Pixel-Level, Cost-Free, Automated Phase Reconstruction

Self-Organizing Map Classification + Prototype-Prior Initialization (SOM Centroids) + Phase Retrieval

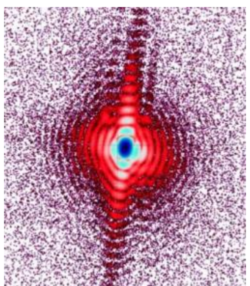
Motivation

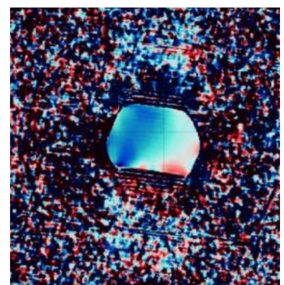
- Current X-ray phase-retrieval workflows often require manual parameter tuning and expert intervention, and can be sensitive to initialization/support and noise/mask mismatch.
- The proposed method is label-free, fully automated, and reproducible (fixed hyperparameters and versioned configs).
- Pixel-level SOM classification provides centroid-based priors for phase retrieval, enabling fine-grained and interpretable structural analysis.
- Ready to integrate with ptychography/coded-aperture measurements and digital-twin simulations.

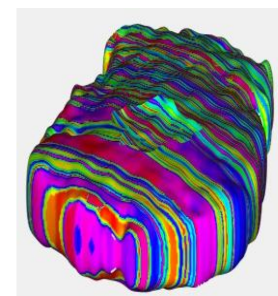
Workflow Overview

Label-free, unsupervised, reproducible pipeline for pixel-level classification and phase retrieval

- Step 1: Automatic pixel-level classification of Set 1 using SOM (unsupervised)
- Step 2: Prototype-prior initialization: use SOM class centroids from Set 1 to seed/regularize phase retrieval on held-out Set 2 (no retraining)
- Step 3: Phase retrieval with centroid priors for structural reconstruction in Set 2





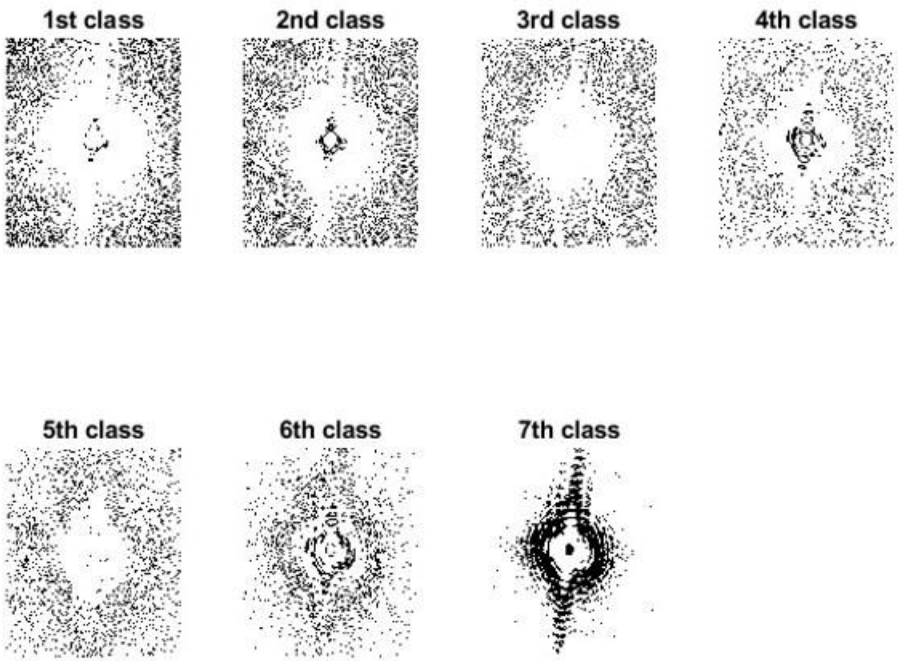


Pixel-level SOM classification (Set 1) → **Prototype-prior initialization (Set 1 → Set 2)** → **Phase retrieval & reconstruction (Set 2)** → **Error analysis (quantitative + visual)**

Source: Simonne *et al.*, *Gwaihir: Jupyter Notebook graphical user interface for Bragg coherent diffraction imaging*, *J. Appl. Crystallogr.*, 2022 (open access, CC-BY). Figures shown are screenshots, not raw detector data.

Automatic Classification (Set 1)

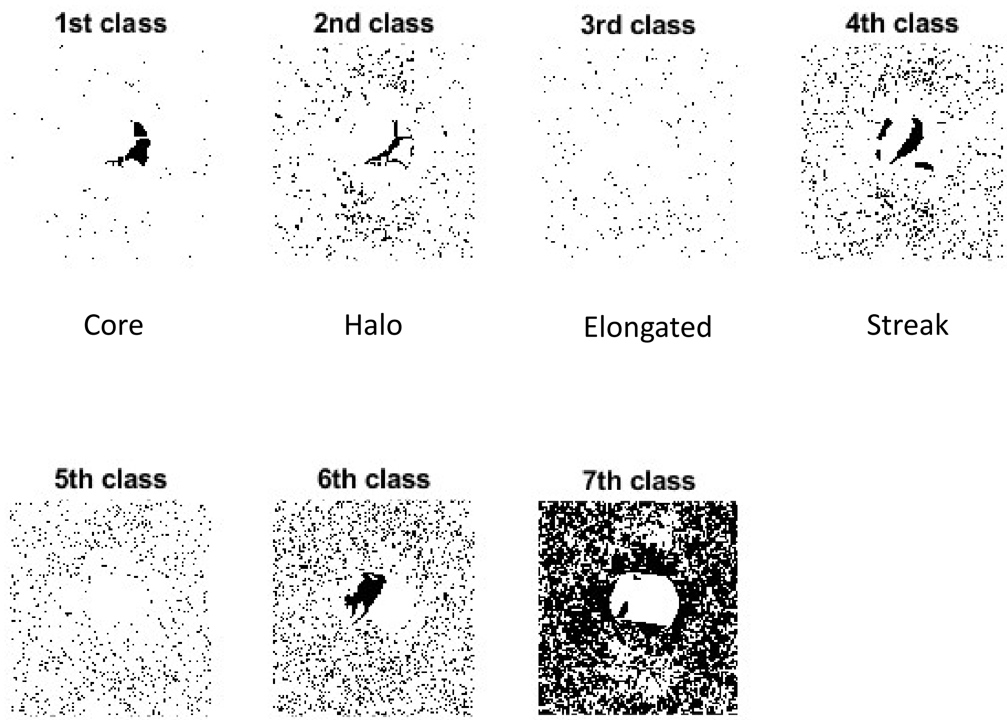
- SOM automatically clusters image features without labels (unsupervised, pixel-level)
- Pixel-level explainability enables detailed structural interpretation
- Outputs: pixel-level class map plus class centroids (prototypes)



Class	Short label (for figure)	Brief description (for notes / caption)
1st	Compact symmetric core	Nearly ideal Bragg spot: concentrated, isotropic intensity, minimal apparent strain or defects.
2nd	Broad symmetric core + halo	Main peak still symmetric but surrounded by a clear halo, indicating moderate strain or defect spread.
3rd	Moderately elongated core	Core stretched along one direction, suggesting anisotropic strain or elongated grain geometry.
4th	Needle-like streak	Highly elongated, streak-like scattering, consistent with strong directional defects or strain bands.
5th	Diffuse cloud-like scattering	No clear peak; intensity distributed in a cloud, representing highly disordered or defect-rich regions.
6th	Ring / vortex-like pattern	Approximate ring or vortex structure, possibly linked to specific dislocation structures or phase change.
7th	Core with strong vertical tail	Bright central spot with a pronounced vertical tail, indicating a strong scattering channel or gradient.

Prototype-prior initialization for Set 2

- No retraining required: directly seed with SOM class centroids from Set 1
- Zero-cost prior reuse significantly reduces computational cost



Core | Halo | Elongated | Streak

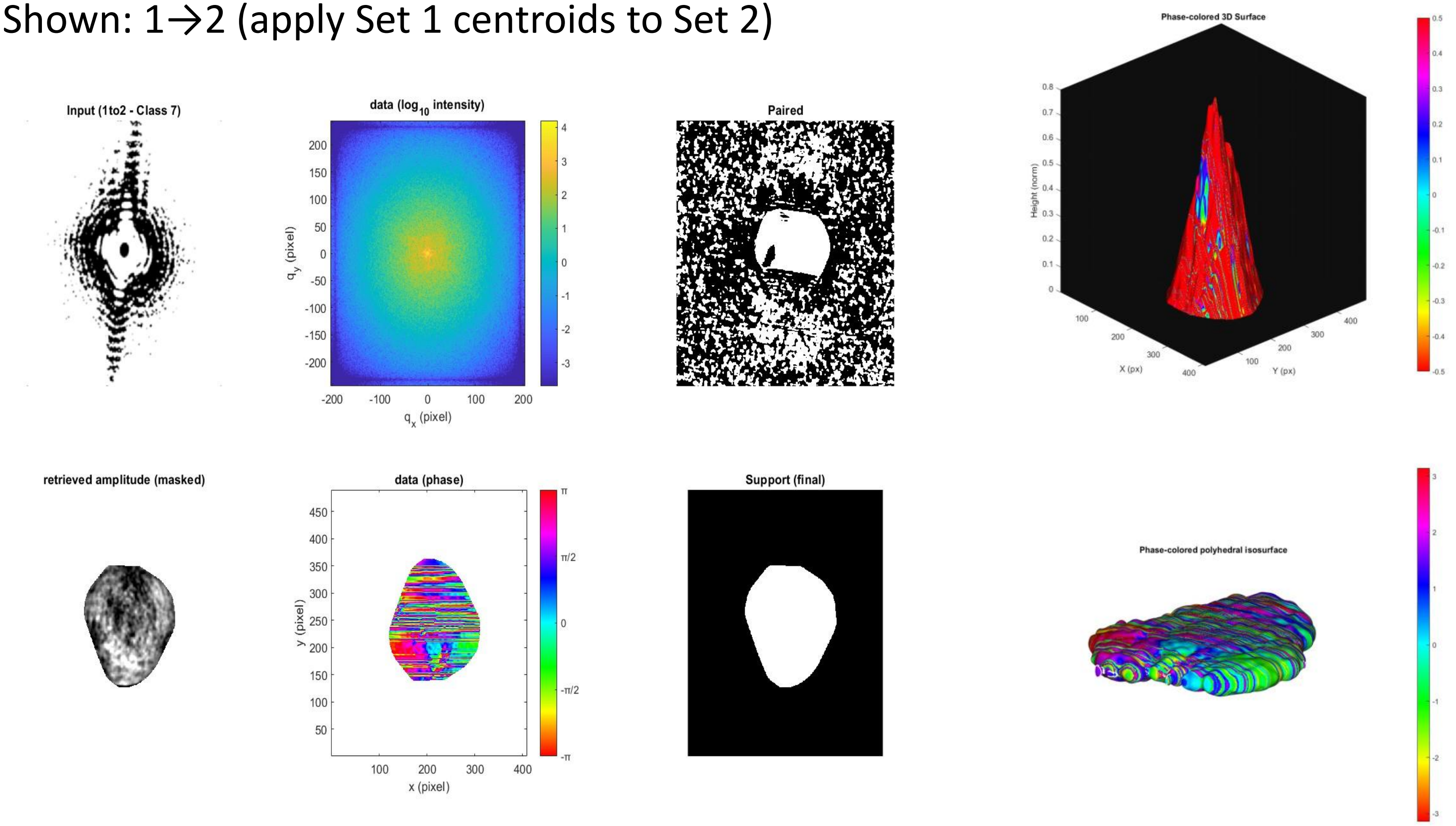
Diffuse | Ring | Tail

Prototype-prior initialization = using SOM class centroids (feature profiles) learned on the training split as initialization/regularizer for phase retrieval on held-out data — no labels or pixels are transferred; no cross-split leakage.

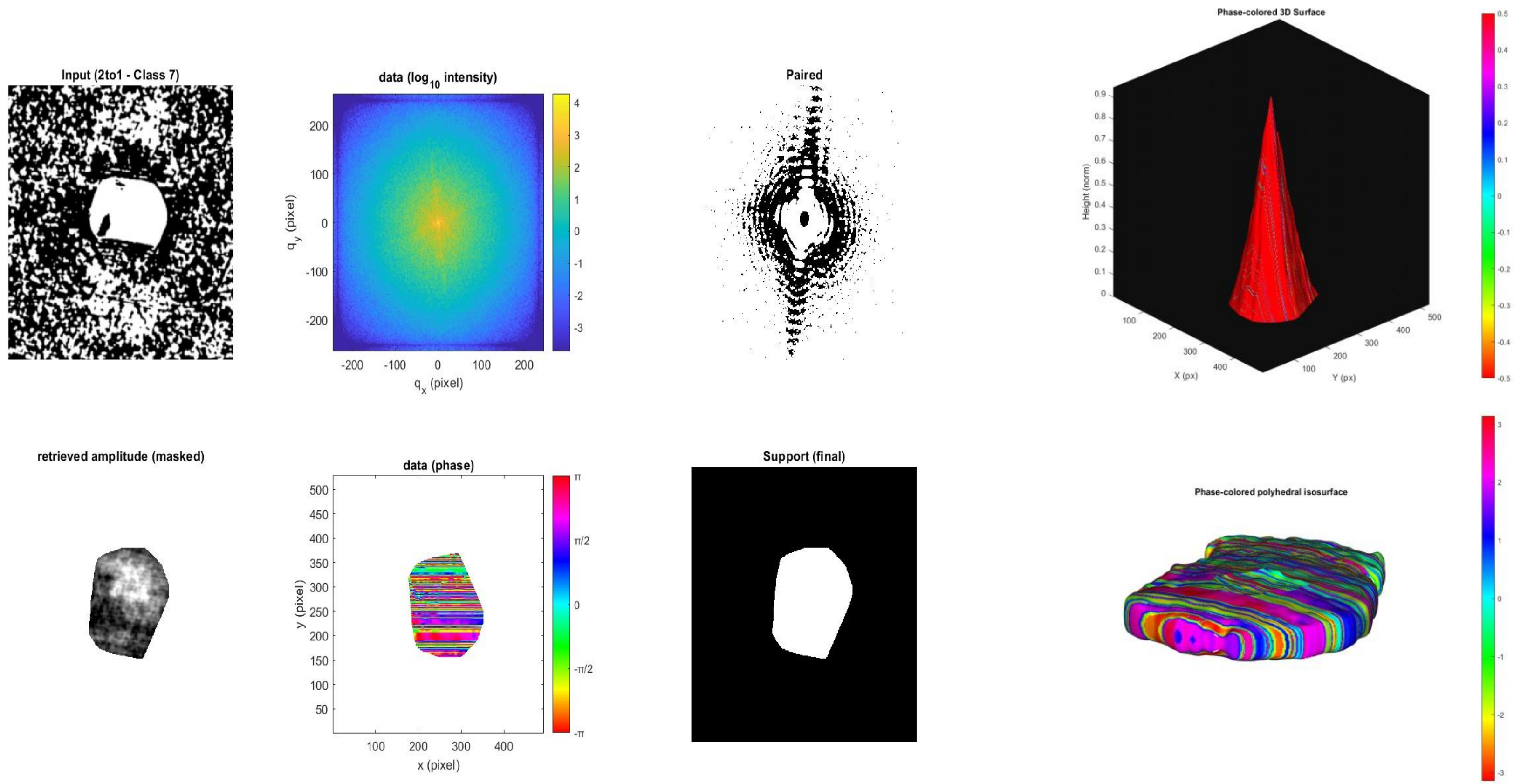
Class IDs (1st–7th) follow the morphology labels defined on the previous slide (compact core, halo, streak, diffuse, ring, tail, etc.).

Phase Retrieval with Centroid Priors

- Reconstruct structural phase using SOM centroid-based priors (from training split)
- Preserves fine-grained structural details and improves stability under noise/mask mismatch
- Shown: 1→2 (apply Set 1 centroids to Set 2)

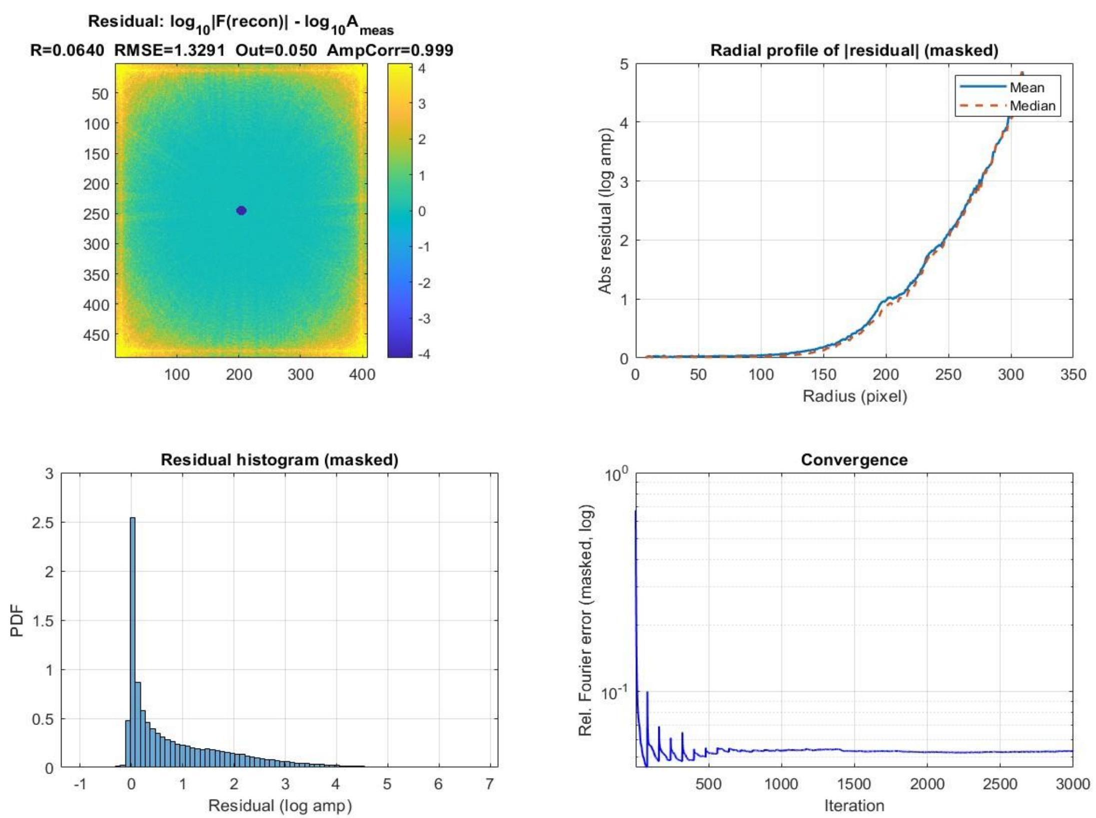


Shown: 2→1 (apply Set 2 centroids to Set 1)

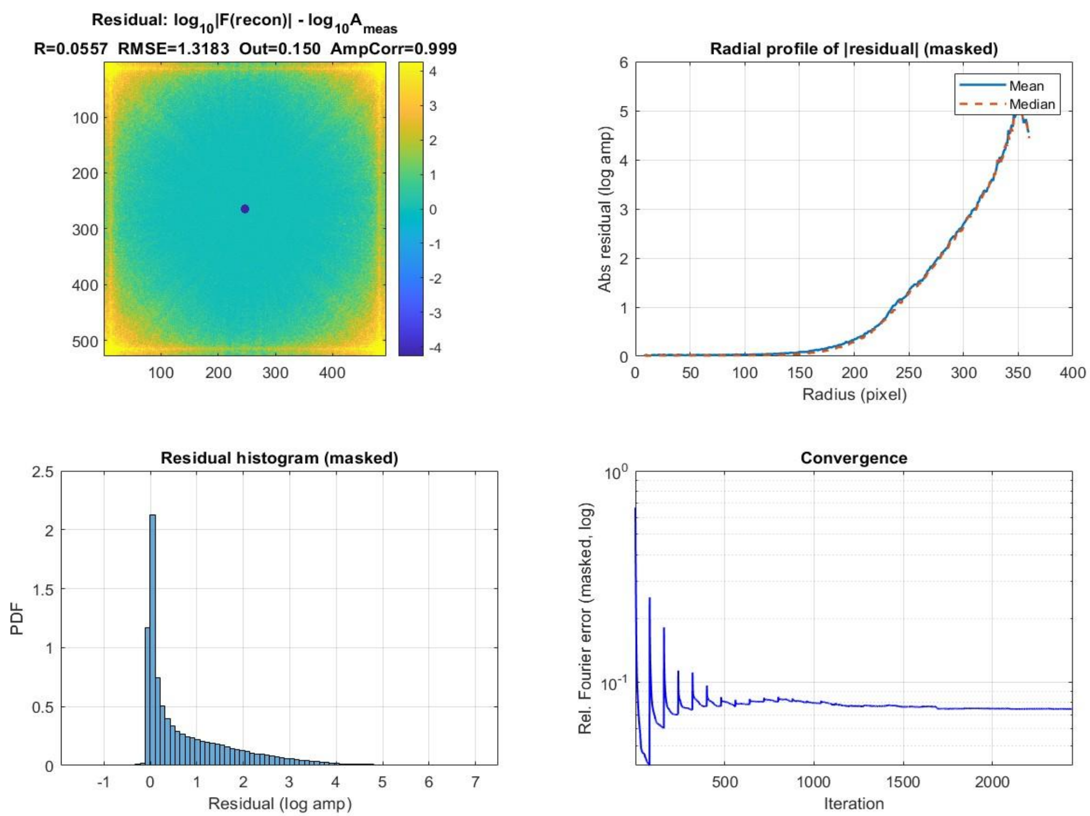


Error Analysis

- Compare reconstructed phase to ground truth: residual map, radial profile, histogram, and convergence
- Residual maps highlight spatial errors; report R-factor / SSIM / PSNR for quantitative comparison.
- Shown: 1→2 (Set 1 → Set 2)



Shown: 2→1 (Set 2 → Set 1)



Conclusion

- Label-free, fully automated, and reproducible pipeline for pixel-level classification + phase retrieval
- No labeling or retraining required; centroid-prior reuse reduces computation
- Preserves fine-grained structural details and improves stability under noise/mask mismatch
- MATLAB prototype is ready to be ported to Python/GPU for HPC integration (NumPy/SciPy/PyTorch; torch.fft)

Implementation: MATLAB prototype; Python/HPC port planned with versioned configs for reproducibility.