# Iterative Phase Retrieval Methods for Weakly Scattering Signals: Transfer of Information and Efficient Regularization

Georgios Varnavides[1,2], Dr Stephanie Ribet[2], Mr Reed Yalisove[2,3], Dr Mary Scott[2,3], Dr Colin Ophus[2]
[1]Miller Institute for Basic Research in Science, University of California, Berkeley, USA, [2]National Center for Electron Microscopy, Lawrence Berkeley Laboratory, Berkeley, USA, [3]Department of Materials Science and Engineering, University of California, Berkeley, USA

When a converged electron probe is scanned across a thin sample, it acquires phase-shifts due to sample interactions which scatter the incident electron wavefunction. Reconstructing these various scattering sources from phase-less measurements of the intensity at far-field detectors is a high-dimensional, non-convex, inverse scattering problem. Iterative electron ptychography is a phase-retrieval technique which attempts to solve this inverse problem using the redundant information in a set of converged-beam diffraction intensities with sufficient real-space illumination overlap [1], e.g., using defocused-probe 4DSTEM measurements [2].

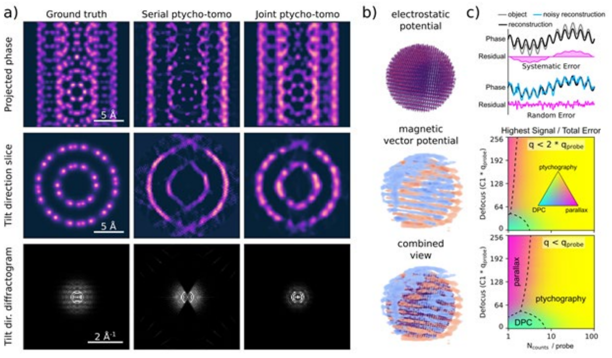
We have recently introduced a general computational framework, implemented in the open-source analysis toolkit py4DSTEM [3], to reconstruct common coherent scattering sources using physically inspired forward and adjoint operators as-well as a suite of regularization constraints robust against common experimental artifacts. Here, we present recent experimental results using the ptychographic framework on a number of materials-science samples, including atomic defects in few-layer hBN, post-acquisition aberration correction on Au nanoparticles, few-layer twisted SrTiO3 moirés, and strain measurements in upconverting core-shell nanoparticles [4], as-well as biological samples, including single-particle analysis of frozen hydrated proteins at sub-nanometer resolution [5].

Moreover, we present simulated results on how the depth-resolution of these phase-retrieval methods can be extended by solving a joint inverse problem for orthogonal tilt-series directly to obtain the three-dimensional nature of scalar and vector scattering sources such as electrostatic (Figure 1a) and magnetic vector potentials (Figure 1b), respectively [3]. In contrast to "serial" ptychographic-tomography, where one performs 2D ptychographic reconstructions for each tilt projection before reconstructing the 3D object using standard tomographic methods, "joint" ptychographic tomography leverages the ability of multislice-ptychography to capture non-linear propagation, together with three-dimensional regularizations, to recover some information inside the "missing-wedge" due to sample-geometry limitations.

Finally, we discuss the transfer of information of iterative electron ptychography and derive various analytical expressions and numerical results for a white-noise model. We compare the results against other common iterative phase retrieval methods, notably differential phase contrast and tilt-corrected BF-STEM [3], to arrive at experiment design recommendations as a function of electron fluence and defocus (Figure 1c).

Phase-retrieval methods in STEM offer particular promise due to their remarkable dose-efficiency, enabling the observation of otherwise imperceptible signals, such as fields inside materials, and of radiation-sensitive materials, such as hybrid organic materials and biological samples.

**Graphic:**




**Keywords:**

phase-retrieval, ptychography, tomography, single-particle analysis

**Reference:**

[1] J Rodenburg, A Maiden, Springer Handbook of Microscopy, (2019), doi: 10.1007/978-3-030-00069
[2] C Ophus, Microscopy and Microanalysis, 25 (2019), doi: 10.1017/S1431927619000497
[3] G Varnavides, S Ribet et al. arXiv:2309.05250 (2023), doi: 10.48550/arXiv.2309.05250
[4] S Ribet, G Varnavides et al. arXiv:2402.10084 (2024), doi: 10.48550/arXiv.2402.10084
[5] B Küçükoğlu et al., bioRxiv (2024) doi: 10.1101/2024.02.12.579607