: Diffractive imaging using coherent x-ray light sources. *Science*, 348(6234):530–535, 2015.

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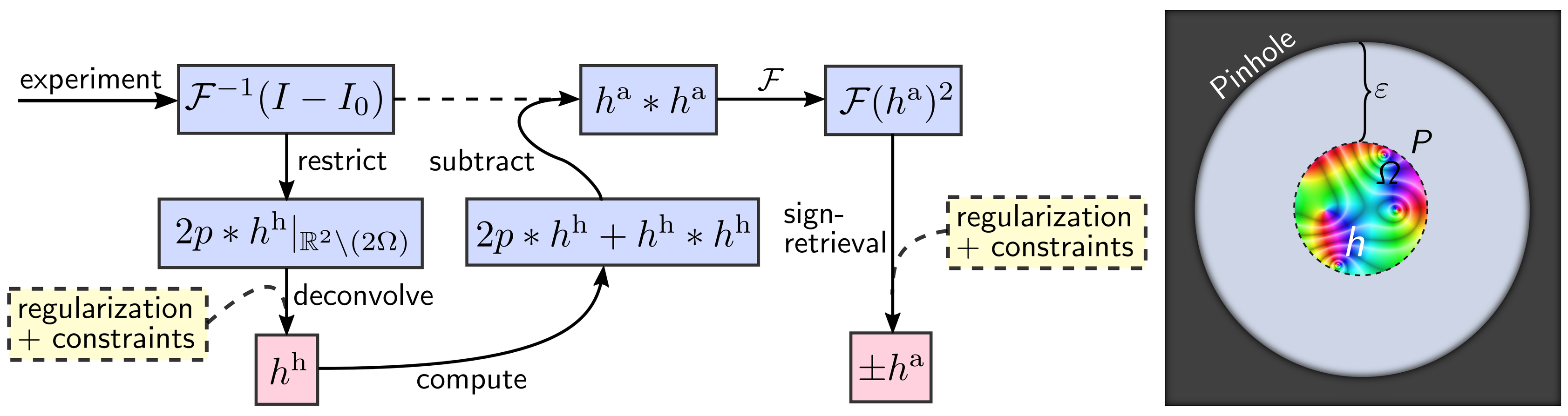
3. Reconstruction Formulas and Uniqueness

Small complex-valued objects: Support Ω fits twice into pinhole: $(2\Omega) \subset P$ (i.e. $\varepsilon \geq \frac{1}{2}$)

Observation: Auto-correlation $h \star h$ vanishes outside 2Ω, incomplete convolution data $2p * h^{\mathrm{h}}|_{\mathbb{R}^2\setminus(2\Omega)} \overset{(1)}{=} \mathcal{F}^{-1}(I - I_0)|_{\mathbb{R}^2\setminus(2\Omega)}$ uniquely determines h^{h}.

***Algorithm 1*:**

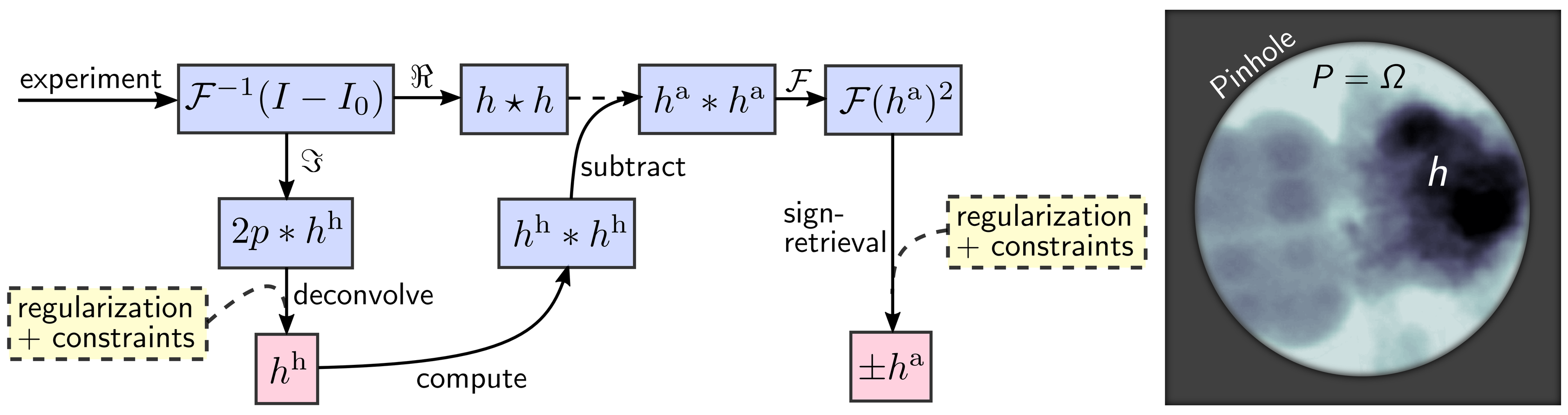


Weak pure phase objects: $h = \mathrm{i}f$, f real-valued. *No support restriction*: $\Omega = P$ ($\varepsilon = 0$)

Observation: Convolution $2p * h^{\mathrm{h}}$ in (1) purely imaginary, $h \star h$ real-valued

$$\Rightarrow \quad 2p * h^{\mathrm{h}} = \mathrm{i}\Im(\mathcal{F}^{-1}(I - I_0)) \quad \text{and} \quad h \star h = \Re(\mathcal{F}^{-1}(I - I_0)) \qquad (2)$$

***Algorithm 2*:**



General scheme and uniqueness:

1. Recovery of Hermitean part h^{h} by *linear* deconvolution $\rightsquigarrow$ *unique + convex*!
2. *Sign retrieval* $\mathcal{F}(h^{\mathrm{a}})^2 \mapsto \pm h^{\mathrm{a}}$ (e.g. by algorithm in [3]) after elimination of h^{h}-terms $\rightsquigarrow$ *unique* up to twin-image

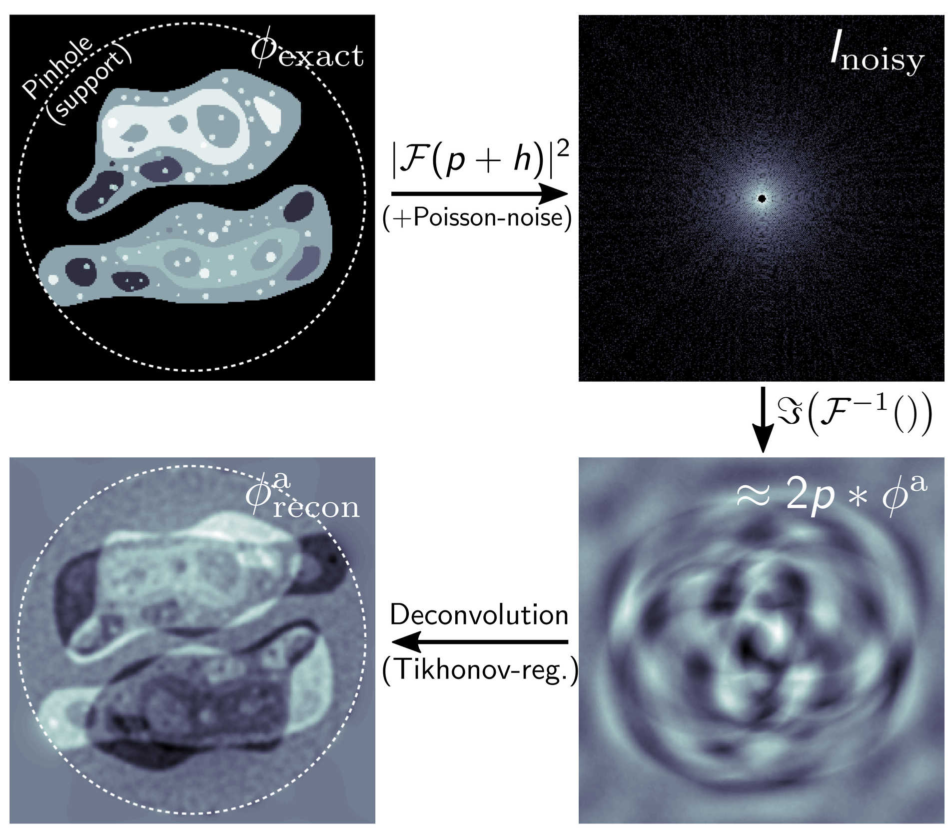
$\rightsquigarrow$ **Phase retrieval simplifies to linear deconvolution + sign retrieval**

4. Numerical Proof-of-Principle

Simulation:

- Phase object $h = p\cdot(\exp(-\mathrm{i}\phi) - 1)$
- Ideal pinhole probe $p = \mathbf{1}_P$
- $I_{\mathrm{noisy}} = |\mathcal{F}(p+h)|^2 +$ Poisson noise (≈ 22 photons per object-pixel)
- Beam stop: missing low-freq. data
- Constraints: support + ϕ real
- Reconstruct $h^{\mathrm{h}} \approx -\mathrm{i}\phi^{\mathrm{a}}$ via linear deconvolution (Algorithm 2)

$\rightsquigarrow$ **Robust to noise, incomplete data and systematic errors**



5. Conclusions and Outlook

- ✓ Beam-shaping pinholes induce holographic reference waves in standard CDI setups
- ✓ Phase retrieval (formally) splits into *linear* deconvolution + sign retrieval
- ✓ Enables uniqueness + improved convergence (e.g. of regularized Newton methods [2])
- ✓ Results and algorithms also valid for *1D*- and *3D*-phase retrieval
- ✗ Resolution limited by knowledge of tailored probe beam $\rightsquigarrow$ *requires accurate optics*

$\rightsquigarrow$ **Pinhole-CDI: A viable technique for coherent X-ray imaging?**

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