3D Phase Retrieval at Nano-scale via Accelerated Wirtinger Flow

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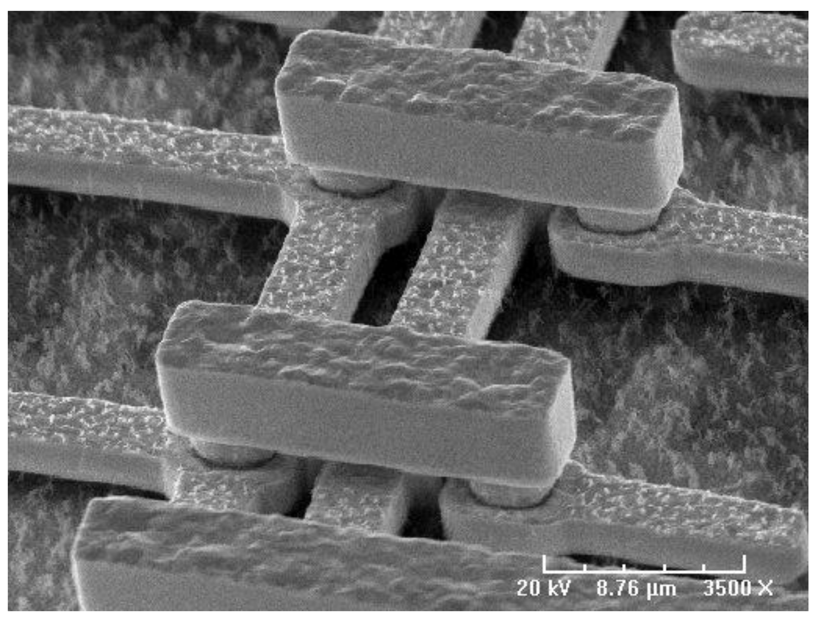
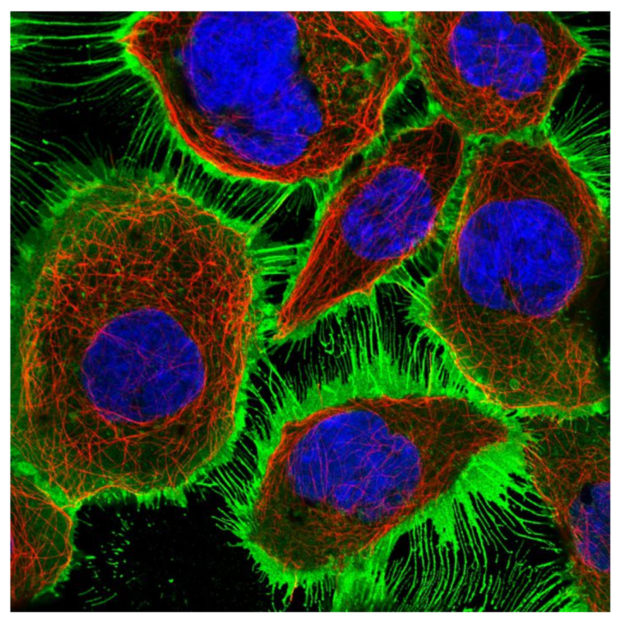
Motivation





Challenges of imaging on the nano-scale

- High energy beams $\Rightarrow$ special devices needed (no optics) $\Rightarrow$ information loss
- Extremely long acquisition time (1000 days!)

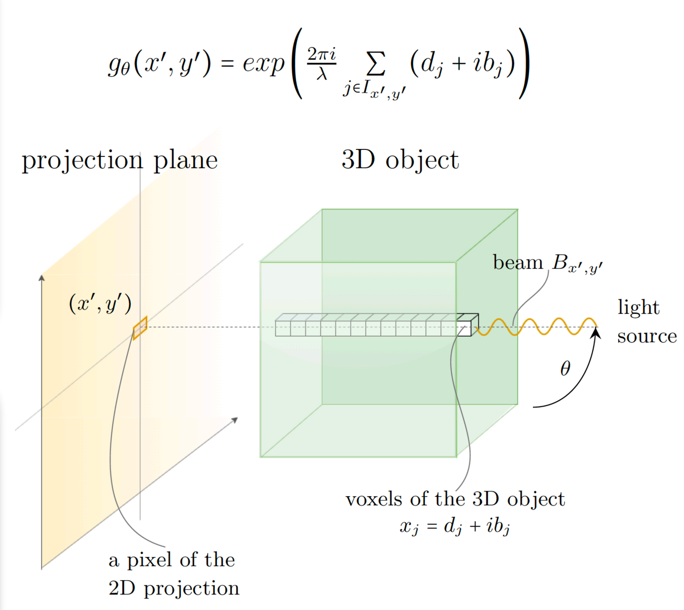
From 3D object to 2D exit waves

Object modeling

- Represented by complex refractive index
- Discretization: voxels on cubic lattice:

$$\mathbf{x} = \mathbf{d} + i\mathbf{b}$$

phase shift — attenuation



Exit wave equation

- Nonlinear projection based on Radon-transform:

$$\mathbf{g}_\theta(x) = exp\left(\frac{2\pi i}{\lambda}\int_{-\infty}^{\infty} (\mathbf{d} + i\mathbf{b})\, dz_\theta\right)$$

From 2D exit waves to measurements

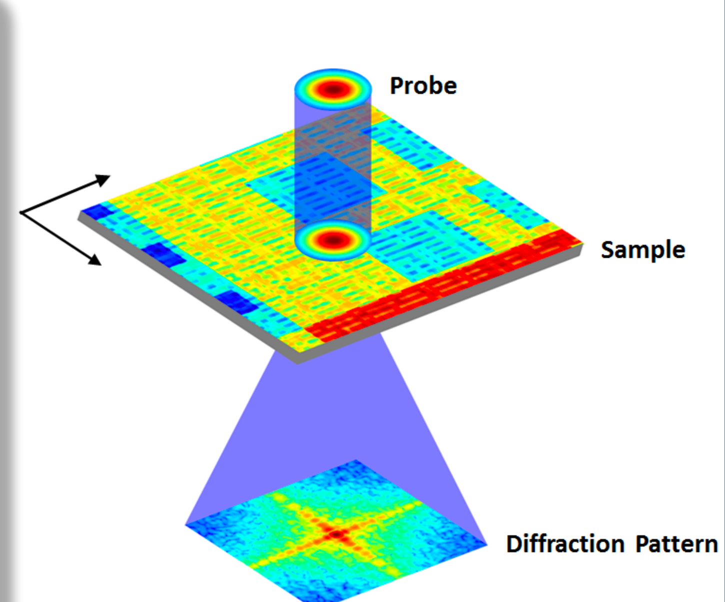
Ptychography

- Exit wave propagation to the far field

$$\mathbf{A} = \begin{bmatrix} \mathbf{F} & \mathbf{0} & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & \mathbf{F} & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{F} & \dots & \mathbf{0} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \dots & \mathbf{F} \end{bmatrix} \begin{bmatrix} \mathbf{I}_{supp(\mathbf{p}_1)} diag(\mathbf{p}_1) \\ \mathbf{I}_{supp(\mathbf{p}_2)} diag(\mathbf{p}_2) \\ \vdots \\ \mathbf{I}_{supp(\mathbf{p}_K)} diag(\mathbf{p}_K) \end{bmatrix}$$

- Magnitude-only measurements

$$\mathbf{y}_\ell = |\mathbf{A}\mathbf{g}_\ell|$$

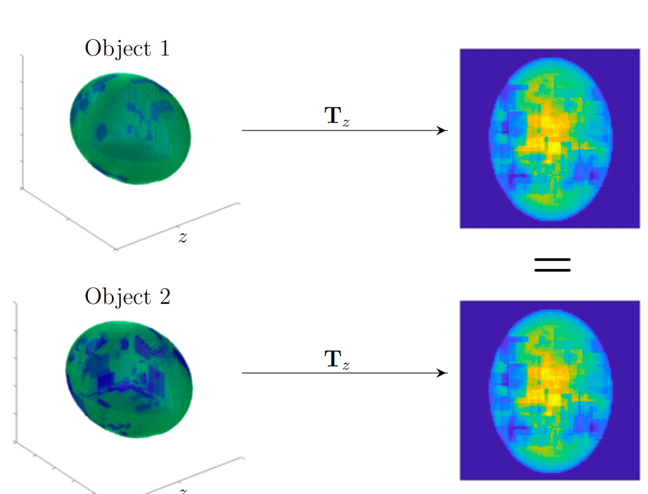


The diffraction pattern in the far field is the Fourier transform of the exit wave multiplied by the probe function.

The ambiguity challenge

Ambiguity of tomography

- Radon-transform has non-trivial null-space, given projection may belong to infinitely many objects
- This can be resolved by sufficiently large number of illumination angles



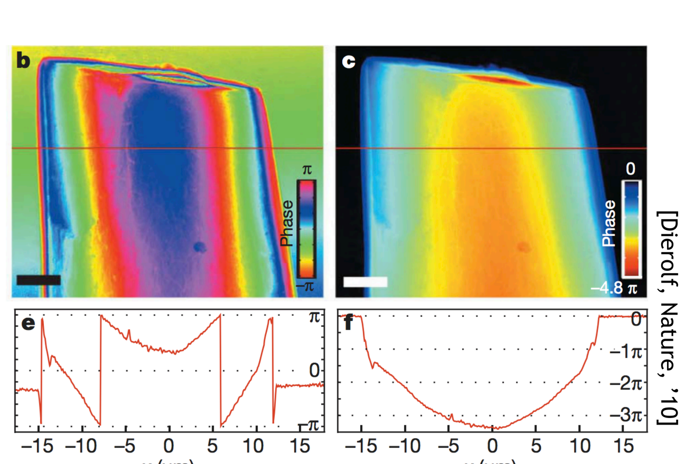
We project object 1 and 2 along the z-axis. Even though the objects are significantly different, the projection images are identical.

Ambiguity caused by phase wrapping

- Beam may accumulate phase shift of $2\pi k$ while passing through the object
- Assume $\mathbf{T}_\ell \tilde{\mathbf{d}} = \lambda \mathbf{k},\ \mathbf{k} \in \mathbb{Z}^N$, then

$$exp\left(\frac{2\pi i}{\lambda}\mathbf{T}_\ell(\mathbf{d} + \tilde{\mathbf{d}})\right) = exp\left(\frac{2\pi i}{\lambda}\mathbf{T}_\ell \mathbf{d}\right) exp\left(\frac{2\pi i}{\lambda}\lambda \mathbf{k}\right) = exp\left(\frac{2\pi i}{\lambda}\mathbf{T}_\ell \mathbf{d}\right)$$

- Voxel-level ambiguity: d_i and $d_i + \lambda k,\ k \in \mathbb{Z}$ produce same measurements



Due to phase wrapping, the phase plot may have jumps of $2\pi k$. We can penalize variations in the object to mitigate phase wrapping.

Reconstruction via 3D-AWF

Formulation as optimization problem

- No closed form solution, we need an iterative method:

$$\hat{\mathbf{x}} = argmin_{\mathbf{x} \in \mathbb{C}^N}\ \mathscr{L}(\mathbf{x}) + \lambda_{TV} \mathrm{TV}_{3D}(\mathbf{x}; \mathbf{w})$$

data consistency — prior knowledge

- Data consistency: the solution is consistent with the measurements:

$$\mathscr{L}(\mathbf{x}) = \sum_{l=1}^{L} \| \mathbf{y}_\ell - |\mathbf{A}\mathbf{g}_\ell(\mathbf{x})| \|_2^2$$

- Prior knowledge: total variation regularizer enforces piecewise constant structure

3D-AWF algorithm

- Acceleration $\quad \mathbf{y}_{\tau+1} = \mathbf{x}_\tau + \beta_\tau(\mathbf{x}_\tau - \mathbf{x}_{\tau-1}) - \mu_\tau \nabla \mathscr{L}(\mathbf{x}_\tau + \beta_\tau(\mathbf{x}_\tau - \mathbf{x}_{\tau-1}))$
- Proximal map: $\quad \mathbf{x}_{\tau+1} = prox_{TV}(\mathbf{y}_{\tau+1})$

Convergence Theorem

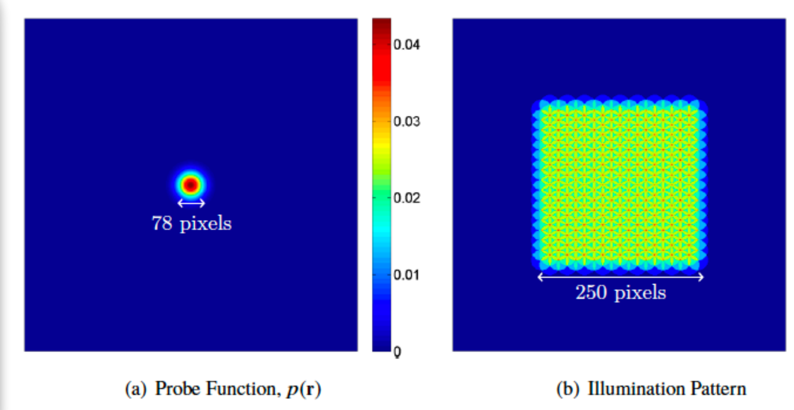
Let $\mathbf{x}^*$ be a global minimum of $\mathscr{L}(\mathbf{x})$. If we run 3D-AWF updates with step size sufficiently small and $\beta_\tau = 0$, then we have

$$\min_{\tau \in \{1,2,\dots,T\}} \|prox_{TV}(\mathbf{y}_\tau) - \mathbf{y}_\tau\| \le \mu \frac{\mathscr{L}(\mathbf{x}_0) - \mathscr{L}(\mathbf{x}^*)}{T+1}$$

Numerical experiments

Experimental setup

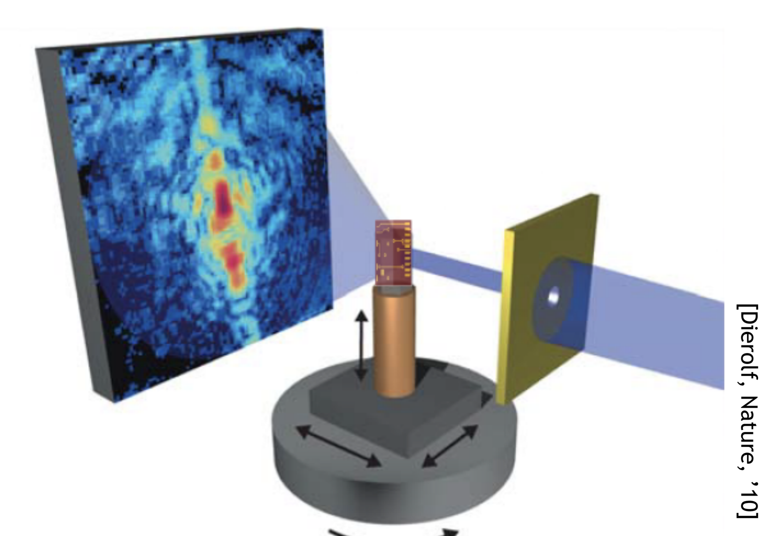
- Highly realistic simulated 3D chip
- Illumination angles: π/L increments with $L \in \{5, 10, 25, 50, 100, 250, 400\}$ # of angles



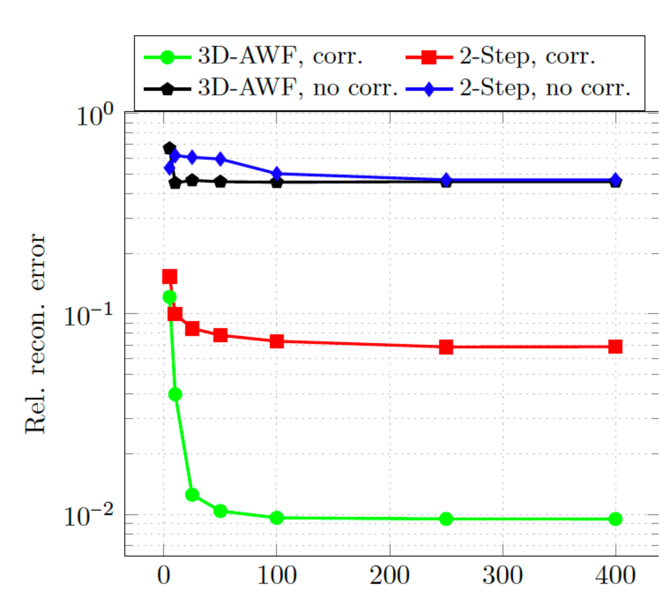
Comparison: a 2-step approach

- 2D phase retrieval and tomography in separate steps
- Uses linear approximation:

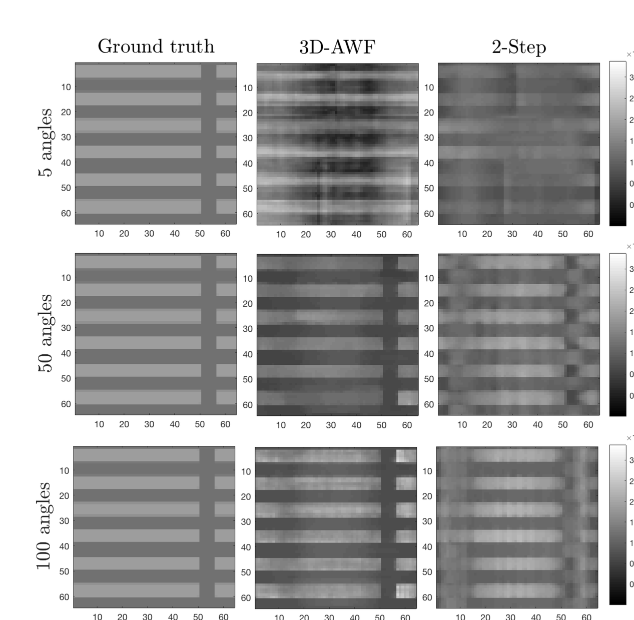
$$exp\left(\frac{2\pi i}{\lambda}\mathbf{T}_\ell \mathbf{x}\right) \approx 1 + \frac{2\pi i}{\lambda}\mathbf{T}_\ell \mathbf{x}$$



Reconstruction results:



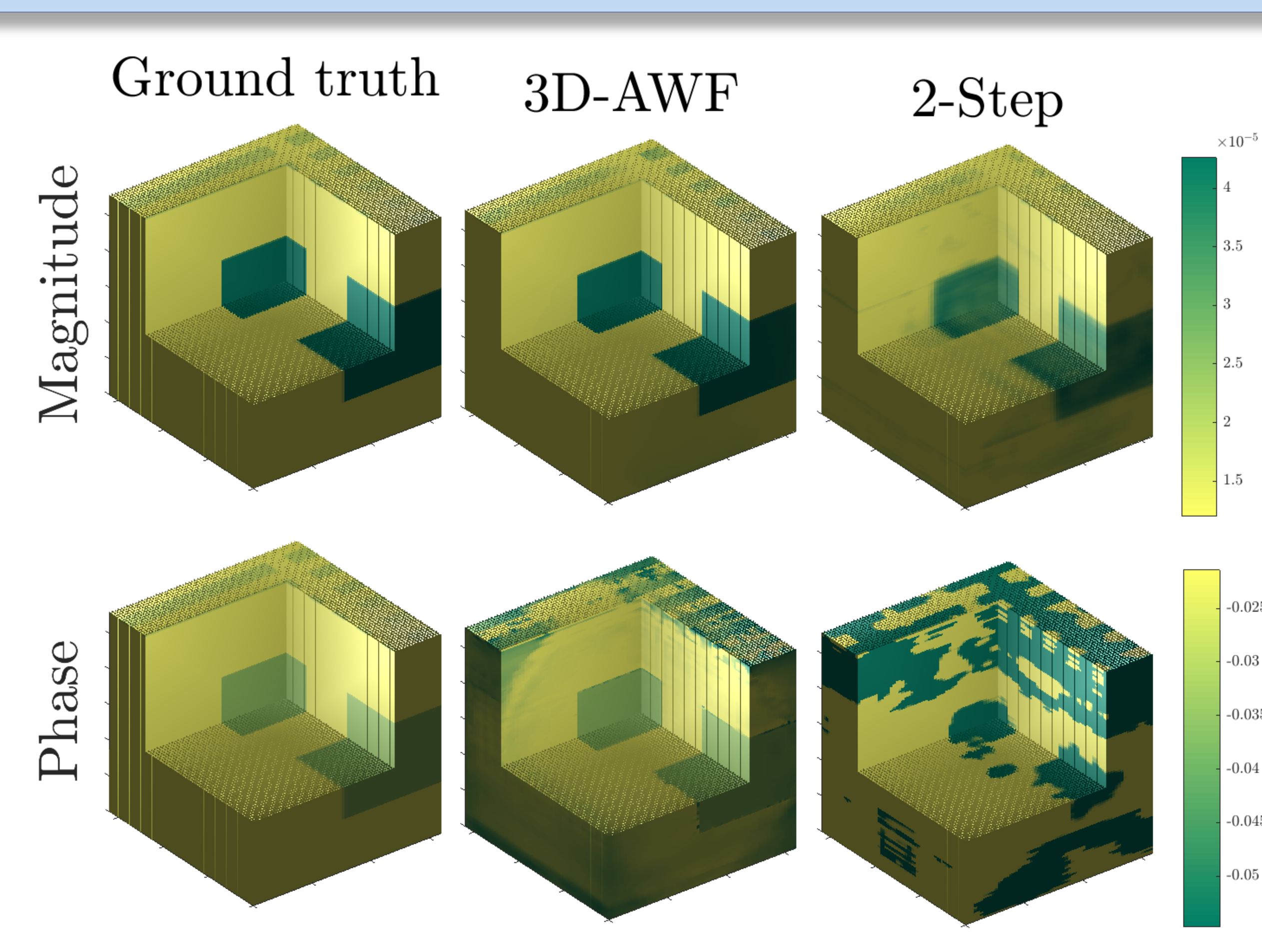
Comparison of relative reconstruction error across various number of illumination angles



Magnitude of ground truth and reconstructions in the x-y plane at z = 1

Key takeaway

- Linear approximation is inaccurate for thick specimens
- Prior knowledge can: (1) reduce acquisition time, (2) mitigate ambiguity



3D rendering of the magnitude and phase of the reconstructed volume