Projected Multi-Agent Consensus Equilibrium (PMACE) for Ptychographic Image Reconstruction

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INTEGRATED IMAGING

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Complex X-ray Imaging

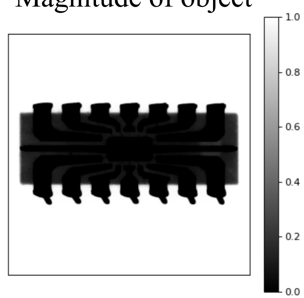
- **Attenuation Contrast**
  - Measures magnitude to estimate image directly.

X-ray source

Object of interest

attenuation

Magnitude of object



$$I(z) = I_0 \exp(-n_a z)$$

- **Phase Contrast**
  - Measures magnitude and estimates phase to produce image.

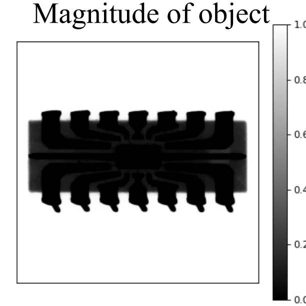
X-ray source

Object of interest

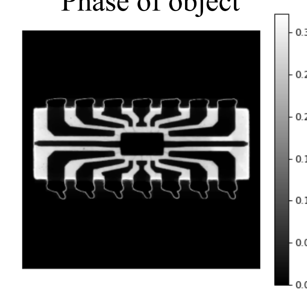
attenuation

phase delay

Magnitude of object



Phase of object



$$I(z) = I_0 \exp\big(-(n_a + i n_p) z\big)$$

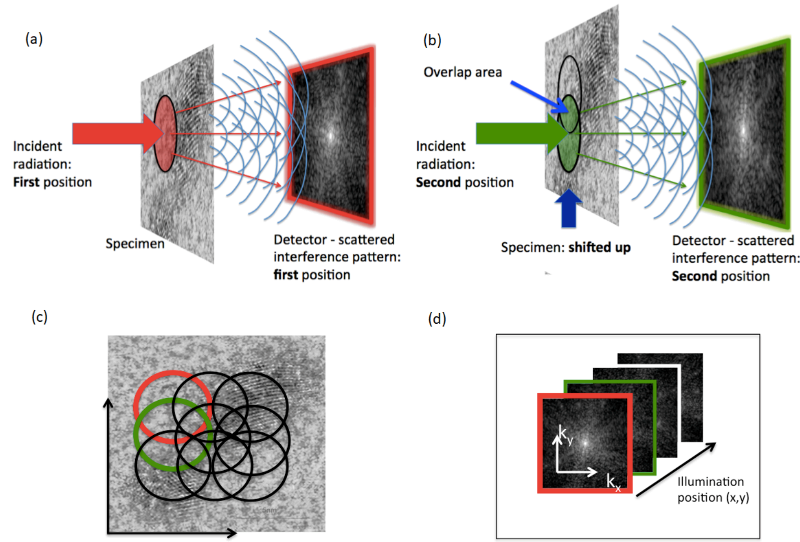
Fourier transform

Detector $(|I(z)|)$

n_a: real refraction index
n_p: imaginary refraction index

Ptychography

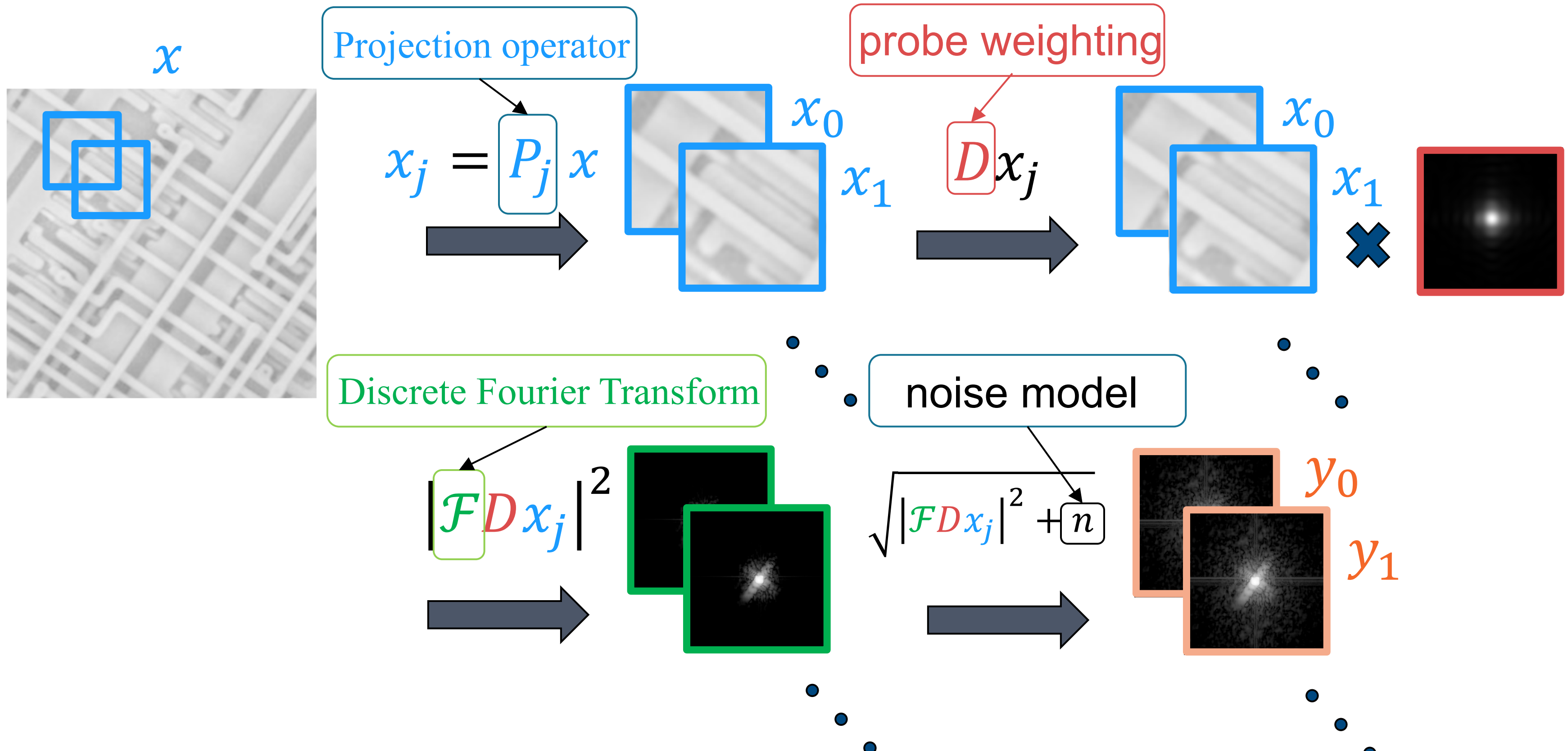
- Imaging technique:
  - Collect real-valued diffraction patterns (without phase).
  - Make measurements at many overlapped locations.



(Image of X-ray ptychography from: Wikipedia.)

- Goal:
  - Reconstruct the complex object from overlapping diffraction patterns.
- Challenges:
  - Recover phase from magnitude measurements.
  - Reduce the number of overlapping measurements.

Forward Model



- Analytical form:

$$y_j = \sqrt{|\mathcal{F} D P_j x|^2 + n} = \sqrt{|\mathcal{F} D x_j|^2 + n}$$

Single Patch Loss Function

- Forward model

$$y_j = \sqrt{\left|\mathcal{F} D x_j\right|^2 + n}$$

$x_j = P_j\, x$

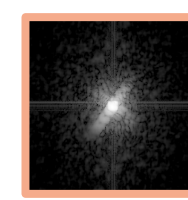
- We introduce the phase θ_j and seek x_j so that

$$y_j^{measure} e^{i\theta_j} \approx \mathcal{F} D x_j$$

- The loss function is

$$f_j(x_j) = \min_{\theta_j} \left\{ \frac{1}{2\sigma_n^2} \left\| y_j^{measure} e^{i\theta_j} - \mathcal{F} D x_j \right\|^2 \right\}$$

θ_j matches the phase of $\mathcal{F} D x_j$



$y_j^{measure}$

Update Agent for Single Probe Location

- Loss function for j^{th} probe location

$$f_j(x_j) = \min_{\theta_j} \left\{ \frac{1}{2\sigma_n^2} \left\| y_j e^{i\theta_j} - \mathcal{F} D x_j \right\|^2 \right\}, e^{i\theta_j} = \frac{\mathcal{F} D x_j}{|\mathcal{F} D x_j|}$$

- Iterative method updates each patch closer to measured data.

- The probe-weighted proximal map is given by

$$x_j \leftarrow F_j(x_j) = \arg\min_{v} \left\{ f_j(v) + \frac{1}{2\sigma^2} \left\| Dv - Dx_j \right\|^2 \right\}$$

$$= \frac{\alpha x_j + D^{-1} \mathcal{F}^* \left(y_j \frac{\mathcal{F} D x_j}{|\mathcal{F} D x_j|} \right)}{\alpha + 1}$$

data-fitting point

current estimate

where $\alpha = \frac{\sigma_n^2}{\sigma^2}$ is noise-to-signal ratio.

Projected Multi-Agent Consensus Equilibrium (PMACE)

- To get a solution consistent across patches, we define $\boldsymbol{x} = [x_0, \dots, x_{J-1}]^t$ and

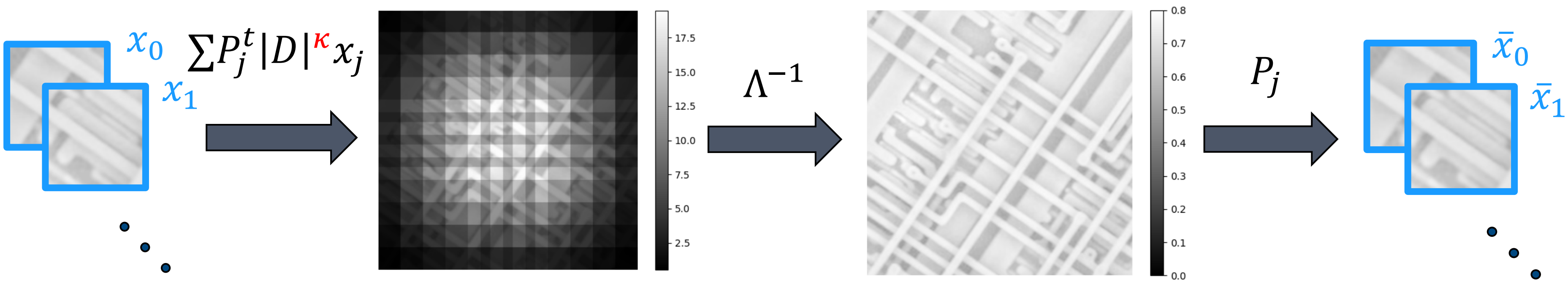
$$\boldsymbol{F}(\boldsymbol{x}) = \begin{bmatrix} F_0(x_0) \\ \vdots \\ F_{J-1}(x_{J-1}) \end{bmatrix} \text{ and } \mathbf{G}(\boldsymbol{x}) = \begin{bmatrix} \bar{x}_0 \\ \vdots \\ \bar{x}_{J-1} \end{bmatrix}$$

where

$$\bar{x}_j = P_j \Lambda^{-1} \sum_j P_j^t |D|^{\kappa} x_j \text{ and } \Lambda = \sum_j P_j^t |D|^{\kappa}$$

— probe exponent

- **G** combines patches with weighted average and re-extracts them.



PMACE Solution

- **Formulation:** To find the PMACE solution, we solve

$$\boldsymbol{F}(\boldsymbol{x}) = \boldsymbol{G}(\boldsymbol{x})$$

- **Algorithm:** We compute the fixed point of the map

$$\boldsymbol{T} = (2\boldsymbol{G} - \boldsymbol{I})(2\boldsymbol{F} - \boldsymbol{I})$$

  using Mann iteration given by

$$\boldsymbol{x} \leftarrow (1-\rho)\boldsymbol{x} + \rho \boldsymbol{T}\boldsymbol{x}$$

- PMACE inherits convergence property from MACE framework. [1]
- Reconstruction result is given by

$$\Lambda^{-1} \sum_j P_j^t |D|^\kappa \boldsymbol{x}_j$$

[1] Buzzard, G.T., Chan, S.H., Sreehari, S. and Bouman, C.A., 2018. Plug-and-play unplugged: Optimization-free reconstruction using consensus equilibrium. SIAM Journal on Imaging Sciences, 11(3), pp.2001-2020

Competing Algorithms

- Accelerated Wirtinger Flow (AWF) [2]
  - applies Nesterov acceleration to the original Wirtinger Flow (WF) algorithm.

- Scalable Hetereogeneous Adaptive Real-time Ptychography (SHARP) [3]
  - implements Relaxed Averaged Alternating Reflections (RAAR) algorithm for ptychographic image reconstructions.

[2] Xu, Rui, et al. "Accelerated Wirtinger flow: A fast algorithm for ptychography." *arXiv preprint arXiv:1806.05546* (2018).

[3] Marchesini, Stefano, et al. "SHARP: a distributed GPU-based ptychographic solver." *Journal of Applied Crystallography* 49.4 (2016): 1245-1252.

Simulated Test Data

- Complex image and probe

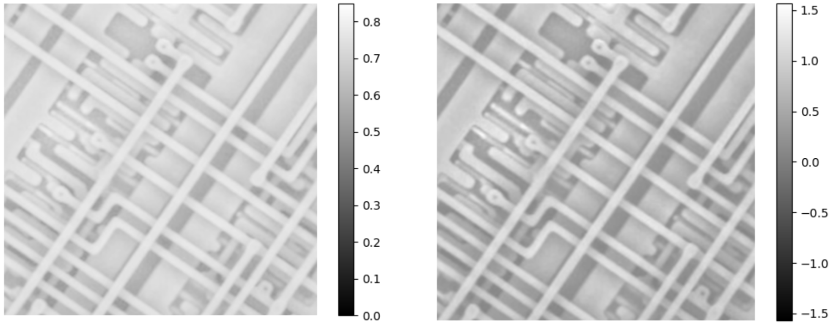


Fig 1. Magnitude (left) and phase (right) of complex test image.

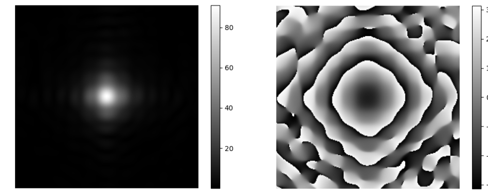
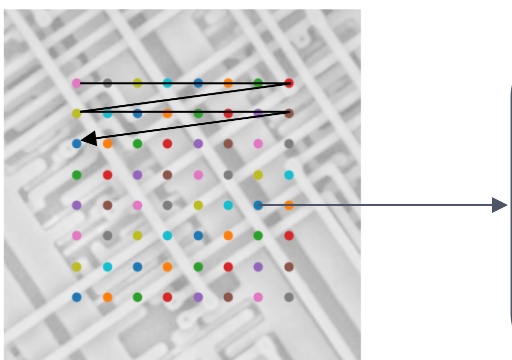


Fig 2. Magnitude (left) and phase (right) of probe.

- Scan pattern



* We simulate Poisson measurements to generate data.

Fig 3. Scan pattern with probe spacing 56 (in pixels).

* Complex image and probe courtesy of Dr. Kevin Mertes, Los Alamos National Laboratory

Reconstructed Amplitudes on Noise-free Data

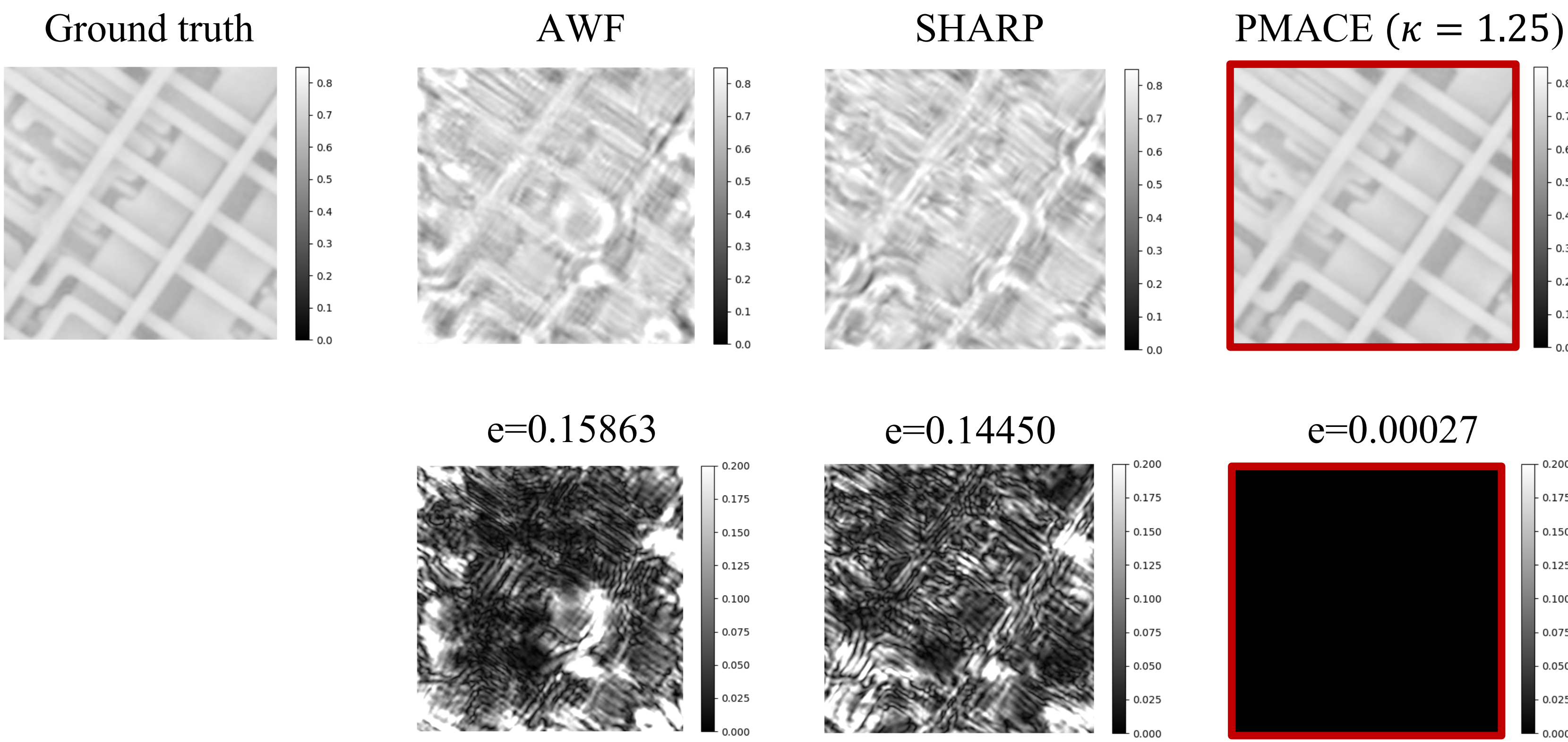


Fig 5. Reconstructed amplitudes (top row) after 100 iterations for noise-free synthetic case with probe spacing 56 (in pixels). The bottom row shows amplitudes of difference between each complex reconstruction and ground truth image.

* e = final Normalized Mean Squared Error (NRMSE)

Reconstructed Phases on Noise-free Data

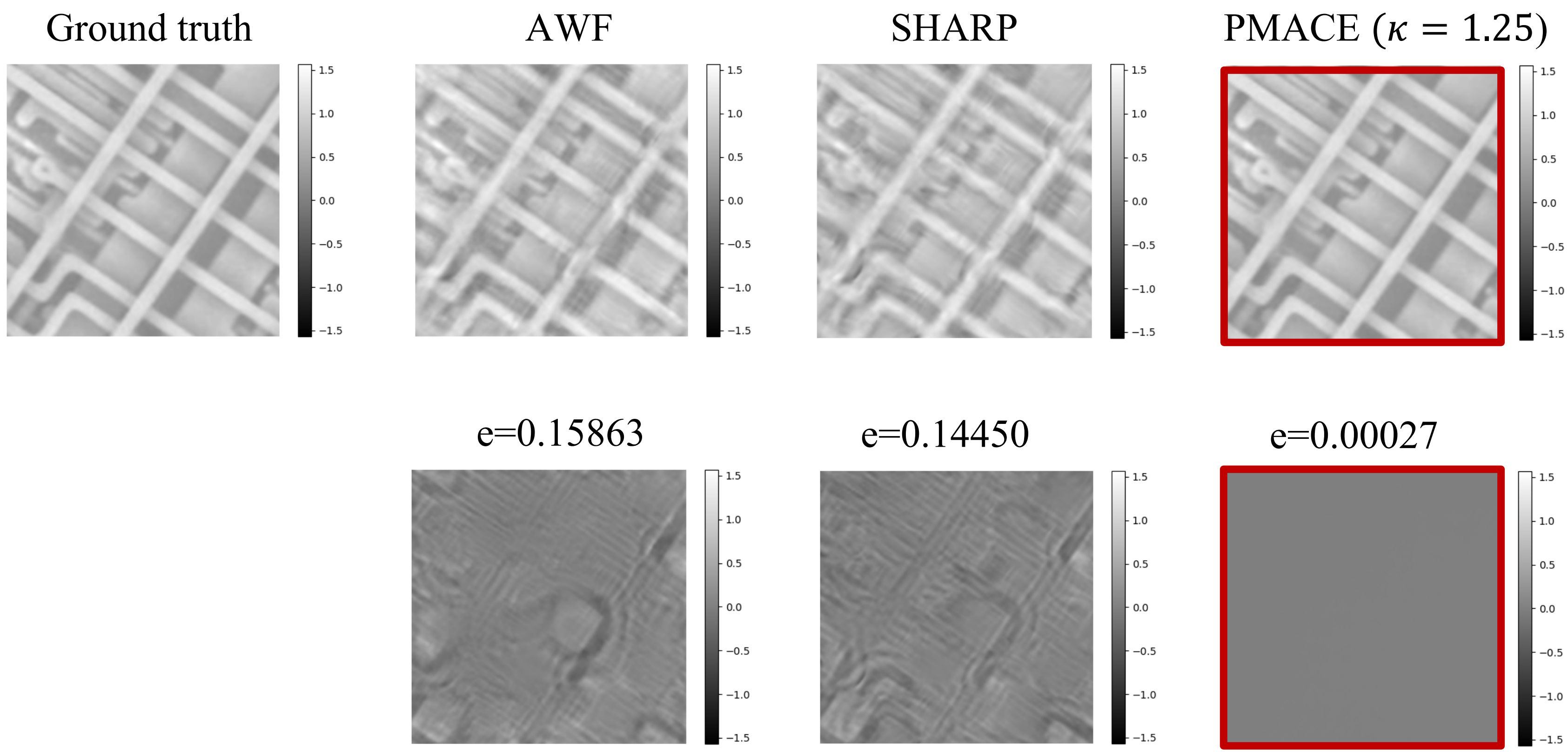


Fig 6. Reconstructed phases (top row) after 100 iterations for noise-free synthetic case with probe spacing 56 (in pixels). The bottom row shows the amplitudes of difference between each complex reconstruction and ground truth image.

* e = final Normalized Mean Squared Error (NRMSE)

Convergence Plots from Noise-free Data

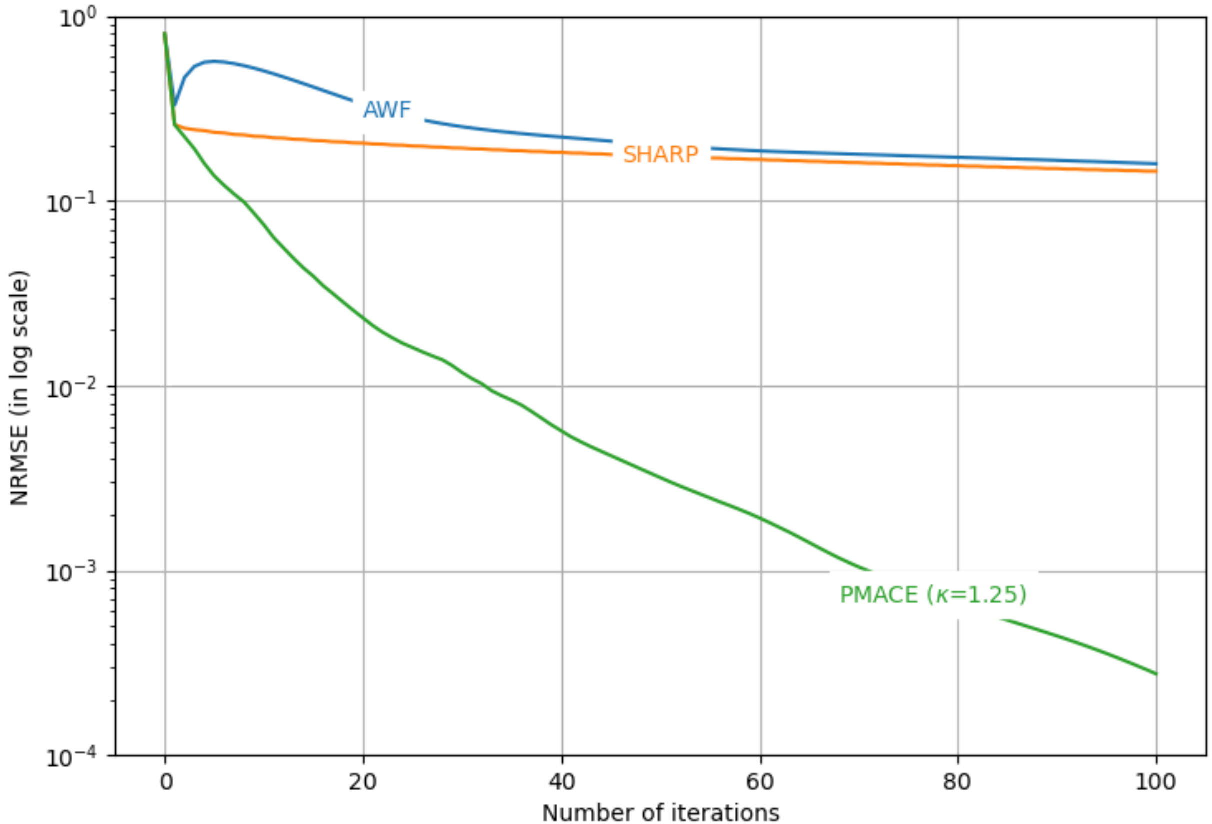


Fig 7. Plots of NRMSE along with number of iterations for noise-free synthetic case with probe spacing 56 (in pixels).

Convergence Plots from Noisy Data

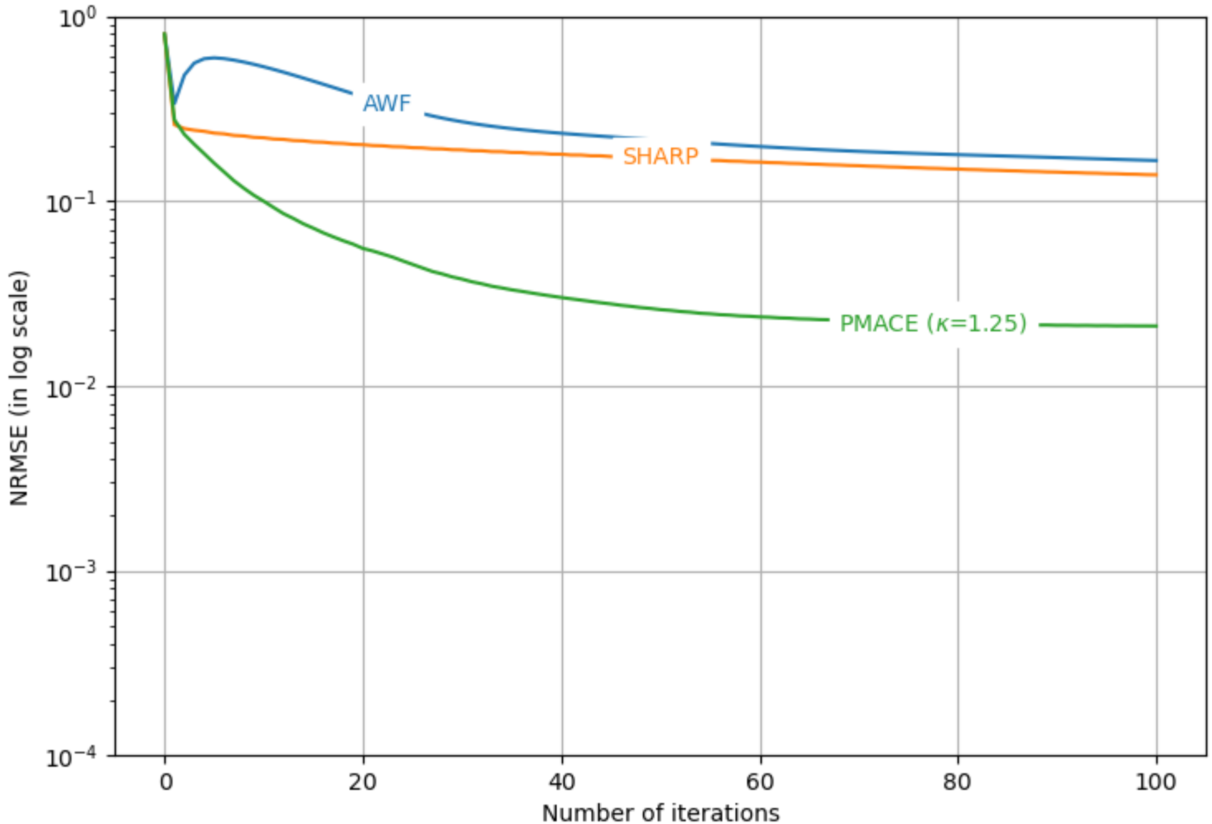


Fig 8. Plots of NRMSE along with number of iterations for noisy synthetic case with probe spacing 56 (in pixels).

Probe Spacing

- **Small Spacing**
  - More overlap between adjacent illuminated areas.
  - More measurements.
  - Reduces uncertainty.
  - More computation.
- **Large Spacing**
  - Less overlap between adjacent illuminated areas.
  - Fewer measurements.
  - More uncertainty.
  - Faster reconstruction.

Fig 9. Scan pattern with probe spacing 40 (in pixels).

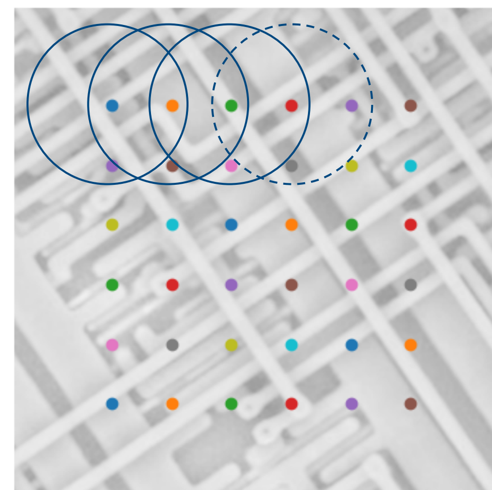
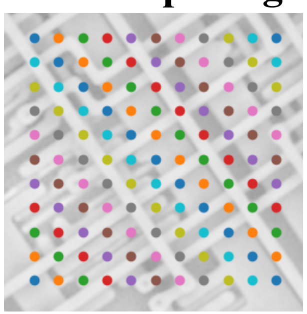
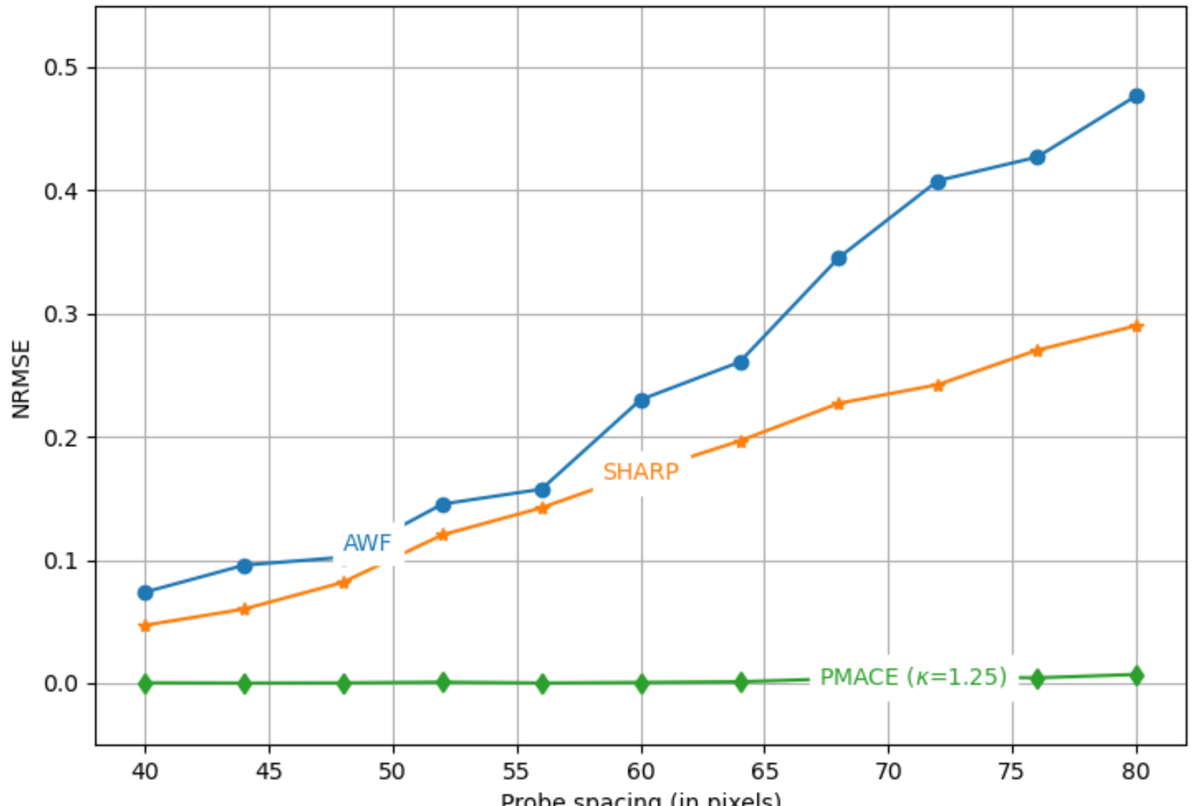


Fig 10. Scan pattern with probe spacing 80 (in pixels).

Final NRMSE vs. Probe Spacing on Noise-free Data

Small Spacing





Large Spacing

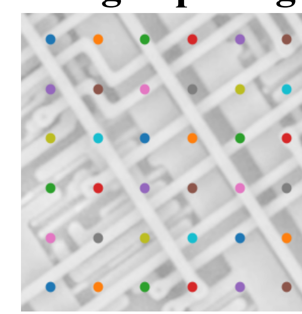
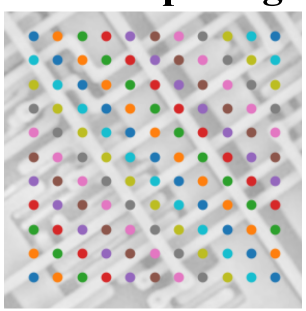
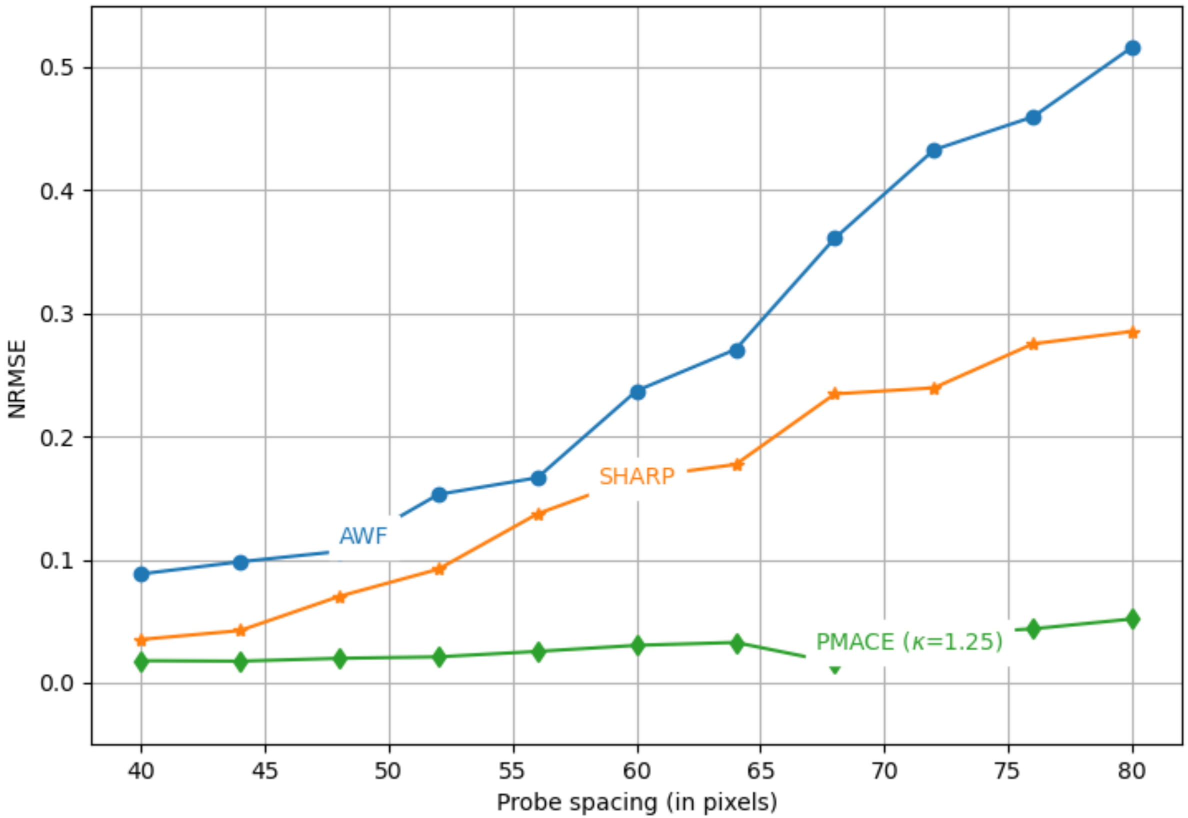


Fig 11. Plots of NRMSE after 100 iterations along with probe spacings for noise-free synthetic case.

Final NRMSE vs. Probe Spacing on Noisy Data

Small Spacing





Large Spacing

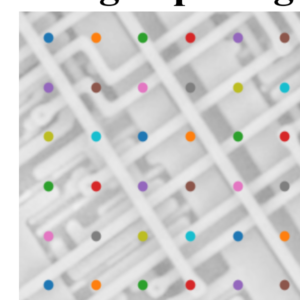
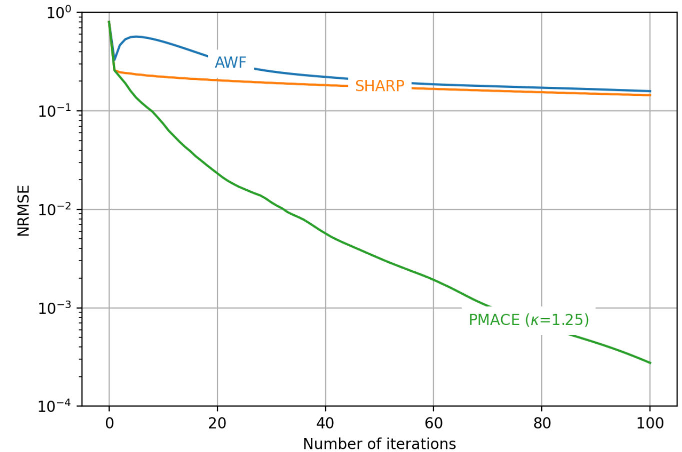


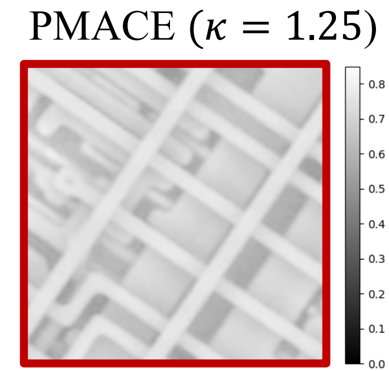
Fig 12. Plots of NRMSE after 100 iterations along with probe spacings for noisy synthetic case.

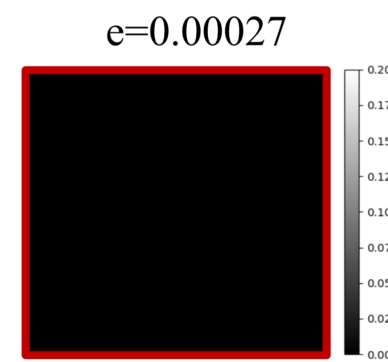
Takeaways



- PMACE has
  - better reconstruction quality
  - faster convergence speed
- PMACE approach:
  - allows problems to be broken into smaller pieces
  - allows parallelization
  - can be applied to ptychography
  - guaranteed convergence under appropriate hypotheses

Thanks


PMACE ($\kappa = 1.25$)
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0


e=0.00027
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000