Third Summer School on ML for Electron Microscopy

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# Reward Functions for Decision Making


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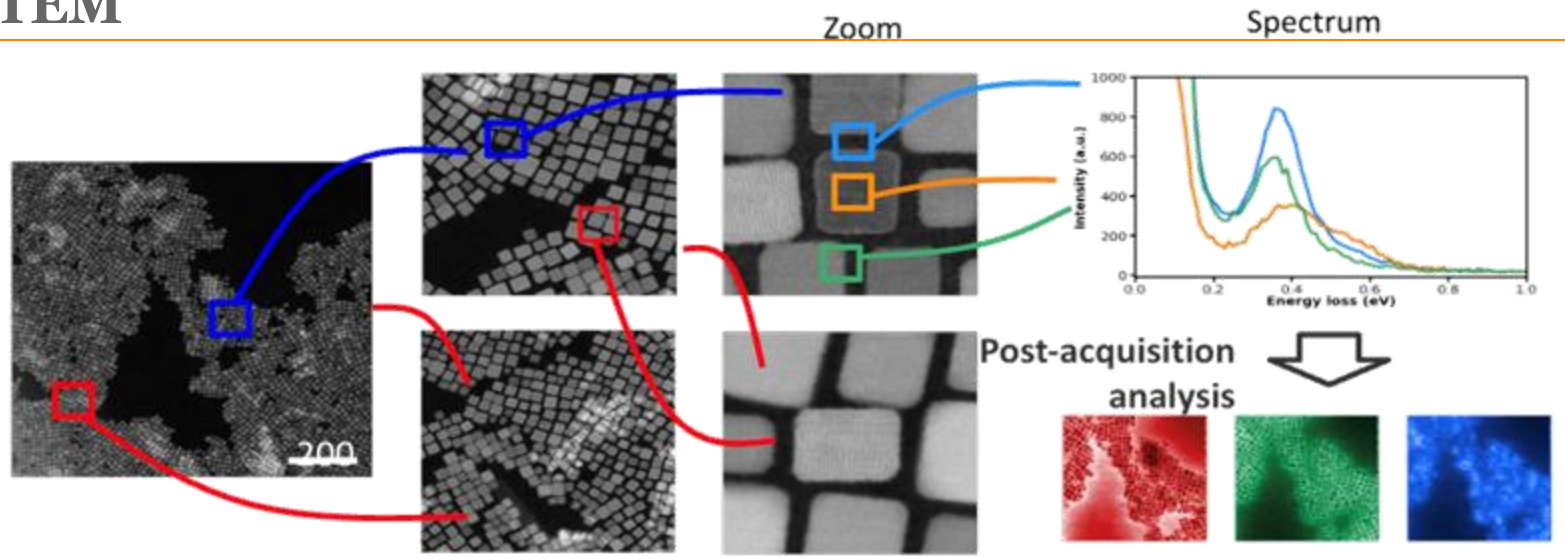
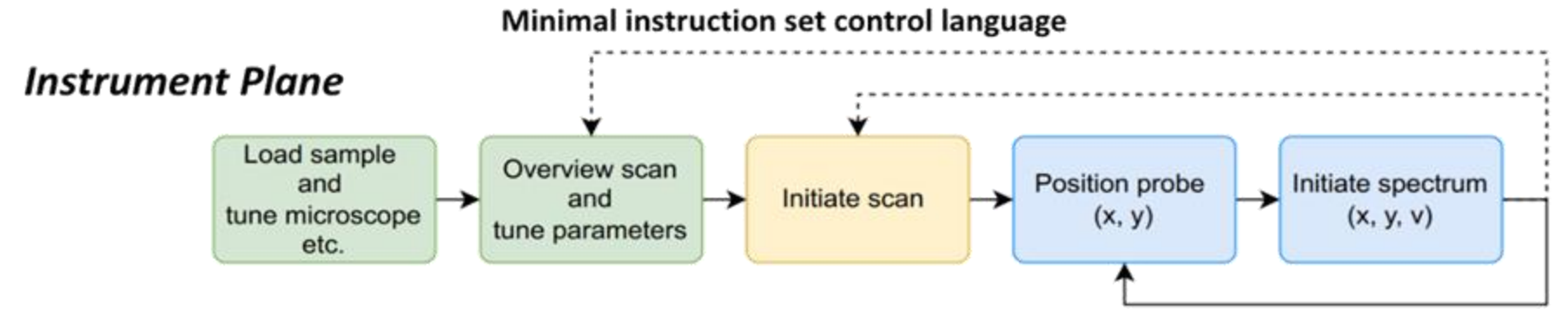
# Workflows in STEM




- Objective: purpose of the experiment (outside context)
- Policy: what do we do depend on observation
- Reward: what do we hope to achieve
- Value: anticipated reward

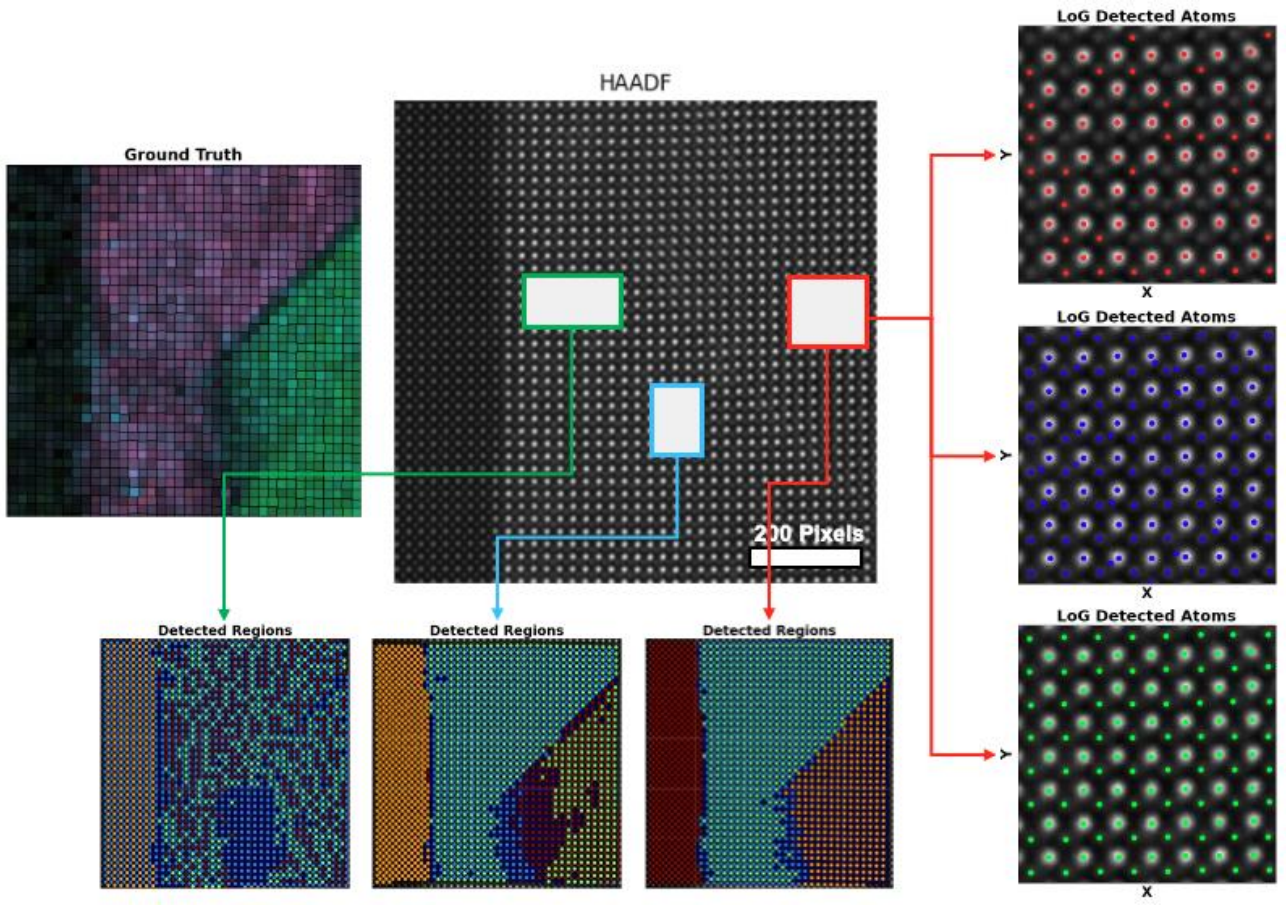
# EXAMPLES

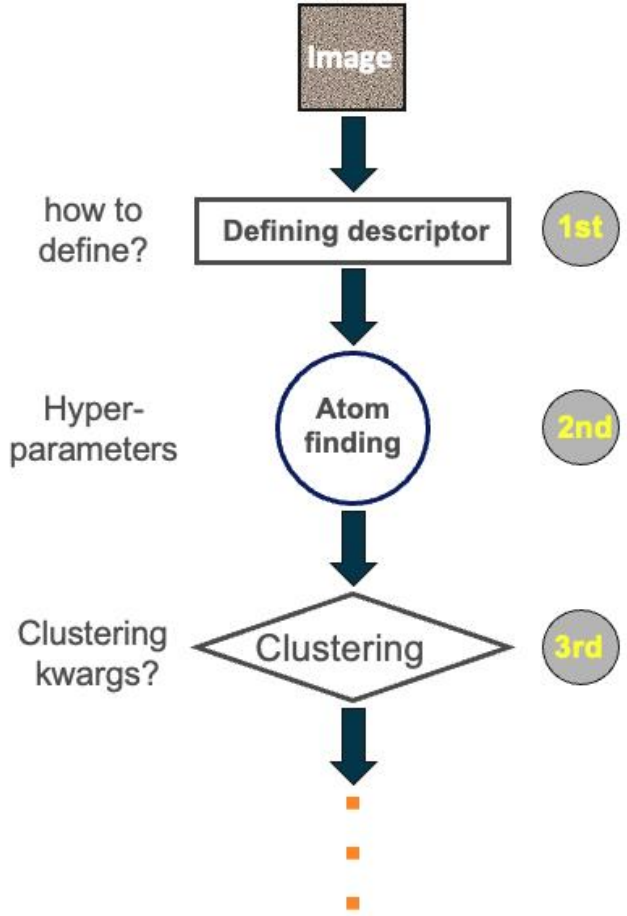
## SmBFO

Increase in data generation:

**Challenges in real Time:**

1. Parameter Sensitivity
2. Labeling

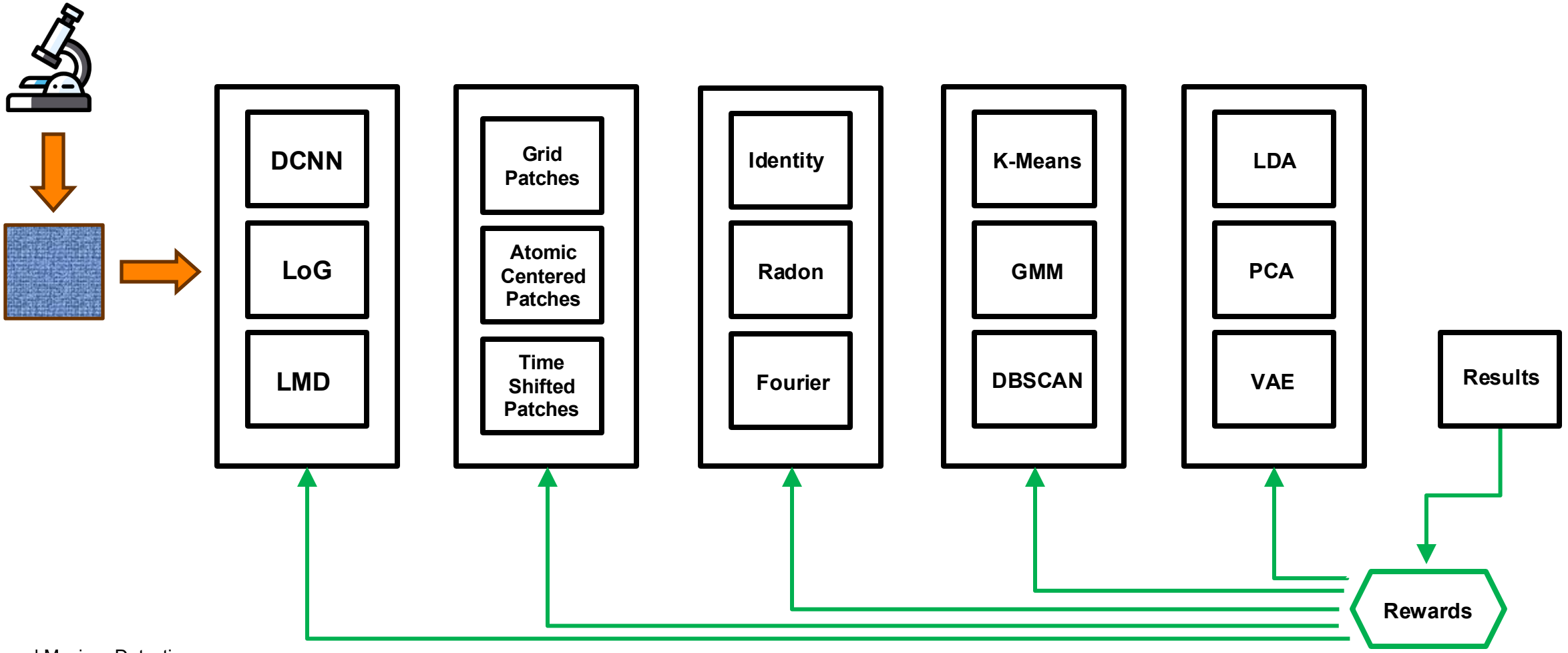



We do not know what may have been overlooked or sacrificed in pursuit of a seemingly desirable result.

# Design Physics Based workflows

What are we looking for? 1. **Explainable 2. Reproducible 3. Fast**



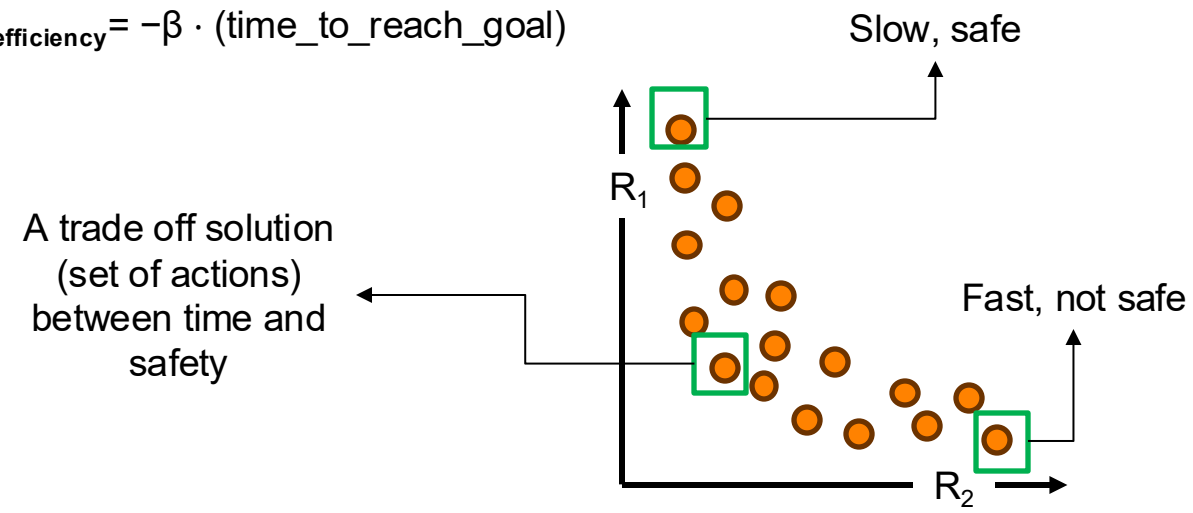

**LMD:** Local Maxima Detection
**LDA:** Linear Discriminant Analysis

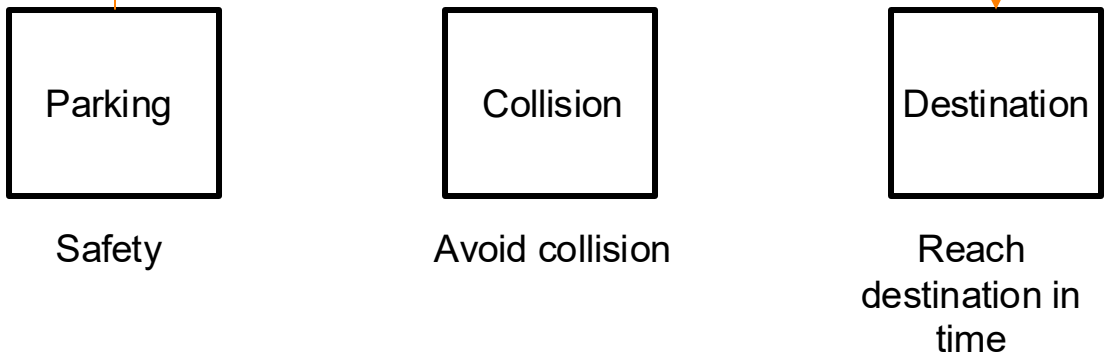
## Key Characteristics of Rewards

1. **Non-myopic:** Evaluates the entire outcome, not just individual actions.
2. **Multi-objective:** Can consider multiple factors (accuracy, efficiency, completeness)
3. **Alignment with goals:** The final reward should directly reflect how well the result meets the experimental objective.

$R_{safety} = -\lambda \cdot collision\_risk$

$R_{efficiency} = -\beta \cdot (time\_to\_reach\_goal)$



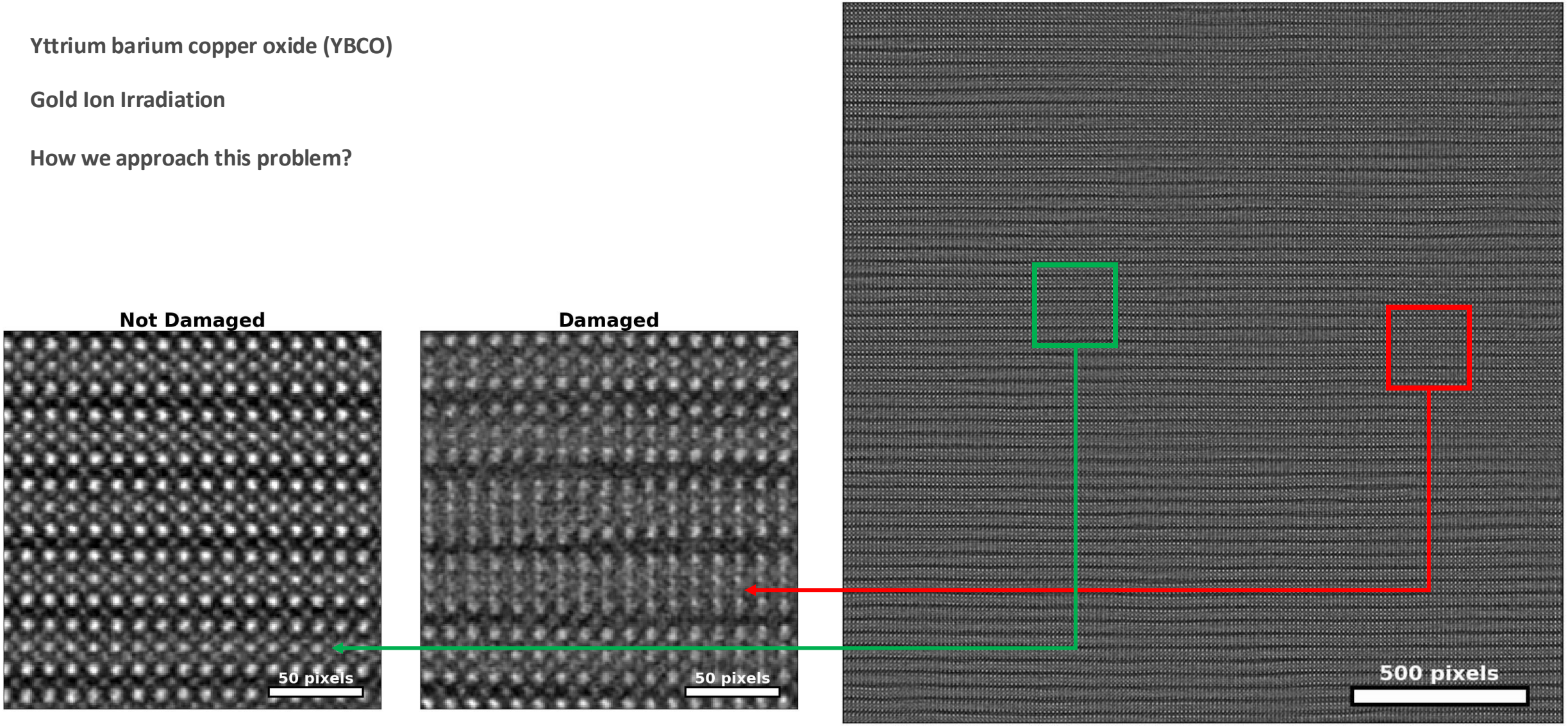



# MODEL PROBLEM

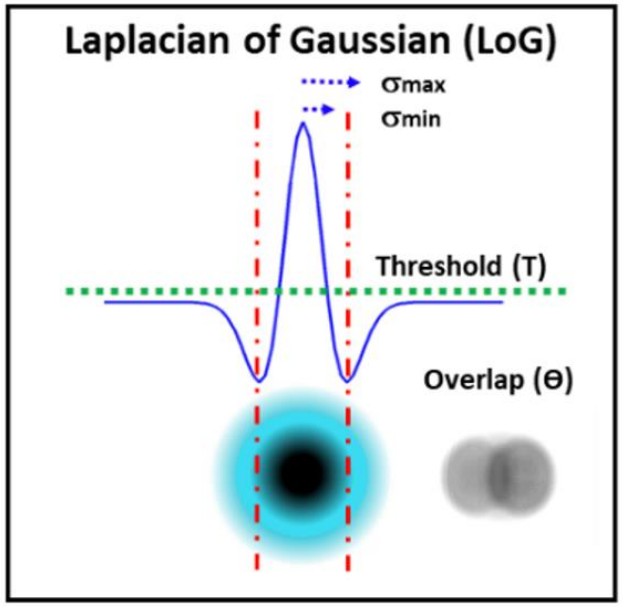
Yttrium barium copper oxide (YBCO)

Gold Ion Irradiation

How we approach this problem?



# LoG vs DCNN




Parameter space: (**6, 2**)

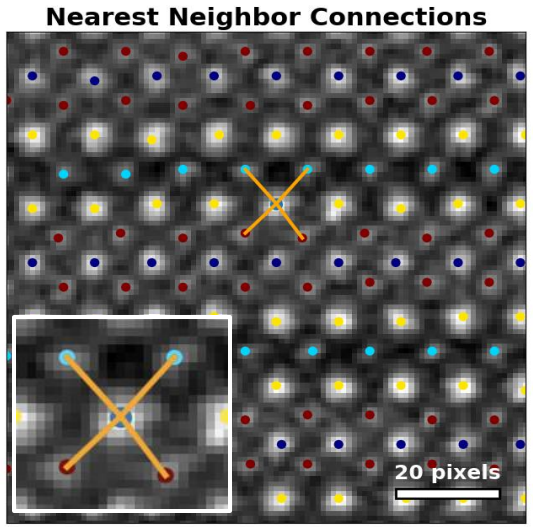
$\sigma_{min}$, $\sigma_{max}$, T, $\theta$, $w_w$, $w_h$

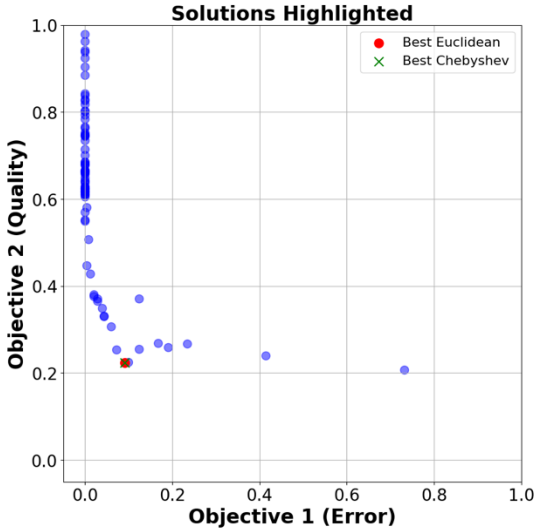
## Multiobjective optimization of LoG

1. Number of atoms via **physical criterion** – like number of atoms in the structure with respect to stoichiometry
2. False positives (Atoms to close): < distance to their 4 nearest neighbor

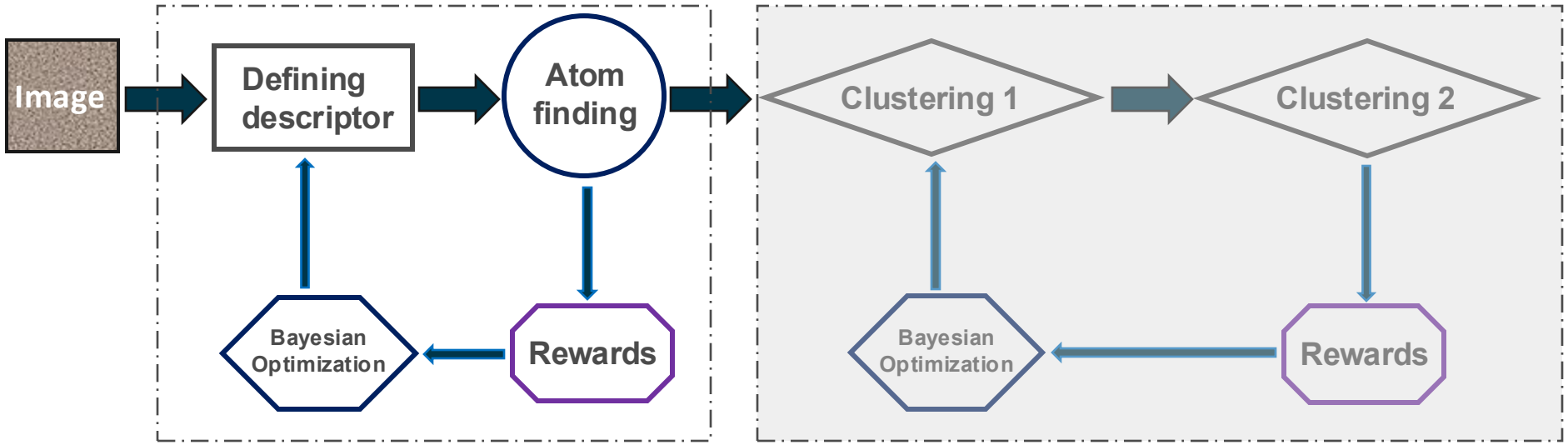
## Benchmarking

- Number of atoms via **DCNN**

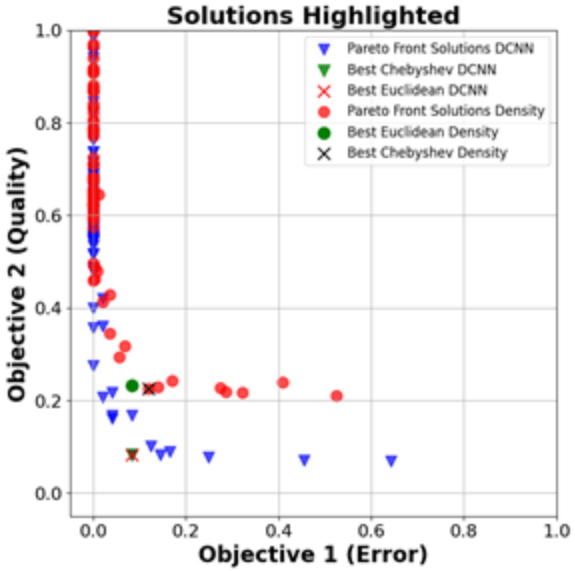


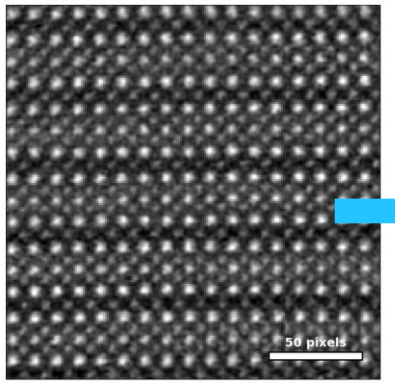



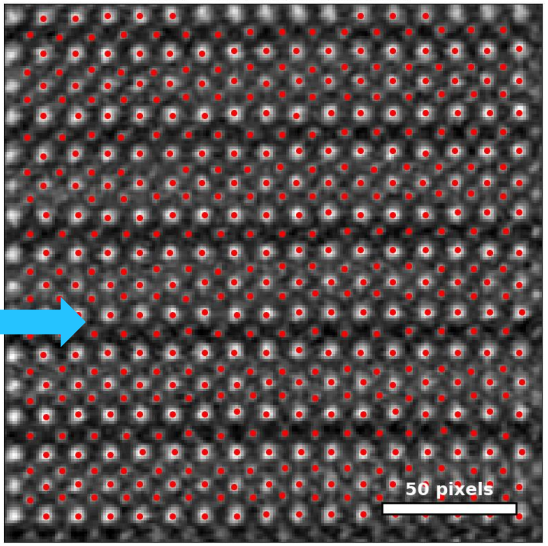
# MODEL WORKFLOW



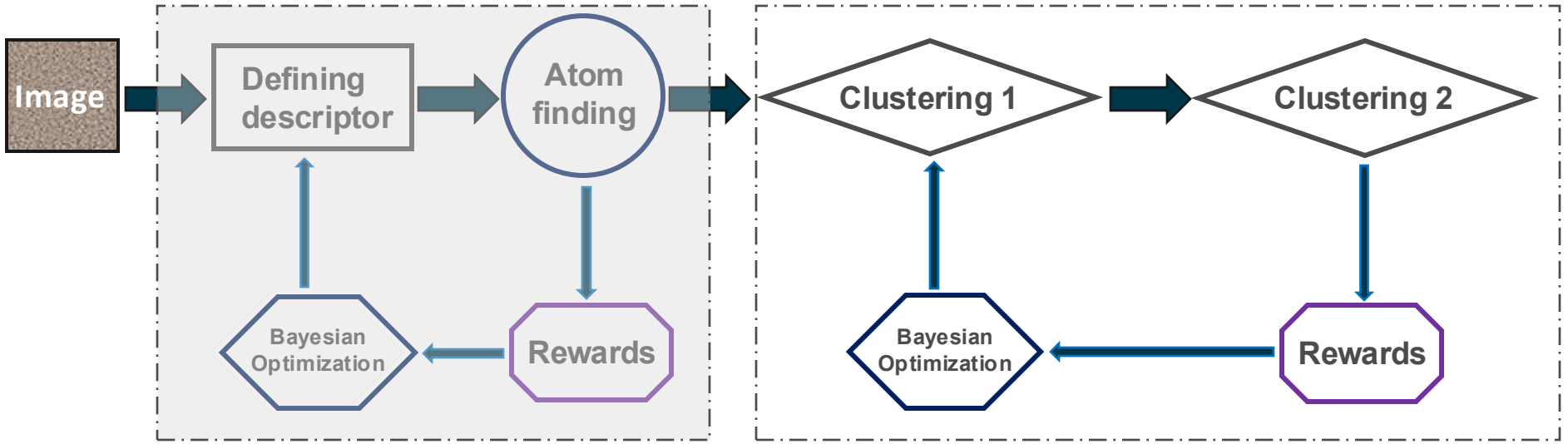

| 1st set Rewards | |
|---|---|
| Objective 1 | Objective 2 |
| Quality | Error |
| Number of atoms | False positives |



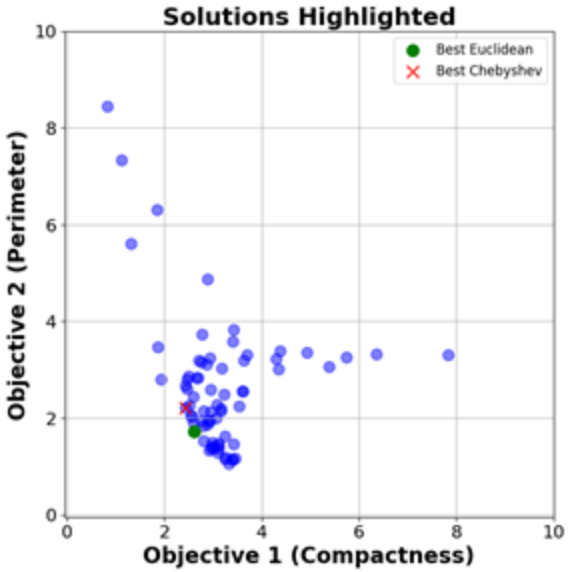
# MODEL WORKFLOW

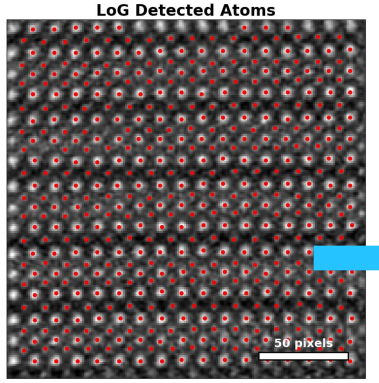


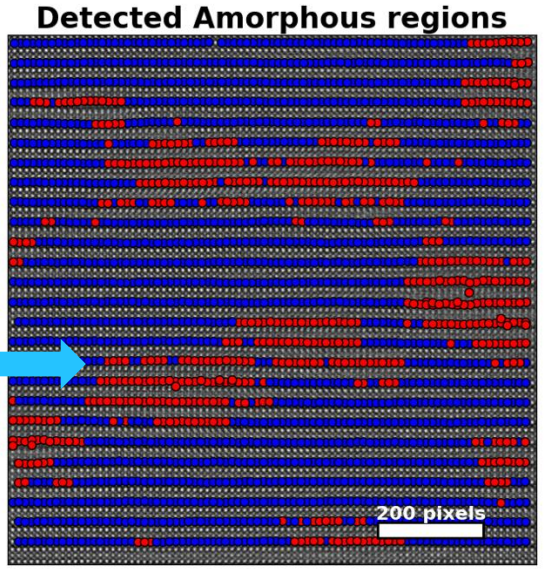

Parameter space: (**3, 2**)

$w_w$, $w_h$, $COV_{\_type}$

| 2nd set Rewards | |
|---|---|
| Objective 1 | Objective 2 |
| Compactness | Perimeter |



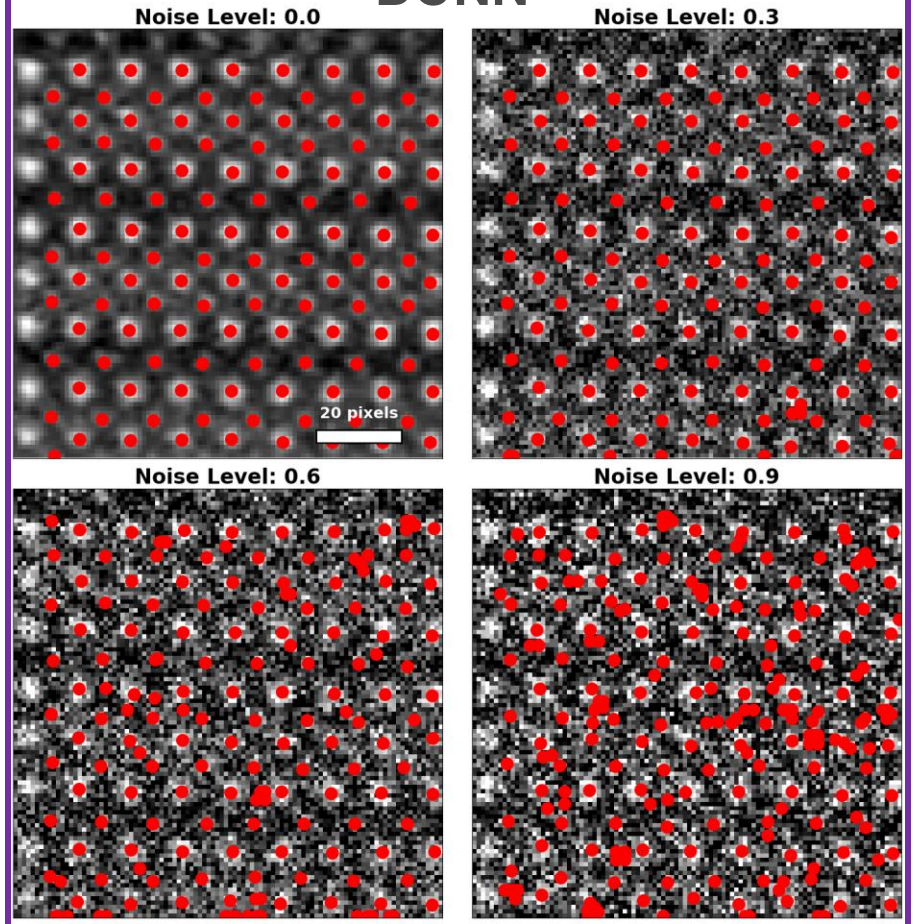



# BENCHMARK VS DCNN

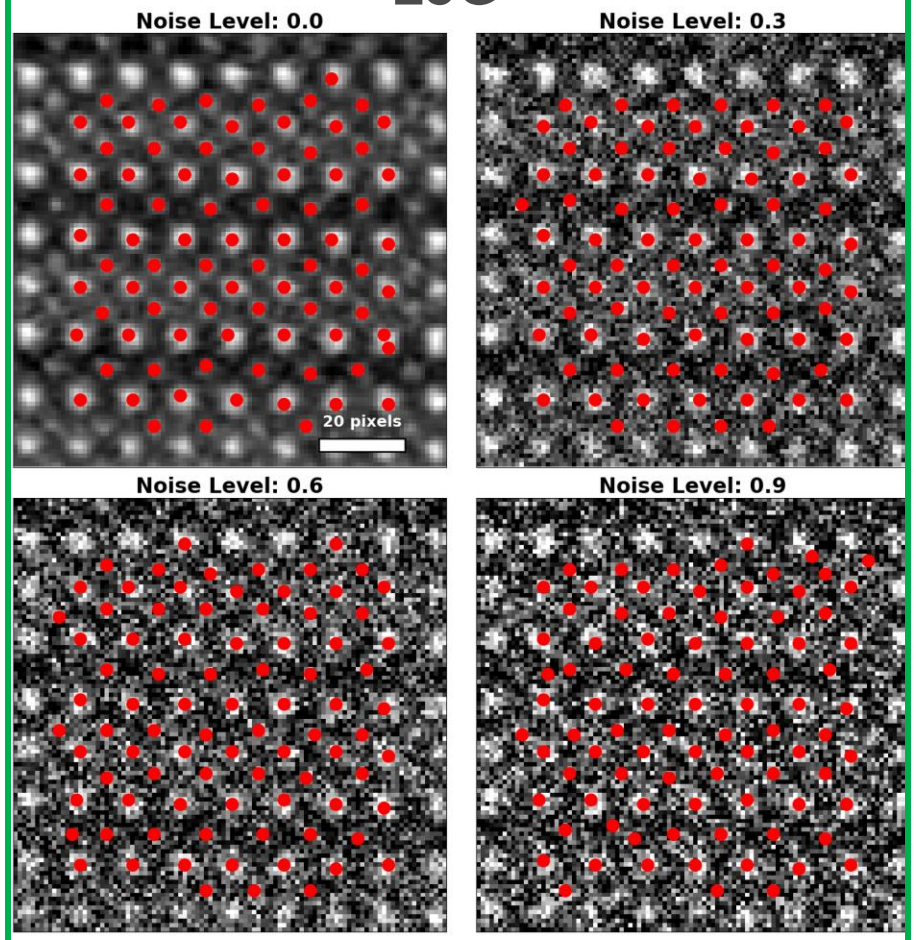
## Stability vs Noise interference

### DCNN

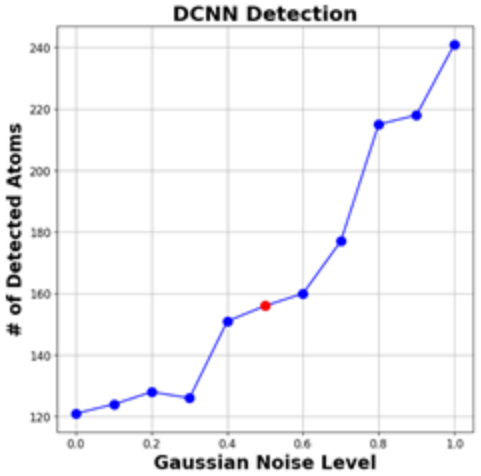



**lack robustness to out-of-distribution shifts**

### LoG*

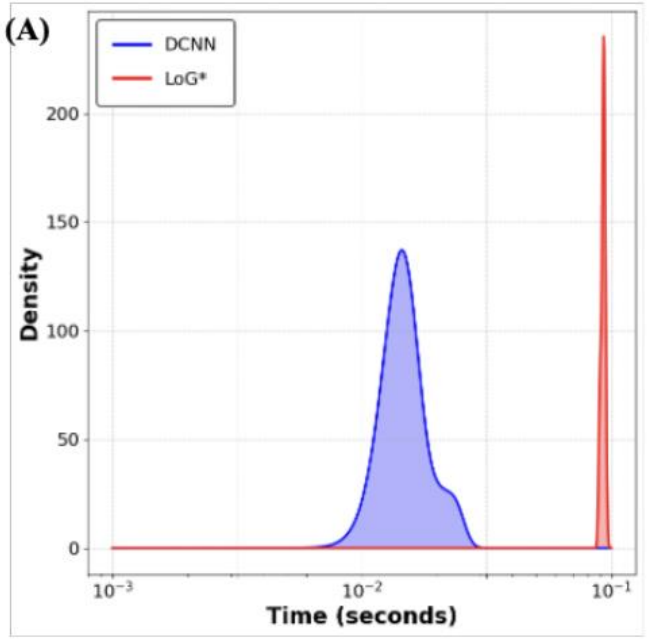



**Rewards constraint false positive predictions**

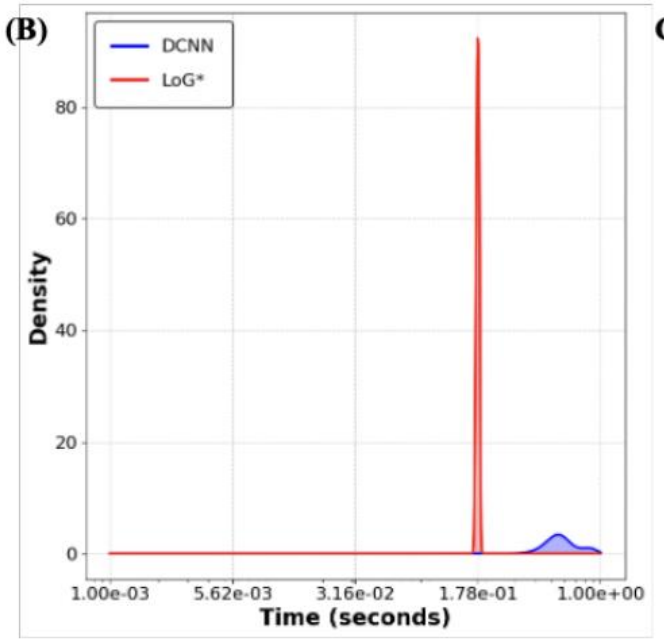



# BENCHMARK VS DCNN

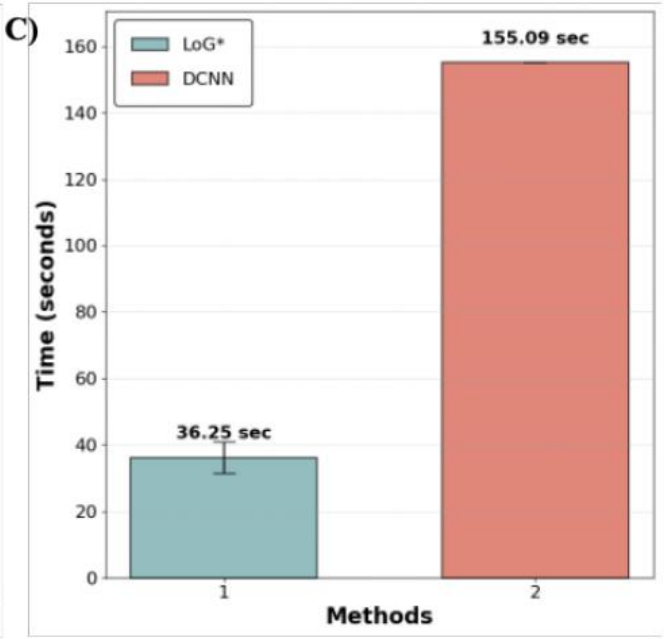
## Time




(GPU)




(CPU)



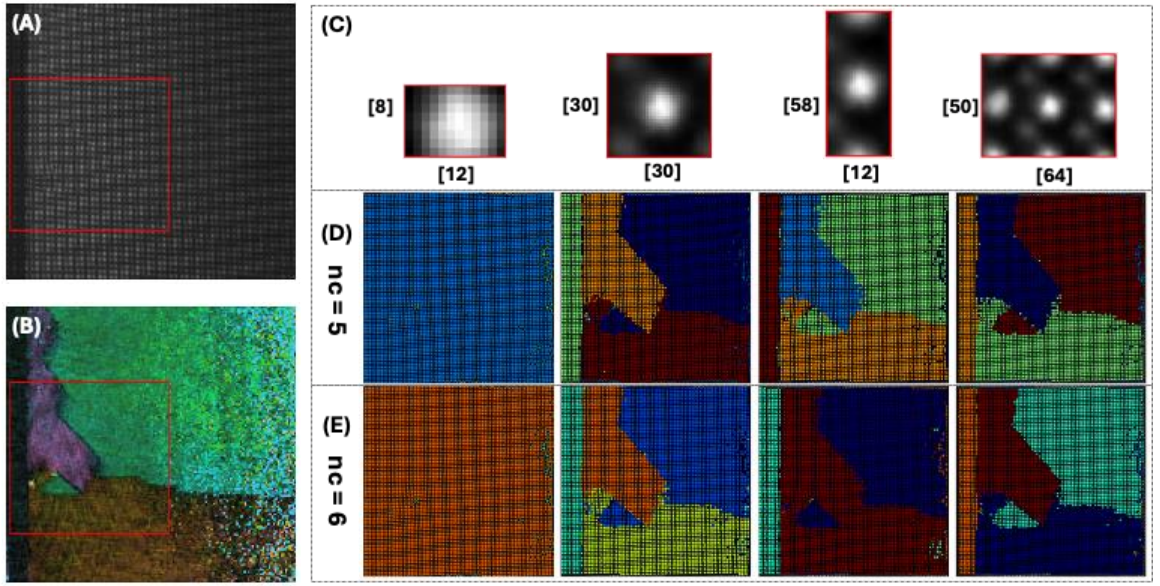

Optimization loop time vs training time

# MODEL WORKFLOW

**Sample**: Sm-doped $BiFeO_3$ (BFO)

**Experimental Goal**: Discovery of polarization and lattice distortion

| set Rewards | |
|---|---|
| Objective 1 | Objective 2 |
| Straightness | Length |

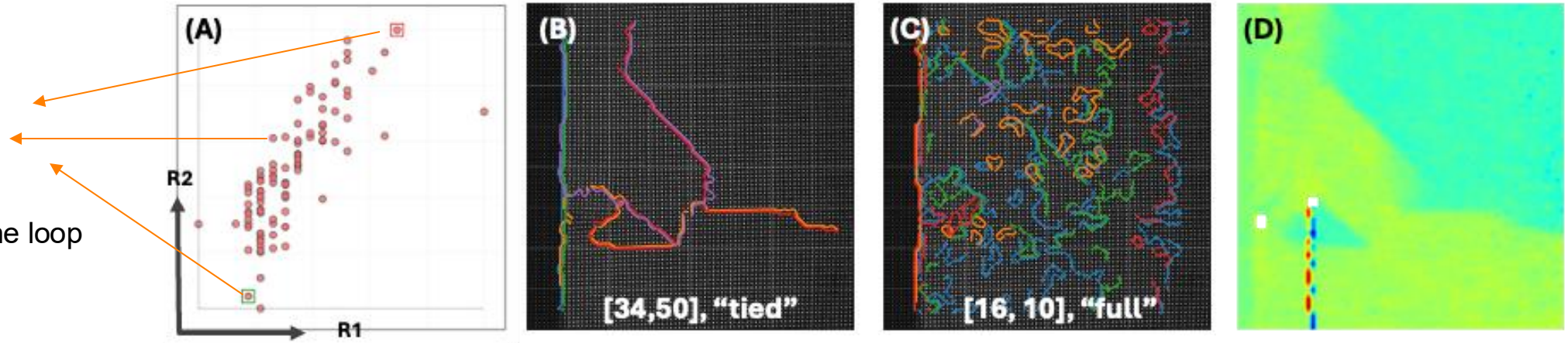



Parameter space: (**3, 2**)

$W_w$, $W_h$, $COV\_type$

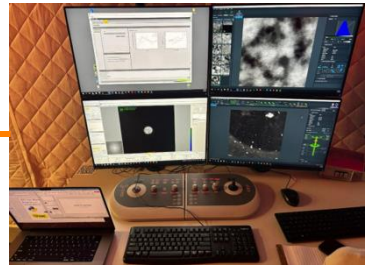
**Control parameters:**

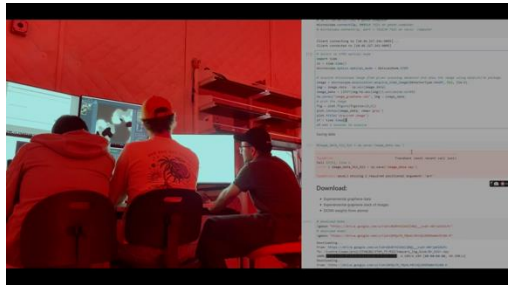
Keep **human** insight in the loop



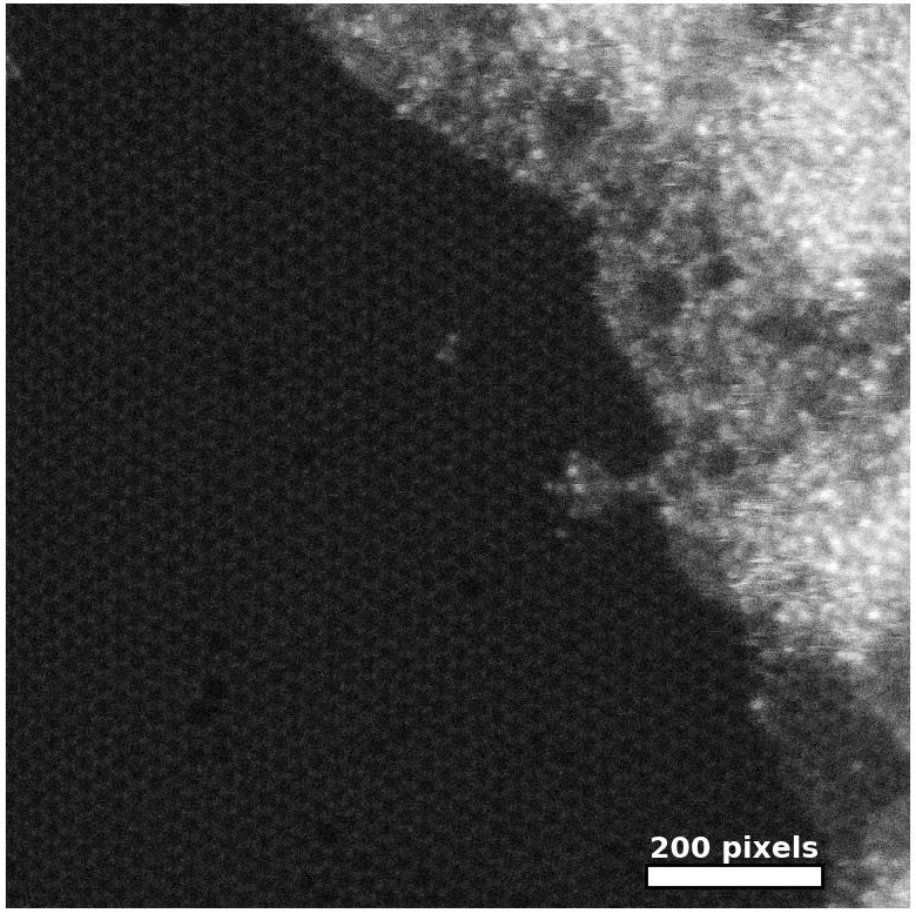
# REAL TIME ANALYSIS

Spectra 300 by Thermofisher

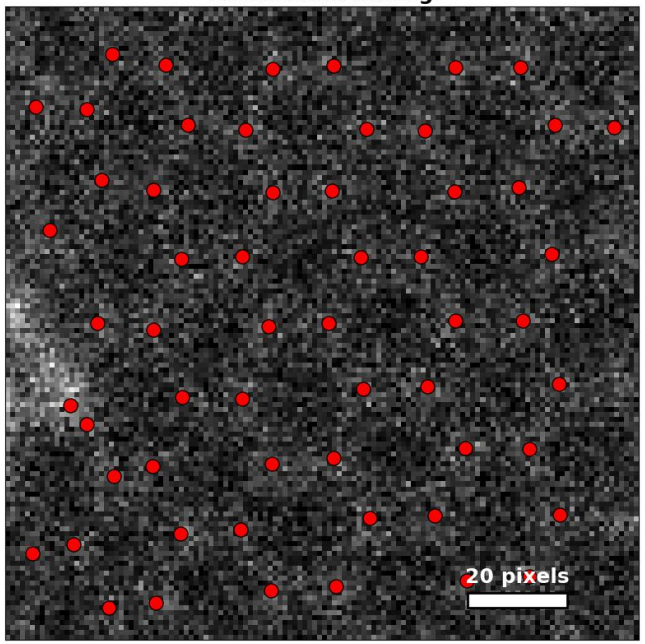




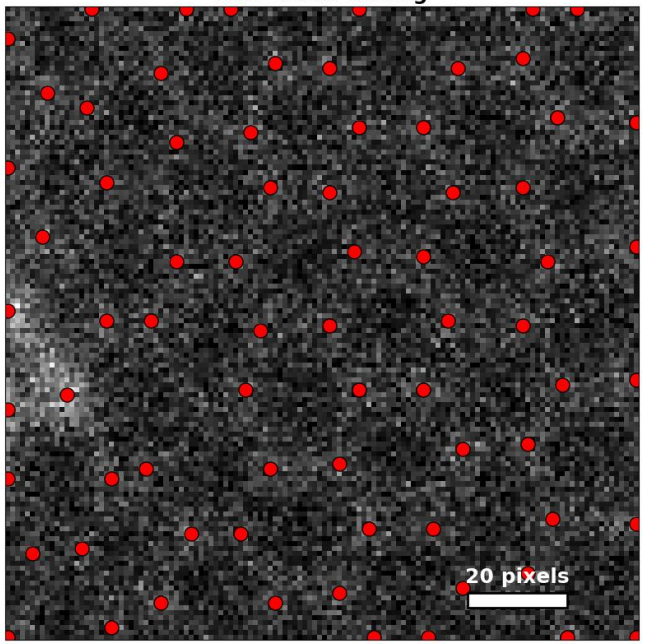
Real time image




DCNN atom finding




LoG* atom finding




**GPU memory required: 5 GB**
**Number of Units: 1**

# Conclusion

- **Reward Driven workflow which enables real time image analysis**
- **Hyperparameter tunning and optimization, keeping human insight in the loop**
- **Focus on physical and chemical concepts while doing the experiment**

# Questions?

## Reference:


[1] Barakati, Kamyar, et al. "Reward driven workflows for unsupervised explainable analysis of phases and ferroic variants from atomically resolved imaging data." *arXiv preprint arXiv:2411.12612* (2024).

[2] Barakati, Kamyar, et al. "Unsupervised Reward-Driven Image Segmentation in Automated Scanning Transmission Electron Microscopy Experiments." *arXiv preprint arXiv:2409.12462* (2024).

[3] Barakati, Kamyar, et al. "Physics-based reward driven image analysis in microscopy." *Digital Discovery* 3.10 (2024): 2061-2069.




# Notebook