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Physics-based reward driven image analysis in microscopy

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The rise of electron microscopy has expanded our ability to acquire nanometer and atomically resolved images of complex materials. The resulting vast datasets are typically analyzed by human operators, an intrinsically challenging process due to the multiple possible analysis steps and the corresponding need to build and optimize complex analysis workflows. We present a methodology based on the concept of a Reward Function coupled with Bayesian Optimization, to optimize image analysis workflows dynamically. The Reward Function is engineered to closely align with the experimental objectives and broader context and is quantifiable upon completion of the analysis. Here, cross-section, high-angle annular dark field (HAADF) images of ion-irradiated (Y, Dy)Ba₂Cu₃O_{7- δ} thin-films were used as a model system. The reward functions were formed based on the expected materials density and atomic spacings and used to drive multi-objective optimization of the classical Laplacian-of-Gaussian (LoG) method. These results can be benchmarked against the DCNN segmentation. This optimized LoG* compares favorably against DCNN in the presence of the additional noise. We further extend the reward function approach towards the identification of partially-disordered regions, creating a physics-driven reward function and action space of high-dimensional clustering. We pose that with correct definition, the reward function approach allows real-time optimization of complex analysis workflows at much higher speeds and lower computational costs than classical DCNN-based inference, ensuring the attainment of results that are both precise and aligned with the human-defined objectives.

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Electron and scanning probe microscopy have emerged as a primary method to provide insights into the microstructure, composition, and properties of a wide range of materials, from metals and alloys to polymers and composites.¹⁻⁴ These techniques generate large volumes of imaging data containing information on material structure that can be further connected to fundamental physics, chemistry, and material processing.⁵ However, the large amount of imaging data requires consistent analysis methods.⁶⁻⁸ Traditionally, this has been accomplished using the collection of the standard image processing techniques including various forms of background subtraction,^{9,10} filtering,¹¹ and peak finding,¹²⁻¹⁴ all applied by the human operator sequentially. The employment of machine learning methodologies, particularly DCNN (Deep Convolutional Neural Network) segmentation,¹⁵⁻¹⁹ has notably enhanced and expedited certain steps within this analytical framework; however, the overall progression of image analysis remains the

same. This type of analysis is also computationally intensive²⁰⁻²³ and requires the ensemble networks to effectively manage deviations from anticipated data distributions.²⁴⁻²⁶ Most importantly, it is strongly biased by the operator's expertise and can potentially be steered towards anticipated answers *via* decisions made at each analysis step.

Here we present a method for image analysis that utilizes a reward function concept.^{27,28} This involves setting a measure(s) of success that can be quantitatively established by the end of the analysis. With the reward function defined, the analysis workflow including the sequence and hyper-parameters of individual operations can be optimized *via* one of the suitable stochastic optimization frameworks. The simple image analysis workflow is optimized by Bayesian Optimization²⁹⁻³² which allows dynamic tuning of the parameters to achieve optimal performance. This concept can be further adapted to more complex, multi-stage workflows *via* reinforcement learning, Monte Carlo decision trees, or more complex algorithms.^{33,34}

In proposing reward-driven workflows, we note that typically human-based image analysis is performed to optimize certain implicit measures of the analysis quality. For example, in atomic segmentation, this task is to identify and classify all the atoms of a certain type, or all defects within the image. Here we propose that analysis can be cast as an optimization problem if

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the reward function based on the analysis results can be formulated. Then the process becomes optimized in the parameter space of the simple analysis functions. Here, we consider two specific tasks, namely atom finding in atomically resolved images and identification of amorphized regions within the material.

As a model system, we chose a 1.2 μm thick $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ thick film, doped with Dy_2O_3 nanoparticles, fabricated using a metal-organic deposition process. The sample then was irradiated with an Au^{5+} ion beam oriented along the c -axis of the Yttrium Barium Copper Oxide (YBCO), and the cross-sectional and plan-view TEM specimens were prepared through standard mechanical polishing, followed by final thinning using Xe Plasma Focused Ion Beam (Xe PFIB).³⁵

As a first model task, we consider the semantic segmentation,^{36–39} or “atom finding” of atomically resolved images.⁴⁰ Traditionally this has been accomplished using the peak finding procedures, correlative filtering, Hough transforms,^{41,42} or versions of Laplacian of Gaussian (LoG) approaches.^{43,44} These approaches require extensive tuning of the parameters of the image analysis function with the human assessment of the results as feedback. The introduction of DCNNs has resulted in broad interest in deep learning segmentation of images,^{45–47} with multiple efforts utilizing versions of U-Nets,^{48,49} Mask R-CNNs,⁵⁰ and other architectures recently reported such as SegNet,⁵¹ DeepLab,⁵² and Pyramid Scene Parsing Networks (PSPNet).⁵³ The use of simple analysis methods requires careful manual tuning of parameters and tends to be very brittle – the contrast variations even within a single image can result in measurable differences of performance. Comparatively, DCNN methods are more robust, but require supervised training and can be sensitive to out-of-distribution drift effects.^{54–56}

Taking atom detection as an initial instance of the reward-driven process, we demonstrate optimization of the conventional LoG algorithm. This approach is characterized by a set of control parameters, including min_sigma (σ_{min}), which sets the smallest feature size that can be detected, max_sigma (σ_{max}), which defines the largest detectable feature size, threshold (T), determining the minimum intensity required for a feature to be detected, and overlap (θ), controlling the degree of permissible overlap between detected features. These parameters collectively define the LoG algorithm's parameter space, as illustrated in Fig. 1(A).

To cast the image analysis as an optimization problem, we define possible physics-based reward (or objective) functions. One such function can be defined based on the expected number of atoms within the field of view, readily available from image size and lattice parameter of material. The LoG algorithm's effectiveness in relation to its hyper-parameters is determined by a metric we refer to as Quality Count (QC), which is defined as the normalized difference between the number of atoms found by LoG and the physics-based reward standard, formulated as:

$$\text{QC} = \frac{\text{LoG blobs} - \text{physics_blobs}}{\text{physics_blobs}} \quad (1)$$

where LoG_blobs represents the number of atoms identified by the LoG algorithm. Physics_blobs represent the expected number of atoms based on the physics-based reward standard.

To avoid reward hacking in this context, we also recognize that the total count of atoms is an overarching characteristic, and for a segmentation algorithm to be effective, it should adhere to more specific requirements. The second constraint is that atoms need to be spaced at distances that are physically plausible. To incorporate this aspect, we introduce a second component to the reward function, which we call the error function.

The error function (ER) will be applied to measure the incidence of atoms in regions that are not aligned with the structural configuration of the YBCO lattice. As shown in Fig. 1(B), the ER calculates the sum of distances from each atom to its four nearest neighbors. If this sum, referred to as the Distance Sum (DS), falls below a certain threshold, the atom is considered incorrectly positioned and is classified as an error. This threshold is determined based on the expected inter-atomic distances within the ideal YBCO lattice parameters (lengths of the unit cell).

$$\text{ER} = \frac{\# \text{ atoms with cumulative interaction value less than DS}}{\text{physics_blobs}} \quad (2)$$

In this setting, the optimization of LoG analysis that we will further refer to as LoG*, becomes that of the multi-objective Bayesian Optimization in the image processing parameter space, where objectives QC and ER are minimized jointly.

In this case, we can further define a benchmark for accuracy, which we designate as “Oracle” in this context. A viable way to create an Oracle for the atomic segmentation task can be performed using the pre-trained DCNN, providing near-ideal identification of all atomic positions. These can be further classified (with human tuning) into specific types. We refer to the DCNN analysis as “Oracle” comparable to human-based analysis and use Oracle to verify the results of the reward-driven workflows accomplished with much simpler tools.

We employed the Skopt library^{57,58} to implement hyper-parameter optimization, specifically focusing on adjusting the threshold and overlap parameters of the LoG function. As represented in Fig. 1(C), a set of optimal solutions, or Pareto front, where no objective can be improved without degrading the other was obtained. Through this framework, a delicate balance between the dual objectives has been established, leading to the discovery of an optimal hyper-parameter configuration for the LoG function. Two common metrics to identify the “best” solutions within the Pareto Frontier are the Euclidean and Chebyshev distances.

Displayed in Fig. 2(A) is the workflow development utilized for Multi Objective-Bayesian Optimization. This workflow outlines the order of steps throughout the analysis procedure. We note that this approach can be readily applied to the scenarios when the image quality or acquisition conditions vary across the image, *e.g.*, due to the mis-tilt or presence of non-



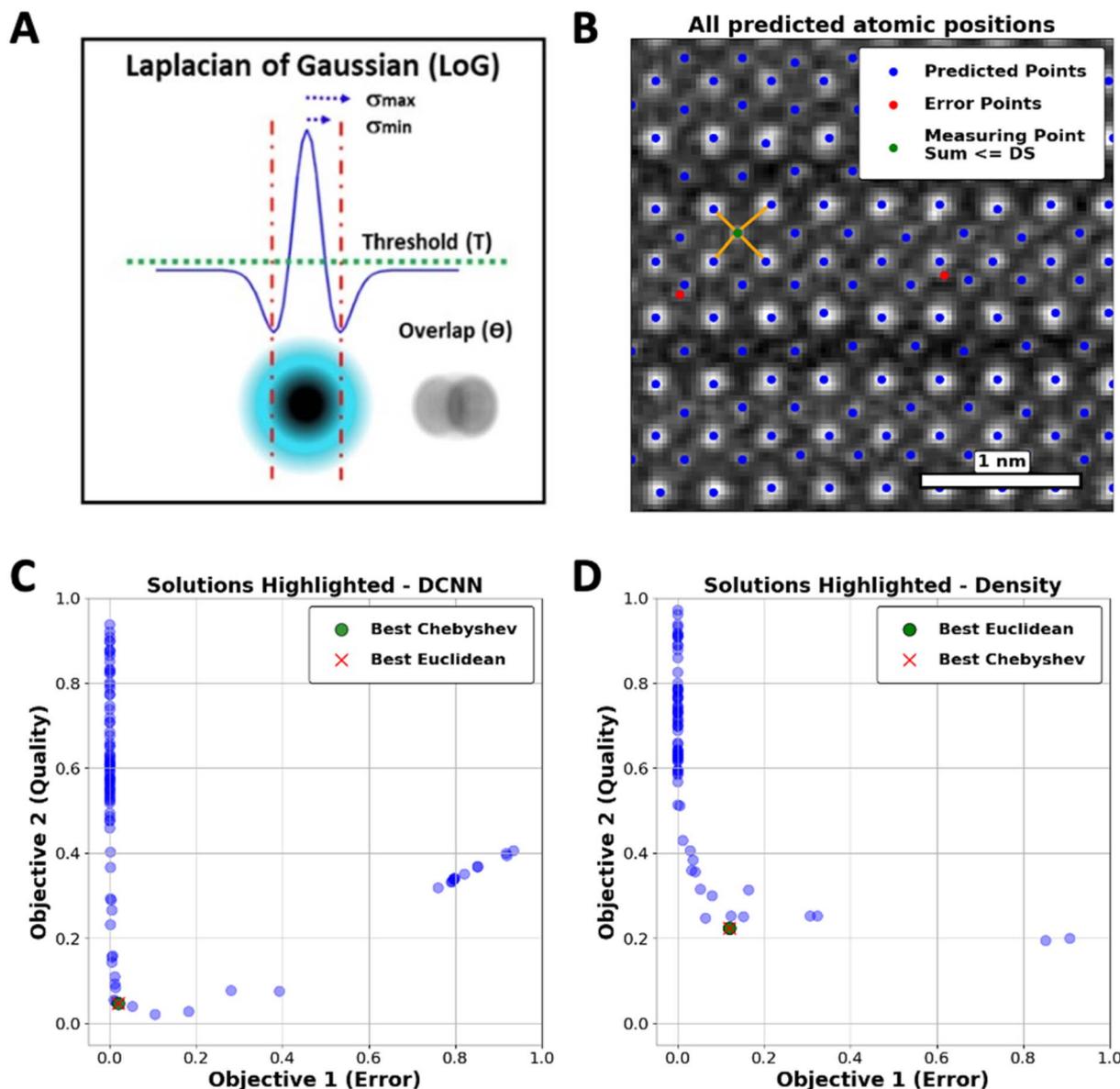


Fig. 1 (A) Laplacian of Gaussian Hyper-parameters, min_sigma (s_{min}), max_sigma (s_{max}), num_sigma (s_{num}), threshold (T), and overlap (q), (B) detected atoms and their nearest neighbor connections. Atoms marked in red indicate those with a sum of distances to their four nearest neighbors less than DS , thus flagged as errors, (C) Pareto Frontier solutions with respect to Oracle-A, and (D) Pareto Frontier solutions with respect to Oracle-B. Each point represents an optimal trade-off point such that improving one objective would compromise another. This balance delineates the optimal hyper-parameter settings for the LoG function, achieved by finely tuning the competing objectives.

crystalline contaminates, *etc.* For these tasks, the algorithm can be implemented in the sliding window setting where the parameters are optimized for each. Further, this workflow can be customized to focus on different rewards such as the identification of the amorphous regions or other objectives of the study as presented in Fig. 2(B).

As a next step, we explore the robustness of the proposed approach with respect to the noise in the image. To accomplish this, Gaussian noise levels from 0 to 1, where 0 is the image without noise have been applied to a specific set of images. Upon noise addition, the number of atoms is identified both by DCNN and optimized LoG* algorithm. Fig. 3(A) depicts the

variation in optimal hyperparameters of the LoG model in response to various levels of added noise. Correspondingly, Fig. 3(D) demonstrates that the best Pareto front solutions, which represent the objectives (QC and ER), adapt in a manner that fulfills the reward requirements.

In DCNN models, elevating the noise level leads to the introduction of artifacts that mimic the appearance of new atoms in the images, thereby generating false positives as depicted in Fig. 3(C). In contrast, the LoG function demonstrates resilience when subjected to comparable increases in noise, avoiding the misidentification of these artifacts as new atoms, as evidenced in Fig. 3(B). This stability can be attributed



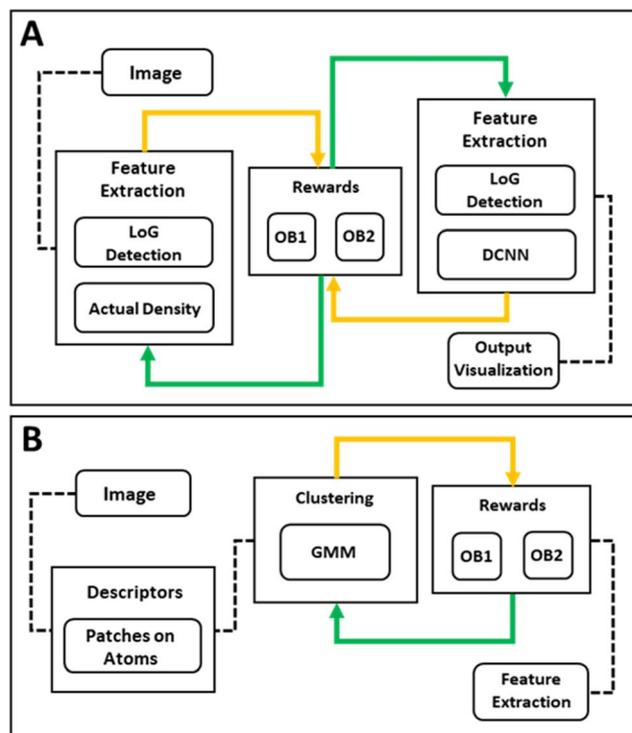


Fig. 2 (A) Workflow for reward-driven methodology in TEM images, data preparation, optimization of the LoG function based on two objectives using multi-objective Bayesian optimization, and processing. (B) workflow for reward-driven methodology in TEM images, task specified version.

to the implementation of the ER function within the LoG framework, which effectively prevents the function from mistakenly identifying features caused by noise as real atomic points.

Fig. 3(F) illustrates the detection capability of the DCNN model regarding Gaussian noise levels. The number of detected atoms increases significantly with the Gaussian noise level after a certain point (Noise level of 0.6), which implies that the DCNN begins to mistakenly identify noise artifacts as atoms, thereby detecting false positives. Fig. 3(E) represents the detection results of the LoG method under the same conditions. In contrast to the DCNN, the LoG detection exhibits a much lower variability in the number of detected atoms across noise levels, maintaining a relatively consistent count. This implies that the LoG approach is more selective, mainly identifying actual atomic points and not creating false positives by noise-related distortions.

We have further explored the applicability of this approach towards more complex tasks of identification of the amorphous regions. Here, the complexity of analysis is that the damage introduces amorphization and change of observed image contrast on oxygen and copper lattices, whereas the bright atoms remain visible. Correspondingly, manual construction of the workflow combining segmentation, multiple possible clustering and dimensionality reduction algorithms can be a very time-consuming and operator-dependent step. Here, we

illustrate that the use of the reward function approach enables us to address this problem through a comprehensive workflow. This workflow includes window-size selection and automated parameter tuning of the Gaussian Mixture Model (GMM) clustering method.^{59,60} We used GMM to model the data as a mixture of multiple Gaussian distributions, which provides a robust framework for clustering complex datasets, and offers a broad range of hyperparameters that enable fine-tuning of the model. In principle, other clustering models⁶¹ can also be used, which makes the selection of the model type a part of the optimization process.

Considering the workflow in Fig. 2(B), we initially implemented GMM clustering techniques to identify the diverse atomic configurations within the YBCO structure. Fig. 4(A) displays the categorization of all atomic types present in the YBCO structure. We organized these into four distinct clusters corresponding to the CuO_2 (planes), CuO (chains), Ba (barium), and Y (yttrium) components, respectively. Given that certain atomic varieties can dominate the clustering outcomes, we refined our approach by reducing the number of cluster types to specifically focus on barium (Ba) atoms. This was achieved by conducting two separate GMM clustering analyses on patches centered exclusively on Ba atoms. As illustrated in Fig. 4(B), two distinct clusters were identified, corresponding to the orientation of barium (Ba) atoms. These clusters are categorized based on their orientation: Ba_1 is aligned along a principal axis, while Ba_2 is configured to exhibit two-fold rotational symmetry with respect to Ba_1 . By concentrating solely on Ba_1 or Ba_2 atoms, GMM clustering enables us to detect the variations in Ba atoms.

In crystalline regions, atoms are generally well-ordered and maintain close alignment with their expected lattice positions, leading to the formation of tightly packed clusters with minimal deviations. However, any observed dispersity within these clusters serves as a clear indicator of deviations from the expected lattice positions, which is characteristic of atoms in amorphous areas. This distinction allows for the differentiation of crystalline and amorphous structures based on the spatial arrangement and variability of atomic positions.

Fig. 4(C) demonstrates that the clustering of atomic points can be controlled through the adjustment of two hyperparameters of GMM: threshold and covariance type. According to our hypothesis, atomic points that surpass a pre-determined threshold, when analyzed using a specific covariance type, should be classified as amorphous. This classification is substantiated by the observed dispersity of these points away from the core cluster, which is predominantly associated with crystalline regions. In this instance, the effectiveness of GMM clustering depends primarily on hyperparameter selection and can be improved by devising a customized reward system that better aligns with desired outcomes.

To direct GMM clustering toward not only pinpointing the location but also assessing the area occupied by atoms deviating from their predicted positions, the compactness of these identified regions should be considered a valuable metric for rewards. Given that compactness is a critical characteristic, the second component of the reward should focus on regions with



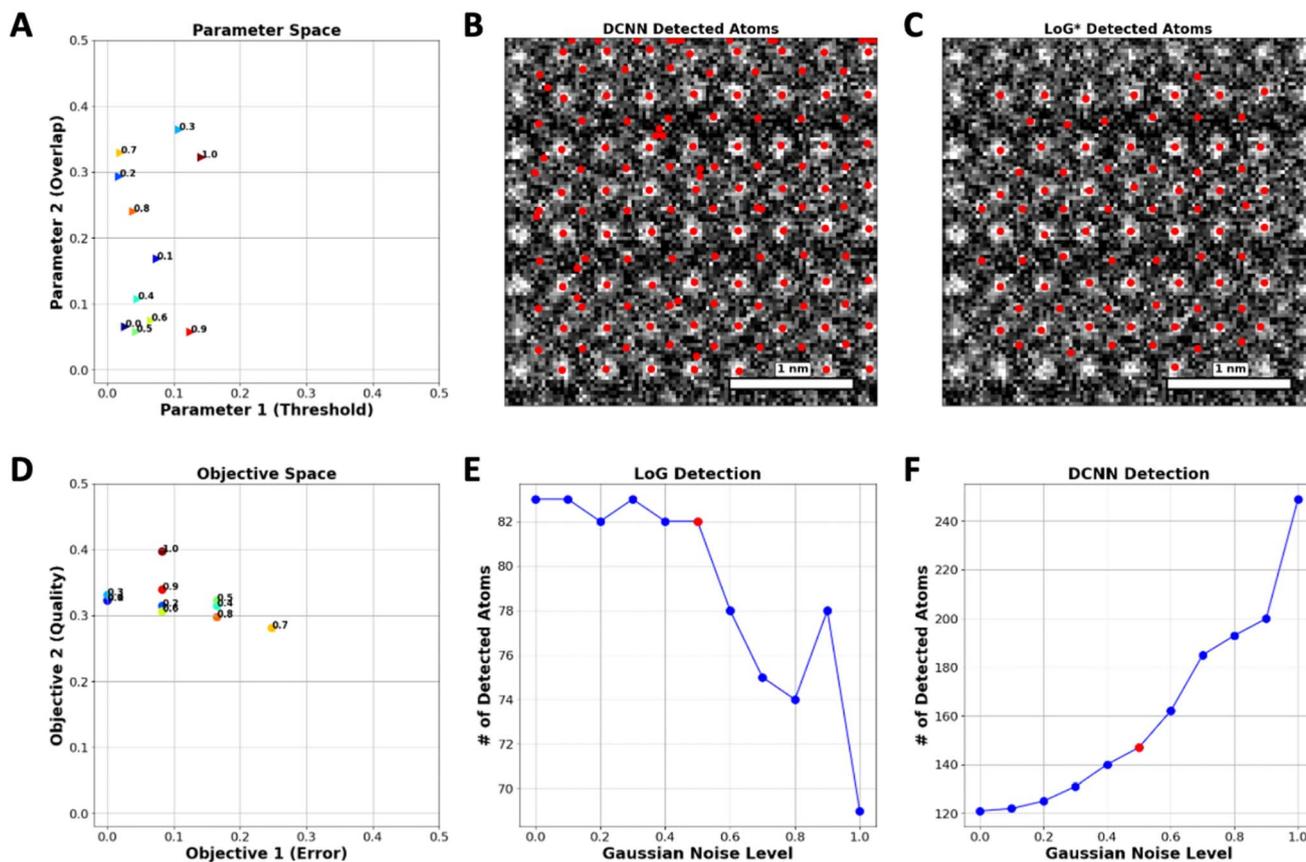


Fig. 3 (A) Optimal hyper-parameter space changes versus noise level in the LoG* optimized method, (B) detected atoms using the LoG* optimized method on the image with a moderate noise level, (C) detected atoms using a (DCNN) model scattered on the image, (D) optimal objective space change versus noise level in the LoG* optimized method, (E) number of detected atoms versus Gaussian noise level using the LoG* optimized method, (F) number of detected atoms versus Gaussian noise level using a (DCNN) model.

minimal perimeter. By integrating both compactness and perimeter as objectives in our analysis, we establish a workflow that is both practical and dependable.

To calculate these two objectives, we start by creating two binary masks to distinguish between crystalline and amorphous regions, where crystalline regions are labeled as “blue” based on provided data and everything else is considered amorphous. We then expand the boundaries of these masks slightly to ensure accurate measurements. Next, we calculate the area of each region by counting the pixels in the masks. For the amorphous regions, we label connected clusters of pixels and measure the length of their boundaries to get the total perimeter. These area and perimeter measurements are then normalized to account for the image size. Finally, we calculate the compactness of the amorphous regions using the formula. This helps in understanding how compact or spread out the amorphous regions are.

$$\text{Compactness} = \frac{\text{area}}{\text{perimeter}^2} \quad (3)$$

As depicted in Fig. 4(D), a set of optimal solutions was identified, demonstrating that no objective can be enhanced

without adversely affecting another. By employing metrics to pinpoint the “best” solutions on the Pareto Frontier, the analysis effectively determined the optimal threshold and covariance type for GMM clustering, as presented in Fig. 4(E). The deployment of the clustering map on the image of the YBCO substrate, as demonstrated in Fig. 4(F), effectively reveals areas within the YBCO structure where there is a higher likelihood of atoms deviating from their predicted positions.

To summarize, here we introduce an approach for the development of complex image analysis workflows based on the introduction of a reward function aligned with experimental objectives. This reward function is a measure of the success of analysis, and can be built based on simple physical consideration, comparisons to the oracle functions, or any other approach imitating human perception. With the reward function being defined, the image analysis problem reduces to that of the optimization in the combinatorial space of image operations and corresponding hyper-parameters, taking advantage of the immense volume of knowledge in his field.

Here, this approach has proven to be effective in a case study involving *in situ* ion irradiated $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ layer images, where it facilitated the accurate identification of atomic positions and detection of amorphous regions. We propose the physics-based



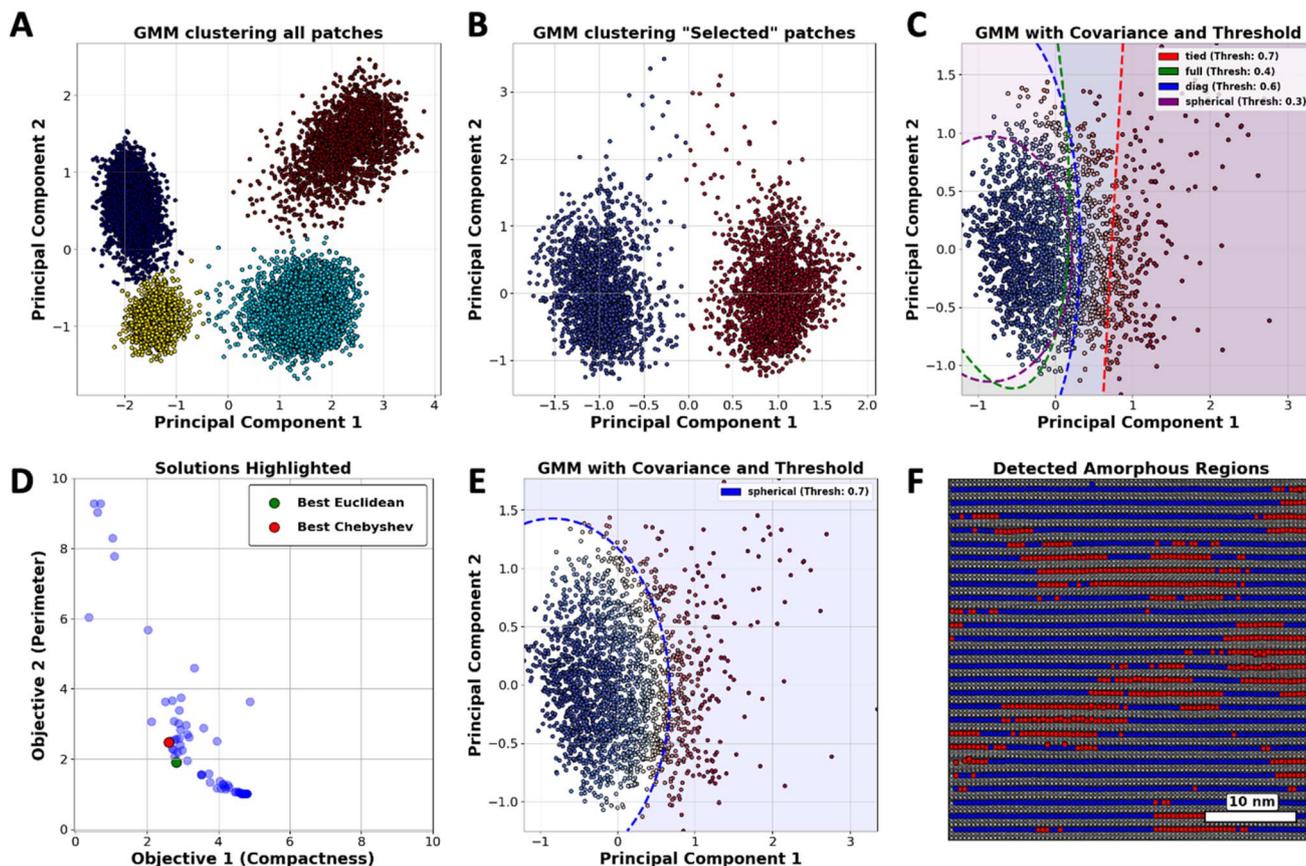


Fig. 4 (A) GMM clusters based on all the patches, providing 4 clusters with respect to 4 types of strong atoms in the YBCO structure. (B) GMM clusters based on the patches centered on Ba atoms, presenting two types of Ba in the YBCO structure. (C) GMM clusters based on only one type of Ba atoms, introducing some variety, which it can be differentiated by different values of threshold and covariance type in GMM clustering. (D) Pareto Frontier solutions with respect to reward possession. (E) optimal threshold and covariance type achieved by MOBO for GMM clustering, and (F) uncovered amorphous areas in the substrate.

multi-objective reward functions for finding atom positions and classification of the amorphous regions and demonstrate the Bayesian optimization in the parameter space of multi-step simple image analysis functions to yield robust identification.

To evaluate the performance of the LoG* workflow as a suitable method for real-time analysis *versus* DCNN in case of time, we conducted a comparative study using 10 subimages of size 256×256 pixels extracted from YBCO sample. The comparison between DCNN and LoG* methods revealed distinct strengths and potential limitations for each, particularly regarding image processing speed and adaptability as presented in Fig. 5. DCNN exhibits a considerable speed advantage, processing images faster than LoG*. This efficiency is primarily due to the optimization of GPUs, which are engineered to manage the intensive computational demands of deep convolutional neural networks. Achieving this speed, however, requires an initial investment of time and resources to create and label the dataset for training the DCNN model. While this training process only needs to be done once, it can be particularly demanding for large datasets.

Although LoG* processes individual images at a slower pace, its key advantage is adaptability and explainability. This

adaptability is particularly important when dealing with an out-of-distribution dataset. Additionally, the transparency of LoG* allows researchers to understand how specific features in the image contribute to the final output, making it easier to interpret results. In such cases, DCNN may struggle to provide accurate predictions because it heavily depends on the representativeness of its training data. If the new data deviates significantly from the training data, the DCNN model may fail, necessitating retraining, which diminishes its initial time efficiency. On the other hand, each time a new dataset is introduced, LoG* undergoes its optimization process, ensuring that it can accurately process data regardless of how different it is from previous datasets. This makes LoG* a more flexible, interpretable, and potentially more reliable choice in dynamic environments where the nature of the data can vary widely. The code utilized in this benchmarking analysis is available for public access on GitHub at [GitHub].

We believe that this approach has three significant impacts on microscopy. First, the introduction of a reward-function-based optimization approach makes the construction of analysis pipelines automated and unbiased, taking advantage of the powerful optimization approaches available today. Secondly,



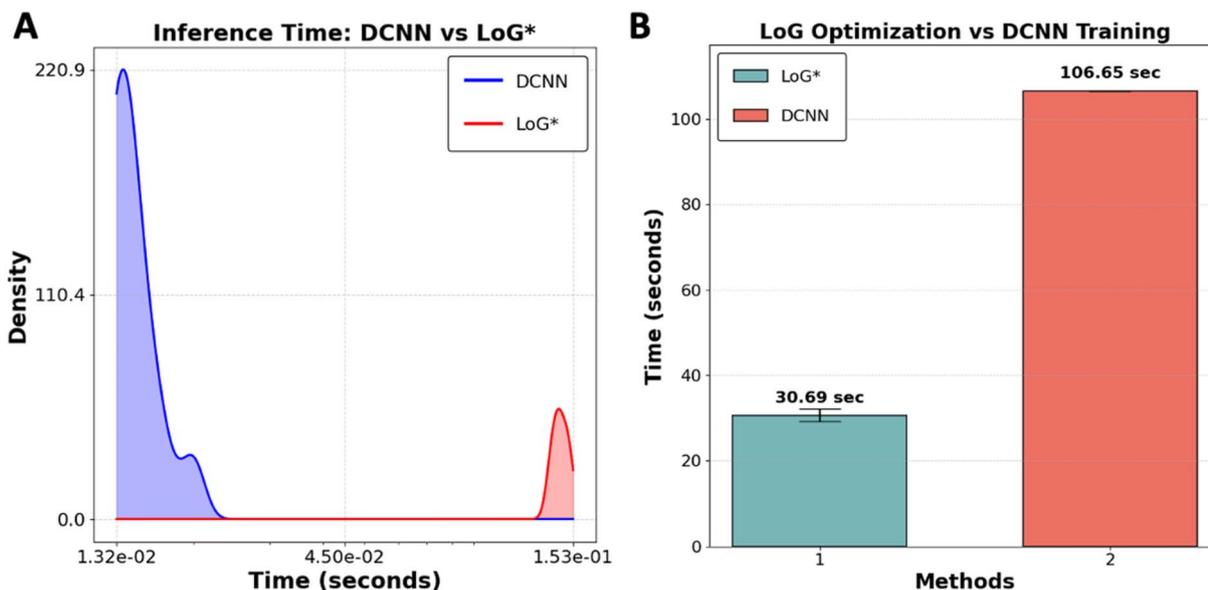


Fig. 5 (A) Distribution of inference times for DCNN and LoG* methods across 10 images ($10 \times 256 \times 256$) pixels. The density plots illustrate the variation in time required for image processing by each method, (B) comparison of DCNN training time using a labeled dataset (1656, 256, 256) pixels versus the average optimization time for LoG* across a set of 10 images ($10 \times 256 \times 256$) pixels.

these analyses have the potential to be integrated into automated experiments and real-time data analytics workflows, enabling on-the-fly adjustments and decisions during data collection. Thirdly, the integration of reward functions across the domains offers a far more efficient approach for community integration than creation of disparate experimental data databases, contributing to the development of the open and FAIR experimental community.

Data availability

The code supporting the findings of this study is publicly accessible on GitHub at <https://github.com/Kamyar-V2/RDW>.

Author contributions

Kamyar Barakati: conceptualization (equal), data curation (lead), formal analysis (equal), writing – original draft (equal); Sergei V. Kalinin: conceptualization (equal), formal analysis (equal), funding acquisition (equal), writing – review & editing (equal), supervision (equal). Hui Yuan: investigation (equal). Amit Goyal: investigation (equal).

Conflicts of interest

The authors have no conflicts to disclose.

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