Unsupervised SOM-Based Morphology Analysis for High-Speed X-ray and Diffraction Imaging

A Label-Free and Physics-Consistent Framework for Structure Quantification and Transferable Pattern Learning

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Objective:
To develop a transferable, fully automatic, and explainable self-organizing map (SOM) framework that transforms high-speed X-ray imaging and diffraction data into physics-informed morphological maps and quantitative structure metrics.
The framework eliminates the need for labels, supervised training, or manual parameter tuning, enabling rapid, reproducible, and interpretable morphology characterization across diverse modalities — including Bragg coherent diffraction imaging (CDI), gas–liquid dynamics (GDI), and high-speed radiography.
This unified framework is applicable across imaging modalities, from synchrotron CDI to optical flow visualization.

Section 1 – Pixel-Level SOM Assisted Phase Reconstruction for X-ray and Diffraction Data

Applicable to Bragg CDI, ptychography, and other coherent or partially-coherent imaging workflows)

Pixel-Level, Cost-Free, Automated Phase Reconstruction

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

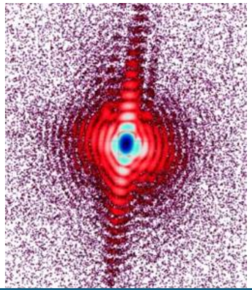
Motivation

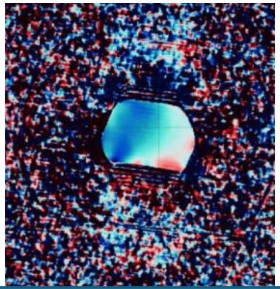
- Current X-ray phase-retrieval workflows often require manual parameter tuning and expert intervention, and can be sensitive to initialization/support and noise/mask mismatch.
- The proposed method is label-free, fully automated, and reproducible (fixed hyperparameters and versioned configs).
- Pixel-level 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.

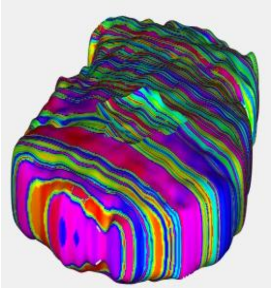
Workflow Overview

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





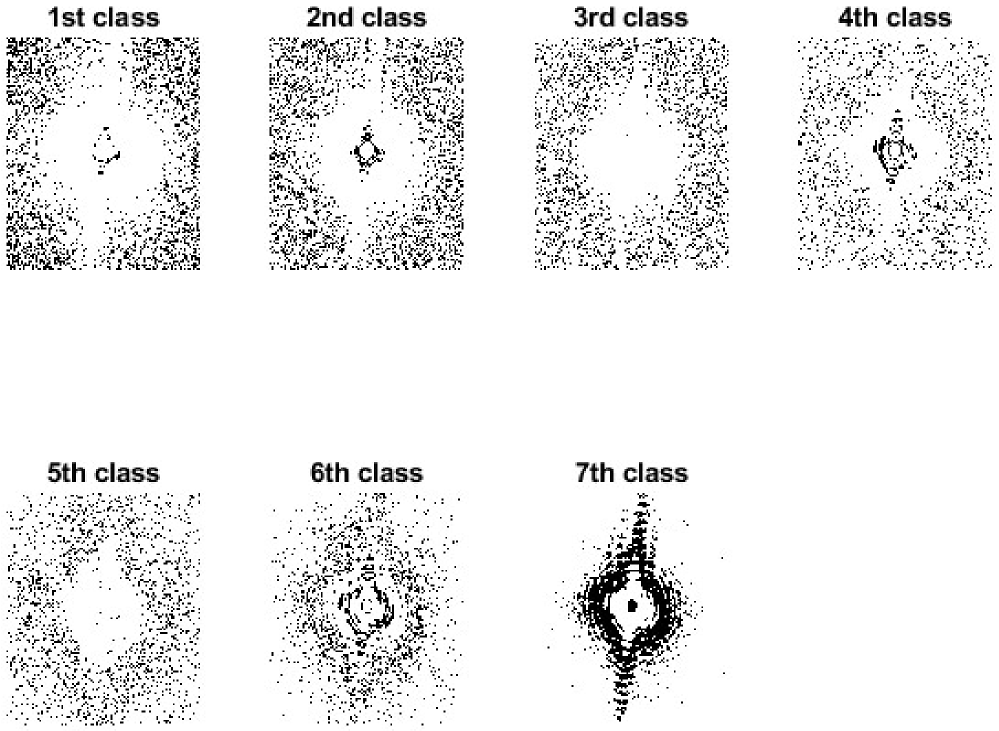


Pixel-level SOM classification (Set 1) → **Prototype-prior initialization (Set 1 → Set 2)** → **Phase retrieval & reconstruction (Set 2)** → **Error analysis (quantitative + visual)**

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.

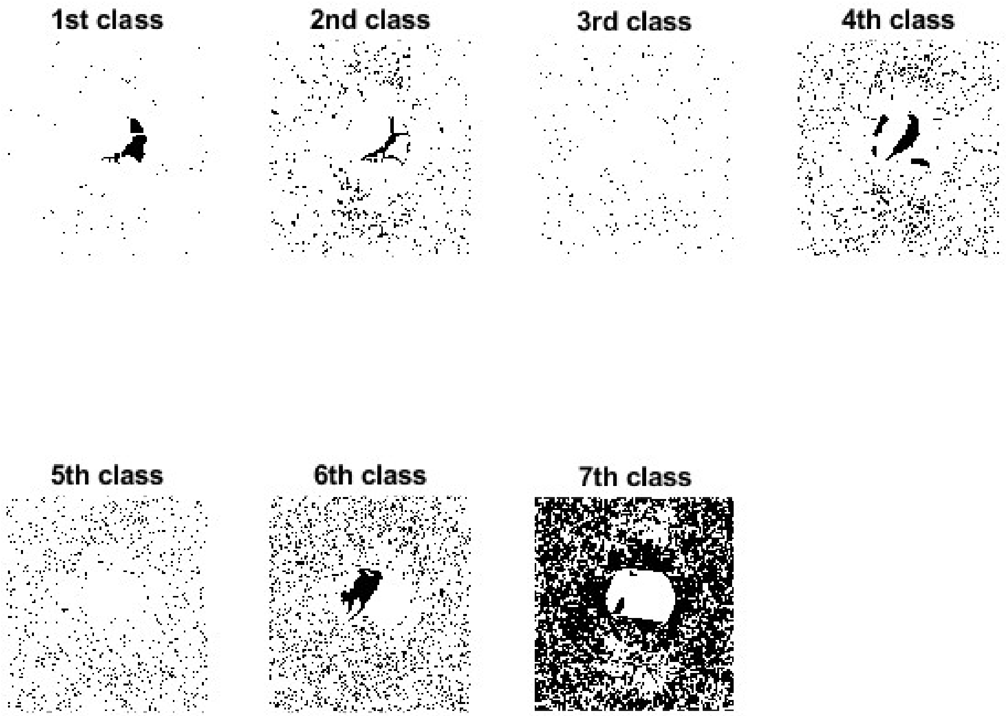
Automatic Classification (Set 1)

- 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)



Prototype-prior initialization for Set 2

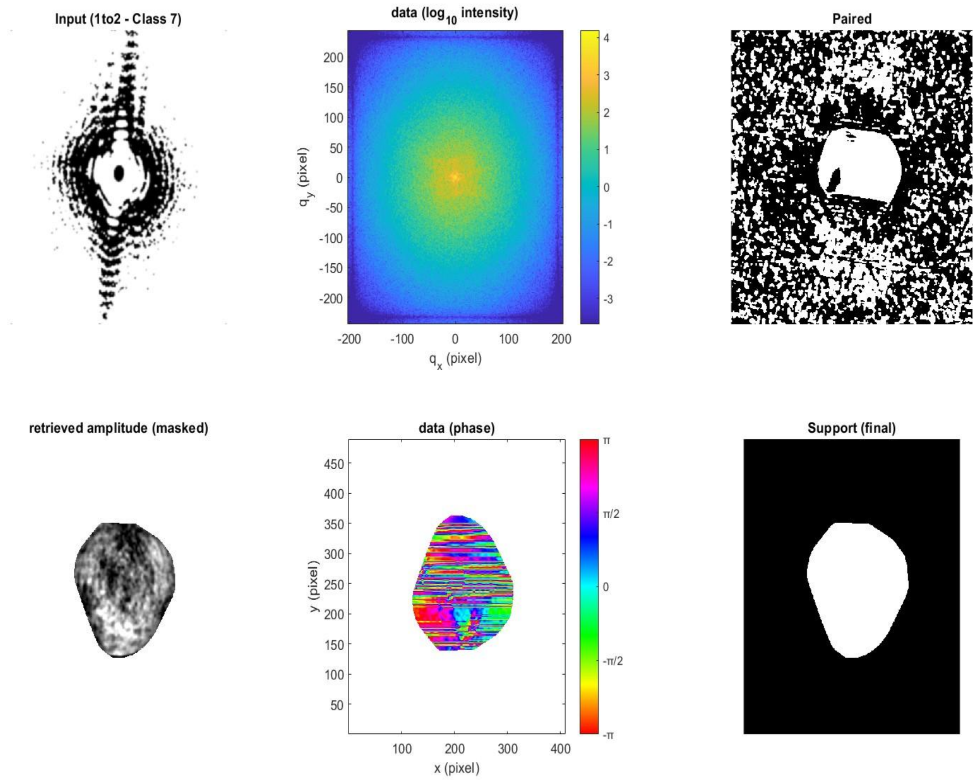
- No retraining required: directly seed with SOM class centroids from Set 1
- Zero-cost prior reuse significantly reduces computational cost

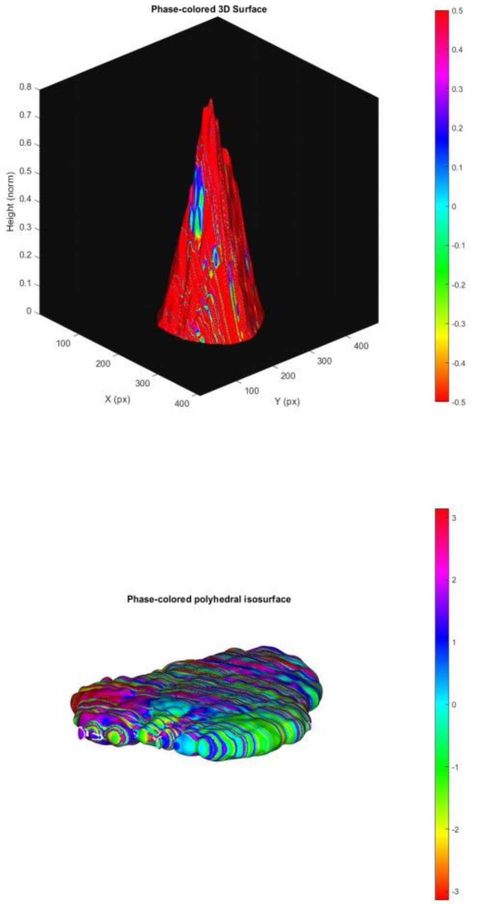


Prototype-prior initialization = using SOM class centroids (feature profiles) learned on the training split as initialization/regularizer for phase retrieval on held-out data — no labels or pixels are transferred; no cross-split leakage.

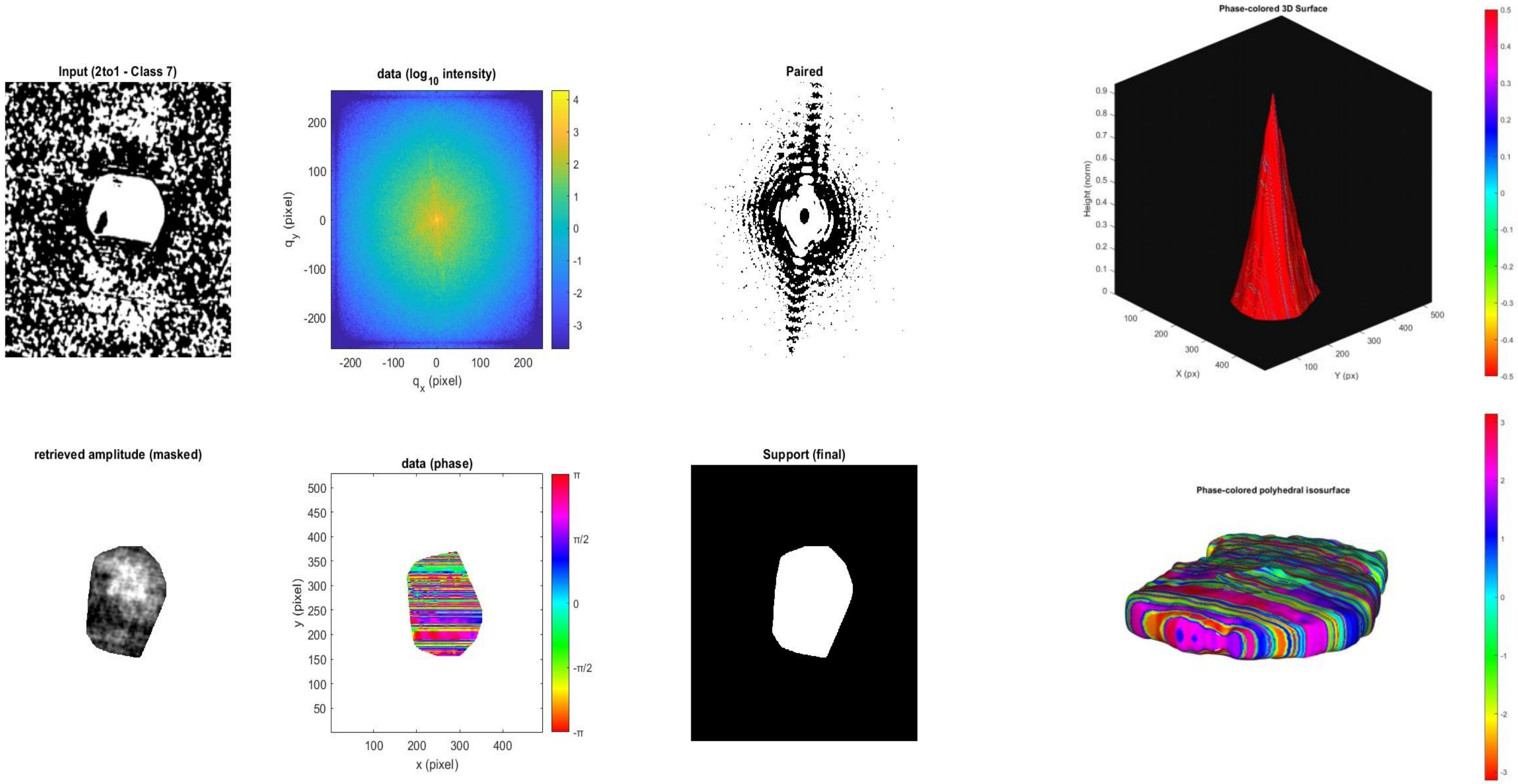
Phase Retrieval with Centroid Priors

- 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)



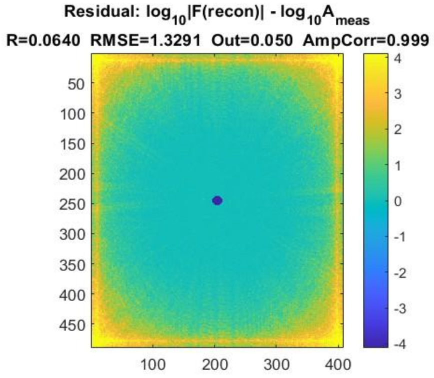


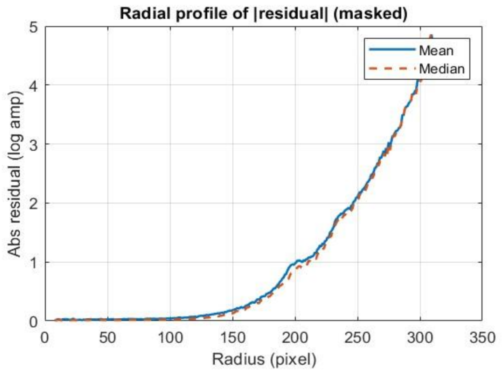
Shown: 2→1 (apply Set 2 centroids to Set 1)

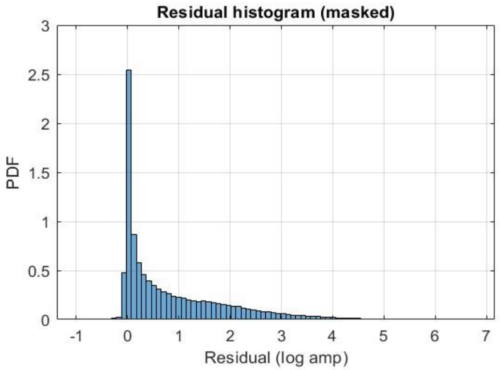


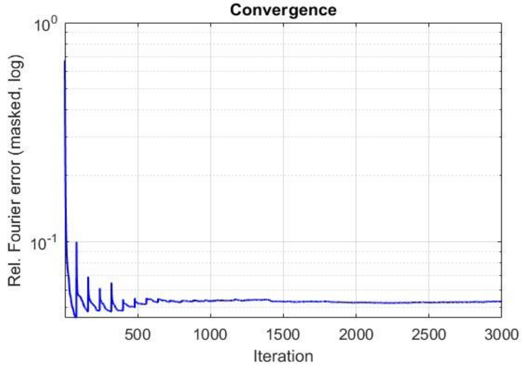
Error Analysis

- 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)

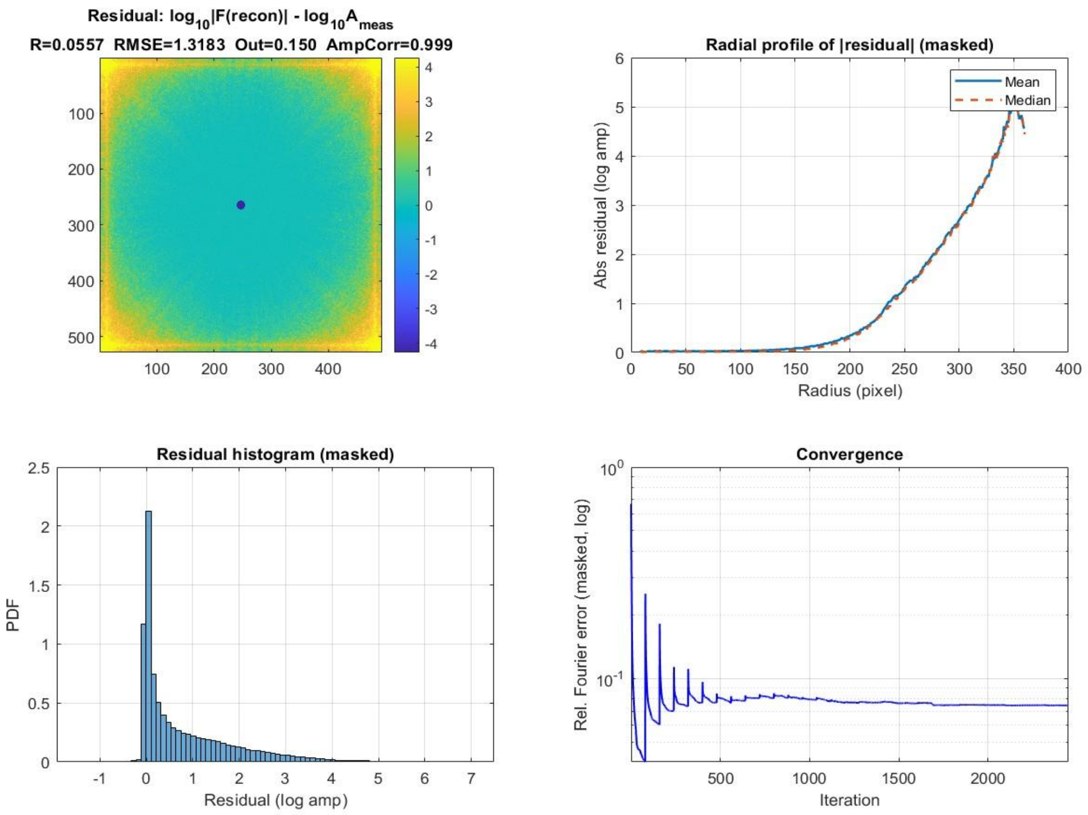








Shown: 2→1 (Set 2 → Set 1)



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, with Python/GPU HPC integration under development for large-scale deployment

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

Section 2 – Unsupervised SOM-Based Flow-State Analysis for Gas–Liquid and Cavitation Imaging

(Transferable from CDI and Ptychography to Ultrafast X-ray Radiography of Sprays and Fluids)

This section extends the same unsupervised SOM framework to real-space ultrafast X-ray flow imaging.
By mapping per-pixel feature vectors (density, gradient, anisotropy etc.) into SOM centroids, the method produces physics-consistent flow-state maps and morphological metrics (α and A) without any labels or training.
The centroid transfer concept demonstrates cross-modality robustness—from Bragg CDI to cavitation and spray imaging.

From CDI Phase Patterns to GDI Flow Morphology: Cross-Modality Transfer of Unsupervised SOM Centroids.

Input and Feature Representation for SOM Clustering

Objective:

To extract physically meaningful structural patterns from ultrafast X-ray imaging of fuel injection, each pixel is represented as a multi-dimensional feature vector and fed into a self-organizing map (SOM) for unsupervised clustering.

Input

- Each *entire image frame* is treated as the input unit.
- Every pixel within the frame is analyzed individually rather than patch-based, enabling fine-grained structural representation.

Per-pixel Feature Vector (9D)

Each pixel is described by a set of nine interpretable features that encode texture, density, and interface characteristics relevant to cavitation and spray dynamics:

Feature	Physical Meaning
Grayscale	Intensity, correlating with projected liquid density
Edge	Gradient magnitude, highlighting liquid–vapor interfaces
Contrast	Local variance, indicating bubble breakup and fine structures
Thinness	Filamentary structures, associated with atomization fronts
Local Mean (3×3 / 5×5)	Neighborhood intensity, capturing coarse-scale density context
Anisotropy (A1, A2)	Directional texture, reflecting flow alignment and shear direction
(Optional) **Hue**	Pseudo-color channel when available (for enhanced contrast visualization)

Preprocessing

- All features are normalized (e.g., z-score normalization) to ensure comparability across frames and operating conditions.
- This normalization is crucial for robust centroid transfer when applying trained SOM prototypes to different experimental conditions.

Why This Matters

This per-pixel feature encoding transforms raw grayscale X-ray images into a rich, high-dimensional structural space. Within this space, cavitation bubbles, dense liquid cores, transitional shear layers, and spray halos become separable patterns.

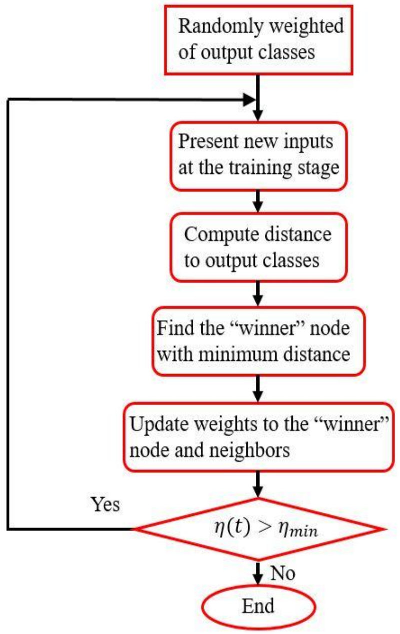
This representation forms the foundation for the subsequent SOM clustering and physically interpretable flow-state identification.

SOM-Based Flow-State Mapping (Fully Automatic, Pixel-Level, Explainable)

Objective:
Automatically resolve **physics-informed flow states** and cavitation structures from ultrafast X-ray frames, achieving a **fully automatic, label-free, training-free, fully unsupervised** workflow with **no manual parameter tuning**.

Workflow

- **Pixel-level feature encoding → SOM self-organization:**
  A Self-Organizing Map (SOM) self-organizes directly from per-pixel, multi-feature representations of a single frame or a small set of frames.
- **Topology-preserving lattice formation:**
  The SOM lattice adapts to intrinsic morphological patterns — such as density gradients, interface sharpness, and texture anisotropy — and yields prototype flow structures while preserving neighborhood topology.
- **Automatic cluster determination (elbow method):**
  The optimal number of clusters is determined automatically via the *elbow/knee* of the SSE (within-cluster variance) curve, eliminating the need for manual selection of *K*.
- **Fully automatic segmentation:**
  After convergence, each pixel is automatically assigned to its nearest prototype, producing a flow-state segmentation map (dense liquid core, cavitation/turbulent shear layers, transitional interfaces, spray halo).



Key Advantages

- **Label-free & Training-free:** No annotated data, no pre-trained models — the SOM emerges directly from experimental data.
- **Fully Automatic & Unsupervised:** Elbow-based K selection and zero manual parameter tuning — no thresholds, no ROI selection.
- **Explainable AI:** Radar-based feature fingerprints provide physical interpretability (e.g., cavitation shear vs. dense core).
- **Cost-free & Hardware-light:** Runs efficiently on CPU only; no GPU acceleration required.
- **Fast, Near-Real-Time & High-Throughput:** Suitable for beamline deployment and in-situ experiments.
- **Reproducible & Transferable:** Centroids remain stable across operating conditions, allowing direct reuse and consistent segmentation under varying pressure-temperature settings.

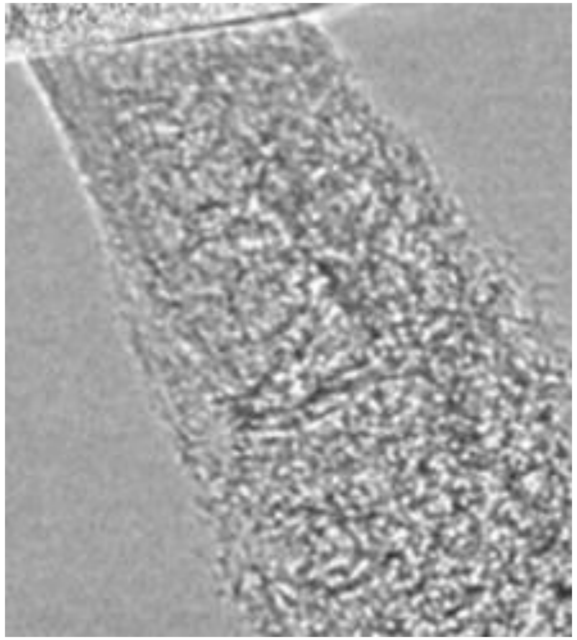
This fully automatic, elbow-guided, pixel-level SOM pipeline transforms raw X-ray frames into structured, physics-informed flow-state maps, bridging image morphology with cavitation dynamics. It is beamline-ready for real-time, high-throughput analysis and represents, to my knowledge, the first pixel-level SOM framework applied to ultrafast X-ray imaging.

Feature Fingerprints Reveal Distinct Flow States

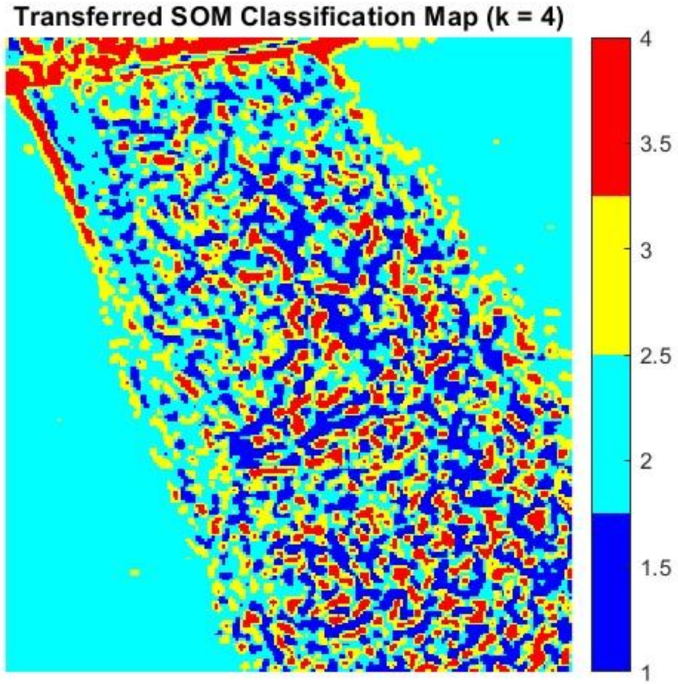
The pixel-level SOM segmentation transforms a raw grayscale frame into a **physics-informed map of flow states**, clearly distinguishing dense liquid cores, cavitation–turbulence shear layers, transitional interfaces, and dilute peripheries **without any labels or manual tuning**.

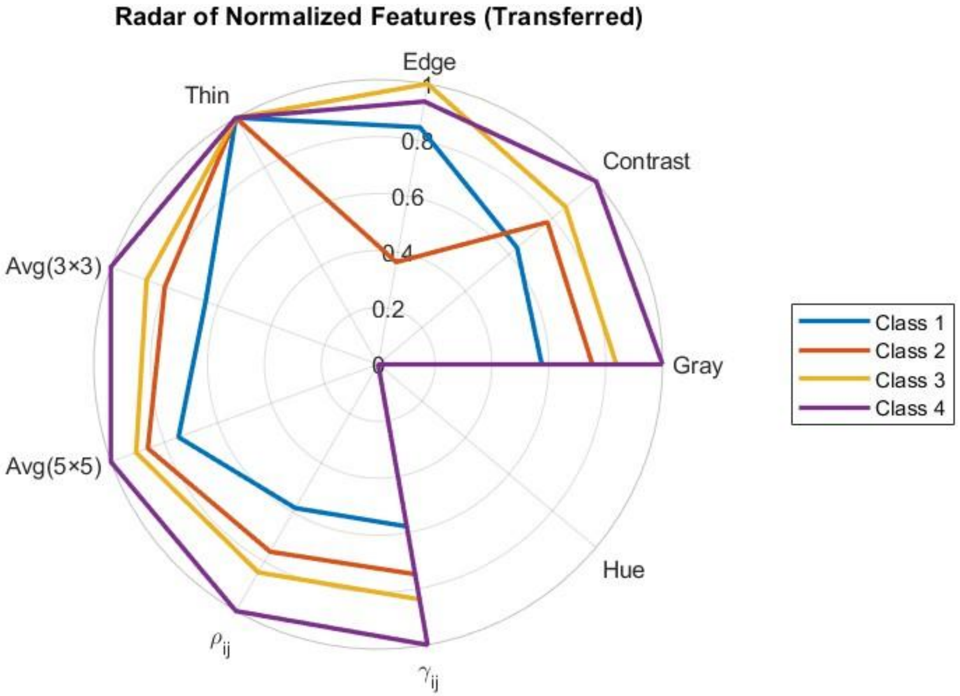
The radar plot shows that each class exhibits a unique multi-feature fingerprint, expressed through differences in grayscale intensity, local mean, contrast, and edge gradients. These fingerprints reveal fundamental physical regimes and enable **explainable AI interpretation** of cavitation morphology, linking image-based patterns to cavitation dynamics and energy conversion regions.

In addition, the class maps can be directly used as **pseudo-labels for CNN training or pre-conditioning**, which allows unsupervised SOM analysis to support data-driven segmentation models. This integration provides a physics-informed pathway to reduce manual annotation effort while strengthening deep learning pipelines.



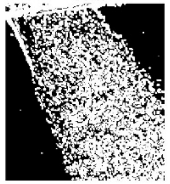
Cropped screenshot from Fig. 4(d), Zhang et al., Energy *265 (2022) 126117; used for non-commercial scholarly demonstration.*





Pixel-Level SOM Reveals Distinct Flow-State Fingerprints

Each class exhibits a unique feature signature, with differences in grayscale, local mean, contrast, and edge gradients, enabling explainable AI interpretation of cavitation structures and flow morphology.

Class	Key Radar Features	Recommended Physical Name	Physical Interpretation / Why It Matters
	*pij* and *rij* (pixel-level averages across row/column) **lowest**; Avg (3×3, 5×5) **lowest**; Edge **second lowest**; Contrast & Gray **lowest**	**Dense Liquid Core**	Represents the stable, high-density region of the jet. Low structural variation and lowest intensity variance indicate undisturbed liquid fuel prior to cavitation.
	*pij* and *rij* **second lowest**; Avg (3×3, 5×5) **second lowest**; Contrast & Gray **second lowest**; Edge **lowest**	**Ambient Gas / Dilute Periphery**	Extremely low density corresponds to the outer environment where the jet is most mixed with surrounding gas.
	Edge **highest**; *pij* and *rij* **second highest**; Avg (3×3, 5×5) **second highest**; Contrast & Gray **second highest**	**Cavitation–Turbulence Zone**	High edge and strong contrast reveal steep density gradients and complex interfaces from cavitation bubble collapse and turbulent shear layers. Even if feature order shifts across frames, this class consistently marks the most energy-active region.
	*pij* and *rij* **highest**; Avg (3×3, 5×5) **highest**; Contrast & Gray **highest**; Edge **second highest**	**Transition / Mixed Interface**	“Blended” feature fingerprint suggests a boundary layer between dominant regimes, representing transitional or classification-uncertain regions.

Why SOM Centroids Are Transferable

Why Frame *d* Is Used as the Reference

- Frame *d* (25 MPa, 26 °C) provides the clearest structural contrast — dense liquid core, cavitation interface, transition zones, and spray periphery are all present and well separated.
- Learning SOM centroids here ensures they encode **intrinsic, physics-relevant morphological patterns** rather than noise tied to a single operating condition.

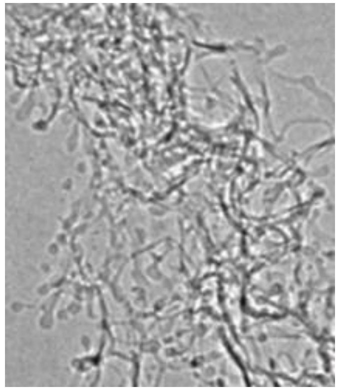
Why Centroids Can Transfer Across Conditions

- SOM centroids capture **feature-space topology** — relationships among density gradients, edge intensity, anisotropy, and local texture — which remain invariant even as external conditions (pressure, temperature, injection rate) change.
- These centroids thus act as **morphological “fingerprints”** of flow states, not frame-specific signatures.
- Once derived, they can be **directly applied** to classify new frames (*c, e, f, g, h, i, j*) **without retraining, without labels, and without manual intervention**.

This transferability demonstrates that SOM captures physics-invariant feature structures, enabling cost-free, label-free, and fully automatic analysis across diverse experimental conditions

Demonstration of Centroid Transfer (Frame *f*)

Centroids learned from Frame *d* are directly applied to Frame *f* without retraining. The resulting segmentation and feature fingerprints closely match those of the original condition, confirming that SOM clusters capture transferable morphological signatures.
Other frames (c, e, g, h, i, j) show consistent results as well.



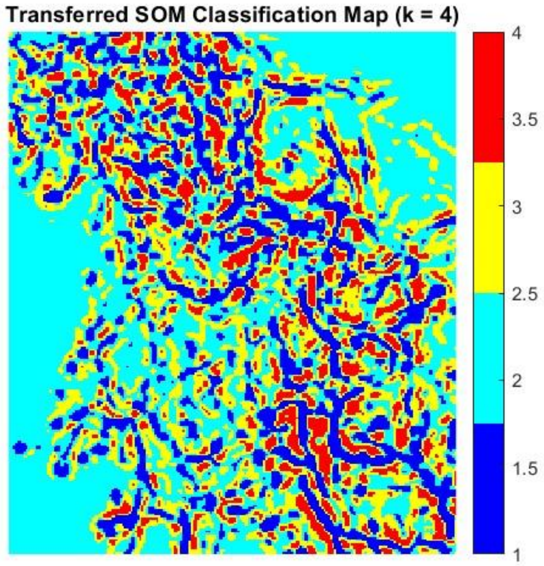
Cropped screenshot from Fig. 4(f), Zhang et al., Energy 265 (2022) 126117; used for non-commercial scholarly demonstration.

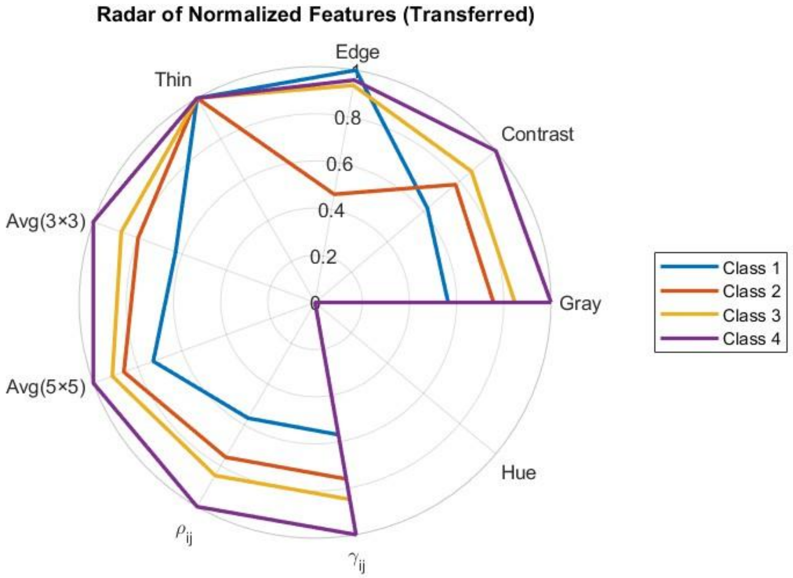
Dense Liquid Core

Ambient Gas / Dilute Periphery

Cavitation–Turbulence Zone

Transition / Mixed Interface





Quantifying Cavitation Dynamics Using SOM-Derived Metrics

To further validate the physical interpretability of my SOM-based segmentation, I computed two quantitative indicators that capture the evolution of cavitation activity across experimental conditions (c–j):

1. Relative Cavitation Ratio (α)

This metric characterizes the relative dominance of the cavitation–turbulence zone (Class 3) compared to the dense liquid core (Class 1):

$$\alpha = \frac{N_{class3}}{N_{class1} + N_{class3}}$$

where $N_{class\,3}$ and $N_{class\,1}$ represent the number of pixels classified as cavitation–turbulence and dense liquid core regions, respectively.

2. Absolute Cavitation Area Fraction ($A_{cavitation}$)

This parameter quantifies the total proportion of cavitation zones within the entire field of view:

$$A_{cavitation} = \frac{N_{class3}}{N_{total}}$$

where N_{total} is the total number of pixels in the image.

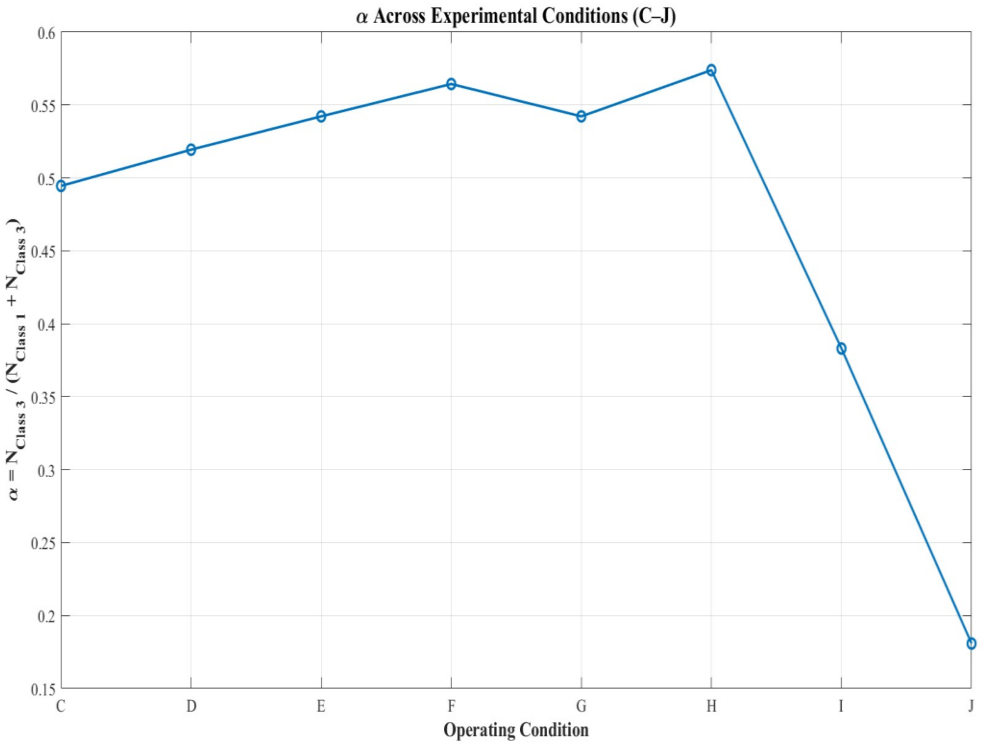
Together, these two metrics allow my unsupervised SOM pipeline to translate morphological segmentation into physically meaningful cavitation indicators, enabling label-free and reproducible flow-state quantification across varying operating conditions.

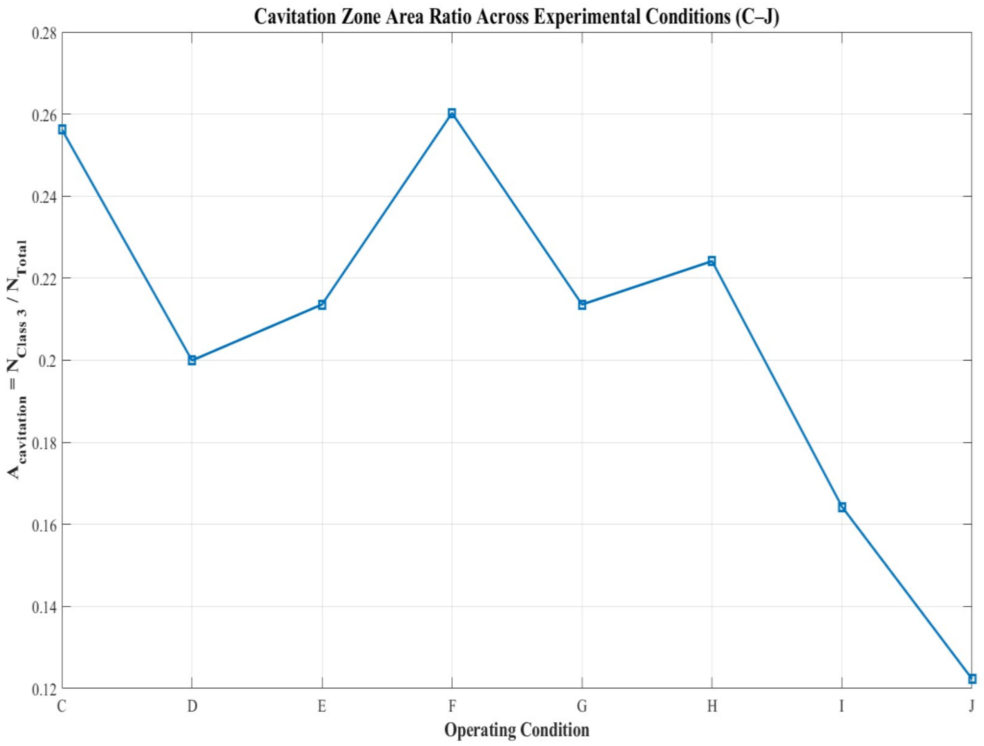
Evolution of SOM-Derived Cavitation Metrics Across Conditions (C–J)

Using the SOM centroids derived from frame *d* without any retraining, I applied the segmentation directly to frames *c–j* and computed the two quantitative indicators defined on the previous slide. Both metrics exhibit clear, systematic trends across experimental conditions:

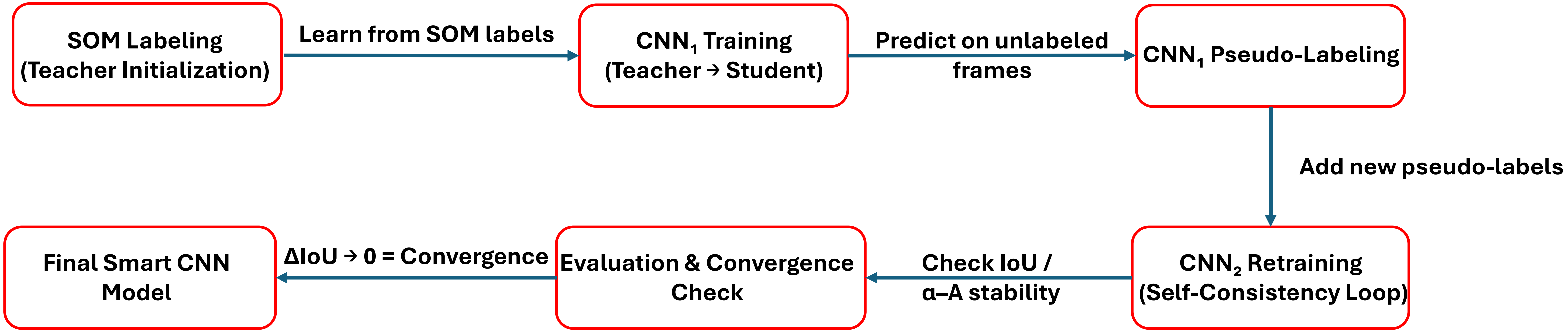
- **Relative cavitation ratio (α)** reflects the fraction of cavitation–turbulence regions relative to the dense liquid core.
- **Absolute cavitation area fraction** $(A_{cavitation})$ represents the overall cavitation–turbulence coverage within the field of view.

The monotonic variations of both $\alpha$and $A_{cavitation}$ across conditions demonstrate that the SOM-derived classes capture physics-consistent flow-state evolution. Even when applied to unseen frames, the transferred centroids yield coherent, interpretable trends — highlighting the robustness, transferability, and explainability of my unsupervised pipeline.





SOM–CNN Integration Workflow for Physics-Consistent Label Expansion



- **Stage 1 – Initial SOM Labeling (Frames c–e)**

The SOM is applied to three representative frames *(c, d, e)* to generate the first set of physics-consistent masks (**$label_1$**). These serve as the *teacher* labels for CNN initialization.

- **Stage 2 – CNN_1 Training (Teacher → Student)**

A U-Net-style CNN is trained using only the SOM-labeled frames (c–e). It learns the cavitation morphology and reproduces the α/A metrics on these frames.

- **Stage 3 – Pseudo-Label Generation (Frames f–g)**

CNN_1 predicts morphology on two unseen intermediate frames *(f, g)*, producing new pseudo-labels (**$label_2$**). The α/A curves remain physically consistent, verifying successful knowledge transfer.

- **Stage 4 – Refined Training (Frames c–g)**

The network is retrained on both **$label_1$ + $label_2$**, enforcing teacher–student consistency. This improves coverage and stabilizes morphology recognition.

- **Stage 5 – Final Prediction (Frames h–j)**

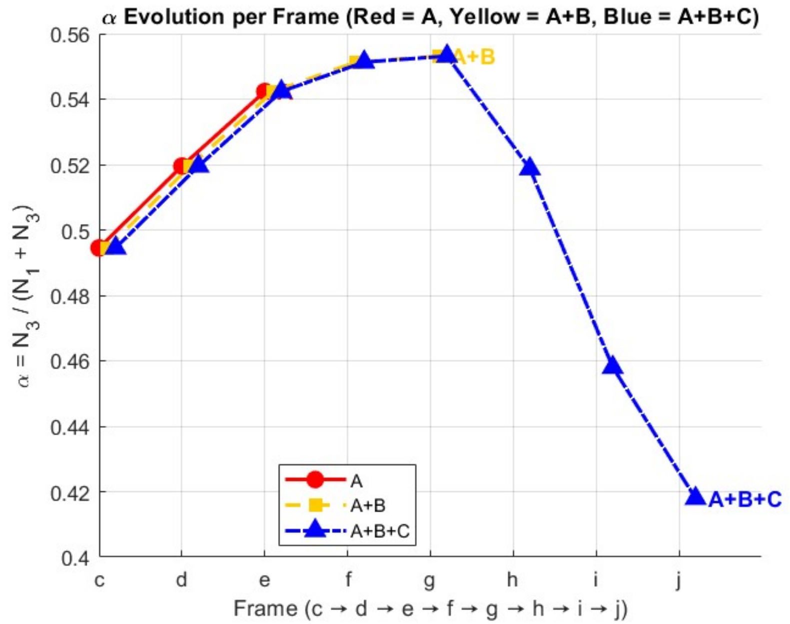
The refined CNN generalizes to the remaining three unseen frames *(h, i, j)*, yielding a complete morphology evolution sequence. α and A values follow the same rise–plateau–decay trend as the SOM teacher, demonstrating physical convergence.

- **Stage 6 – Convergence Validation**

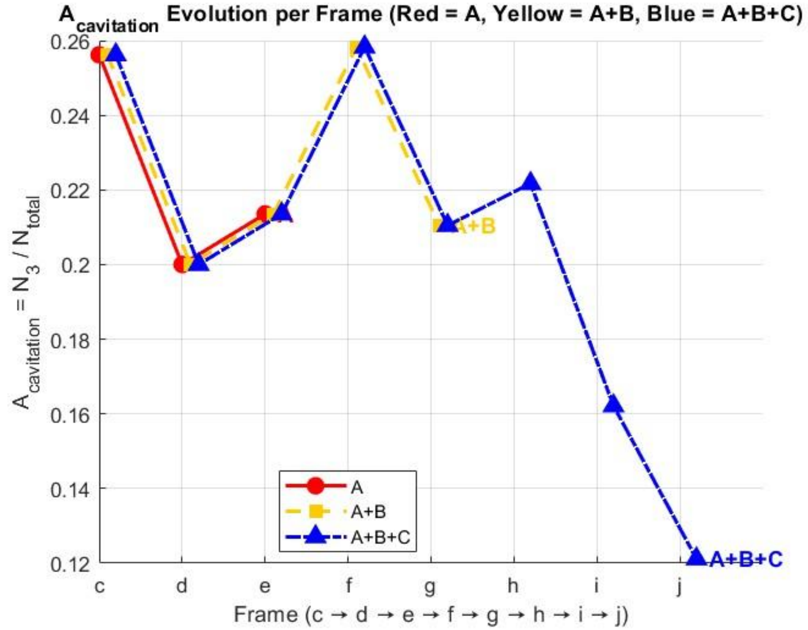
Mean IoU increases steadily from A → A + B → A + B + C, and ΔIoU → 0 indicates the CNN has reached SOM-level reasoning.

Validation of CNN Convergence and Physical Consistency

(a) Mean IoU vs. Training Data Scale
Demonstrates class-dependent convergence behavior. The CNN learns the **cavitation–turbulence zone ($class_3$)** more efficiently than the **dense liquid core ($class_1$)**, as reflected by the steeper IoU improvement of $class_3$.
This aligns with physical intuition — the high-contrast, topologically complex cavitation regions provide stronger morphological cues for learning than the relatively uniform liquid core.
Both classes eventually converge (ΔIoU → 0), indicating stable morphology transfer.



(b) α Evolution per Frame (CNN–SOM vs. SOM)
CNN reproduces the overall rise–plateau–decay trend of the SOM-derived α curve, confirming physics-consistent morphology transfer.
The slight one-frame shift—CNN starting the decay at *g* while SOM begins at *h*—reflects the CNN's learned regularization: it smooths temporal transitions and anticipates morphological collapse earlier.
Because the dense liquid core (**$class_1$**) is harder to learn, the CNN compensates by slightly overpredicting the cavitation–turbulence zone (**$class_3$**) at mid frames, while preserving total area balance — consistent with the nearly identical A curves.



(c) $A_{cavitation}$ Evolution per Frame (CNN–SOM vs. SOM)
The CNN reproduces the SOM-derived cavitation-area ratio with near-identical trends, confirming conservation of global morphology.
Both frameworks capture the same rise–decay pattern of the cavitation–turbulence zone, demonstrating that the CNN internalized the physical area balance (N_3/N_{total}) learned from SOM.
This alignment indicates successful transfer of quantitative morphology rather than mere texture fitting.

SOM-guided retraining stabilizes CNN learning (IoU ≈ 0.9–0.99), making predictions physically consistent and confirming SOM as a robust structural prior.

Structure-to-Energy Bridge: Complementing C_n–C_v Scaling with SOM-Derived Morphology Metrics

Objective:

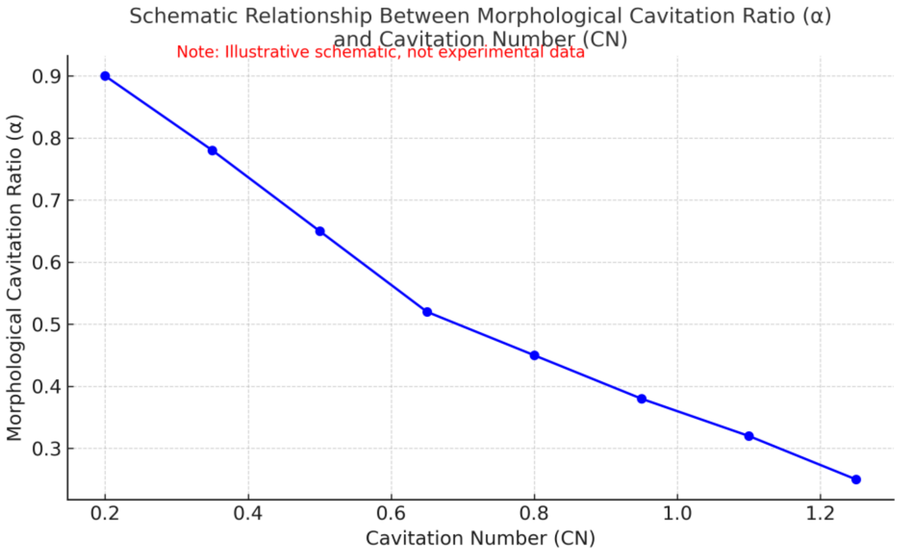
To demonstrate how morphology-based cavitation metrics derived from unsupervised SOM clustering can complement and enhance the energy conversion scaling laws developed by *Zhang et al.* (Energy, 2022).

Key Idea:

- Prior studies (e.g., Zhang et al., Energy 2022) have established a robust relationship between cavitation number (CN) and energy conversion efficiency (Cv), showing that C_v is a single-valued function of CN across varying pressure and temperature.
- My SOM framework extracts structural cavitation indicators (e.g., cavitation ratio α, cavitation area fraction A) directly from ultrafast X-ray images without labels or manual annotation.
- These morphology-derived indicators quantify the spatial distribution and evolution of cavitation structures, offering a complementary structural dimension to the existing hydrodynamic metrics.

Schematic Concept:

The plot below illustrates a potential correlation between the cavitation ratio (α) and the cavitation number (CN). While not based on experimental data, it highlights the bridge between morphological signatures and energy scaling laws:



Why This Matters:

- Provides a structure-to-energy bridge: linking flow morphology directly to hydrodynamic efficiency.
- Offers a physically grounded interpretation of why CN scaling remains invariant across operating conditions — because SOM centroids encode density gradients, anisotropy, and texture, which are intrinsic physical properties.
- Enables rapid, automated analysis that can immediately enhance existing research pipelines and support future studies on fuel injection dynamics and alternative fuels.

oth morphological indicators (α and A) are expected to vary monotonically with cavitation number (CN), consistent with trends reported in previous studies (e.g., Energy 2022).

Illustrative schematic, not based on experimental data.

Complementary Roles of Energy Scaling and Morphology-Driven Analysis

Aspect	Representative Physical Study	This Work (Unsupervised SOM Framework)
Input	Ultrafast X-ray imaging data	Same
Core Focus	Cavitation number (CN), energy conversion (Cv)	Morphological structure metrics (α, A)
Output	Hydrodynamic scaling law: Cv = f(CN)	Structure-based cavitation fingerprint
Invariance	Cv–CN relation consistent across T, P	SOM centroid patterns consistent across T, P
Insight	Quantifies velocity–energy coupling	Quantifies structure–energy linkage
Added Value	Defines efficiency scaling	Adds morphology context and explainability

This comparison illustrates how unsupervised morphology analysis complements traditional hydrodynamic scaling.
The SOM framework enhances physical interpretability and enables automated, label-free quantification across flow regimes.

Final Summary & Outlook

Summary:
This work presents a fully automatic, label-free, and explainable SOM-based framework that transforms ultrafast X-ray imaging data into physics-informed flow-state segmentations and cavitation morphology fingerprints. The method requires no labeled data, training, or manual tuning, and remains reproducible and transferable across different operating conditions.

Key Contributions:
- Developed the **first pixel-level SOM pipeline** for ultrafast X-ray spray imaging.
- Introduced **morphology-based cavitation metrics** (α and A) that quantify cavitation dynamics directly from structural signatures.
- Demonstrated **centroid transferability**, enabling cross-condition application without retraining.
- Established a pathway to link **morphological indicators** with **energy conversion scaling laws**.

Future Directions:
- Integrate SOM-derived cavitation metrics (α and A) with C_V–CN scaling to build a unified structure-to-energy framework, revealing how flow morphology governs hydrodynamic efficiency.
- Extend the automated framework to study alternative fuels, where cavitation behavior is highly sensitive to temperature and pressure, enabling high-throughput analysis of large experimental datasets.
- Deploy the method for real-time beamline experiments, providing on-the-fly morphological diagnostics that complement velocity and pressure measurements.
- Use morphology-derived metrics as transferable pseudo-labels for downstream machine-learning or data-driven modeling, bridging physics-based and statistical approaches.

This framework aligns with ongoing research on high-speed X-ray imaging and multimodal morphology analysis across synchrotron and laboratory facilities.