THE UNIVERSITY of TENNESSEE KNOXVILLE

Deep Kernel Learning – III
Forensics and human-in-the-loop interventions

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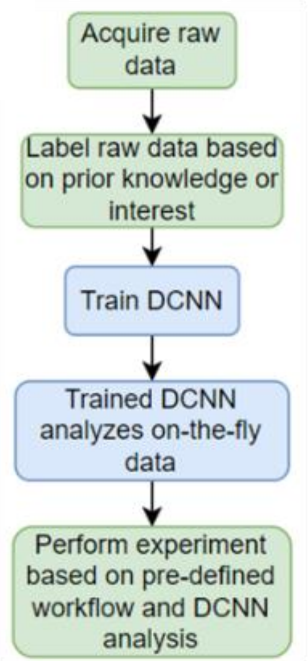
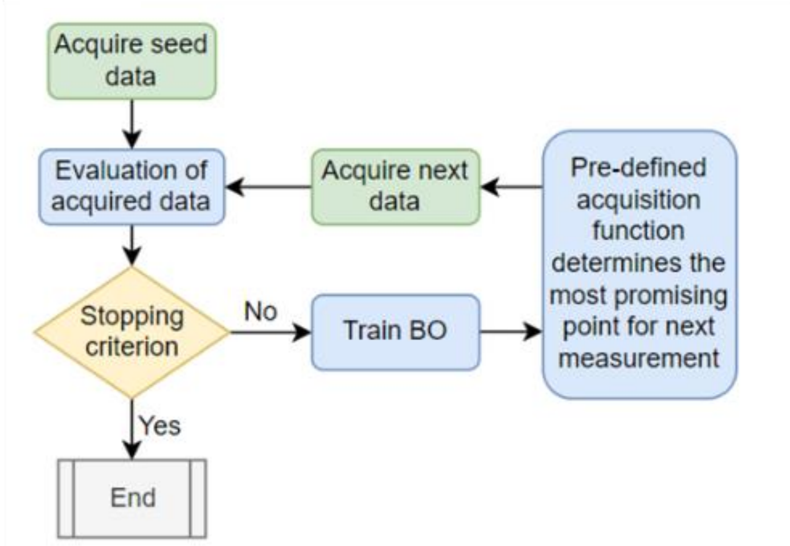
Types of automated experiment

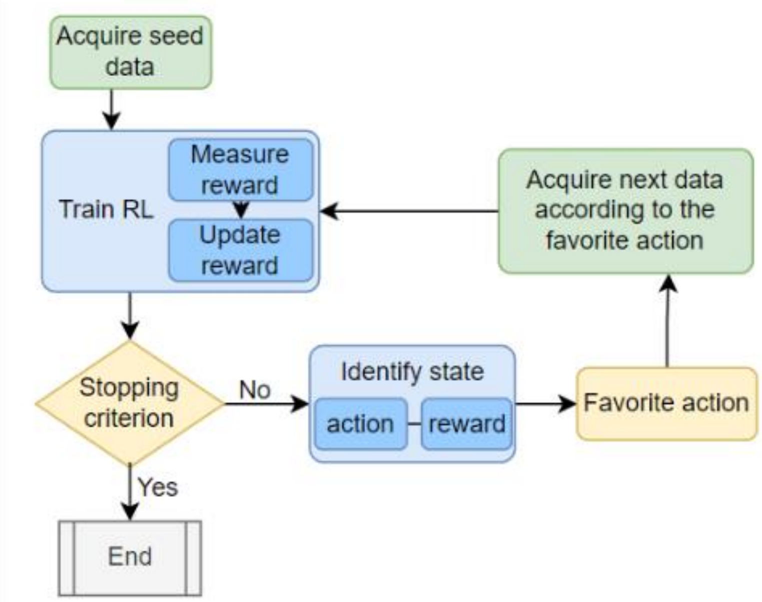
Direct



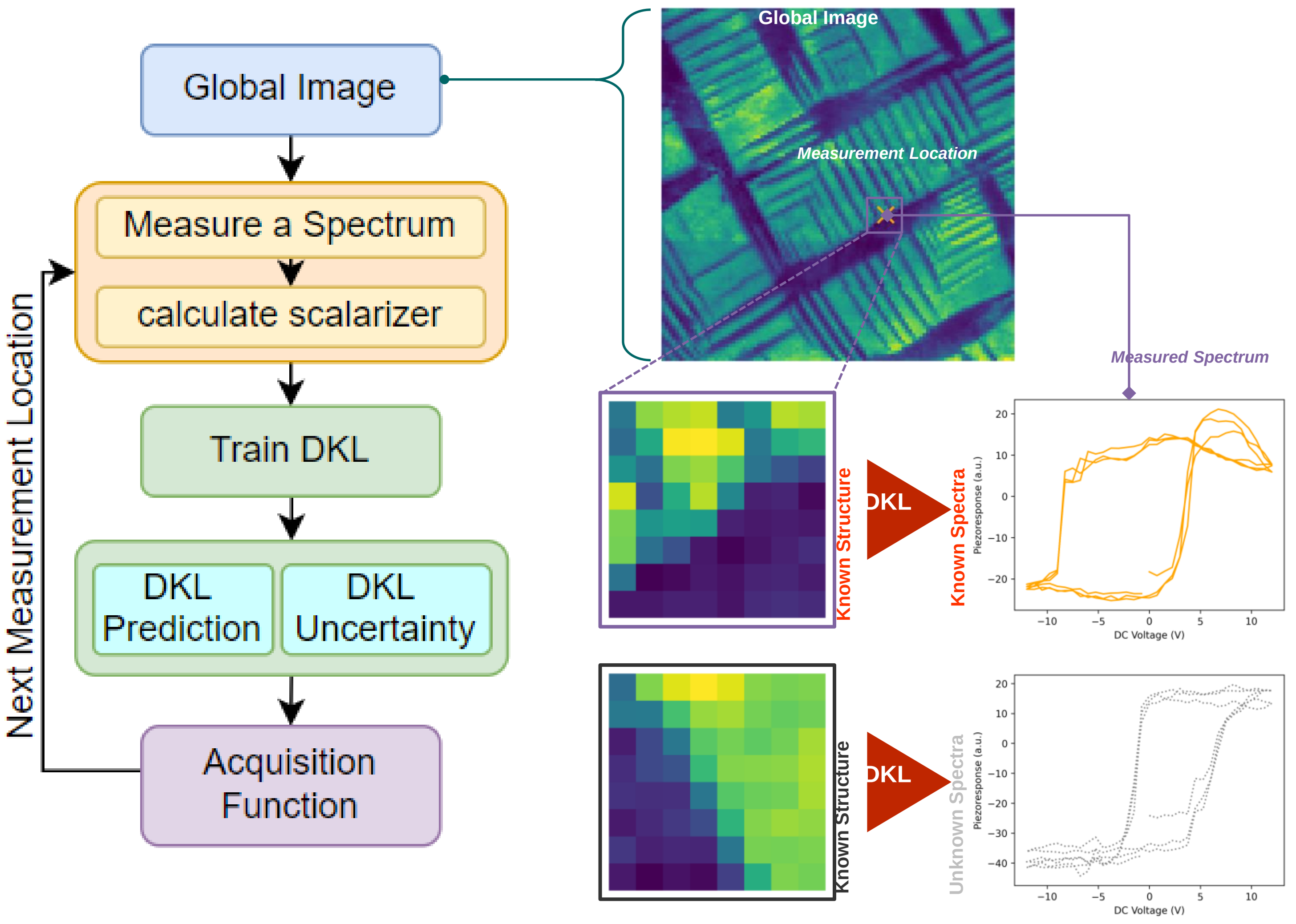
Myopic discovery



Multistage discovery



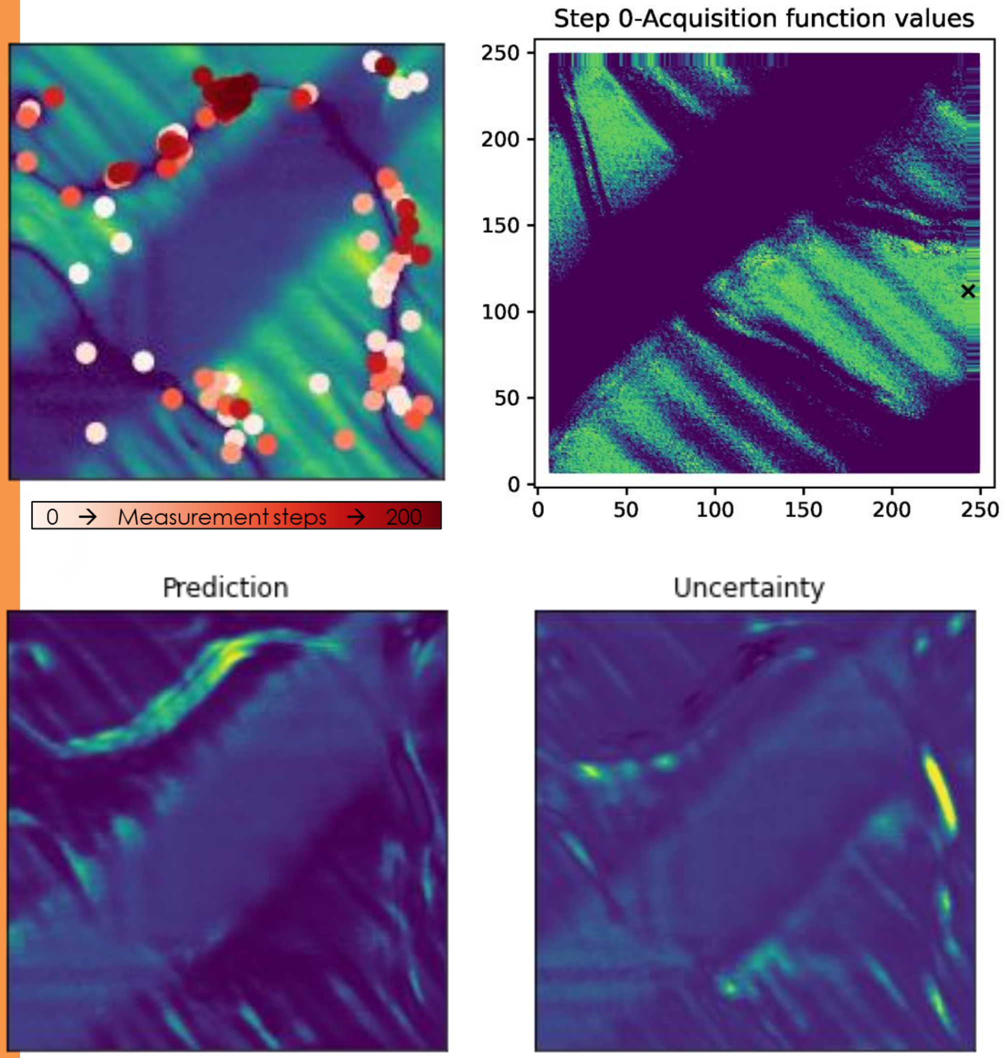
Deep Kernel Learning Automated Experiment



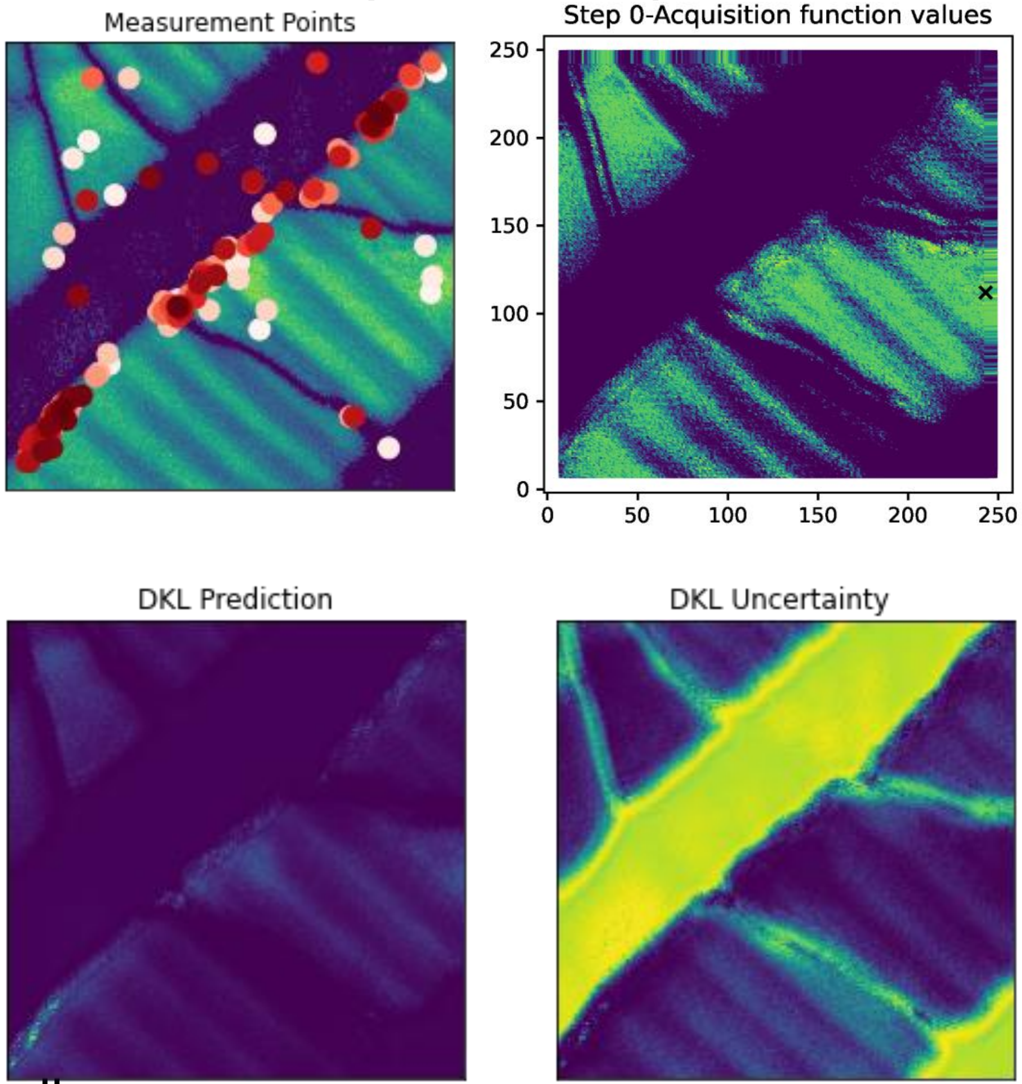
- Global image available at the beginning of the experiment
- We create the set of image patches describing local structures
- Spectra are measured sequentially
- Scalarizer is used to convert the spectrum to a single descriptor of interest
- We run automated experiment to learn which microstructural elements (patches) maximize the scalarizer.

DKL SPM

Guided by: On field loop area



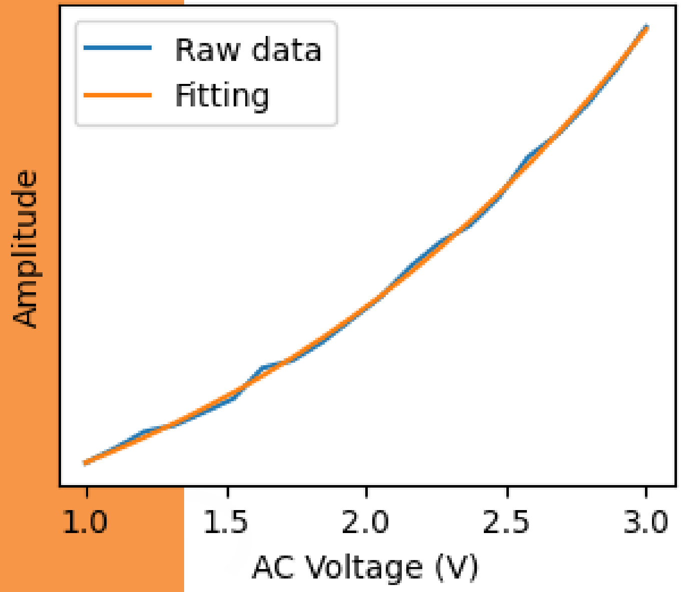
Guided by: Off field loop area



- Large loop opening corresponding 180º domain walls
- This behavior can be attributed to the large polarization mobility of 180º walls

Liu, Yongtao, et al, Nature Machine Intelligence 4, 4 (2022): 341-350.

Exploring Non-Linearity



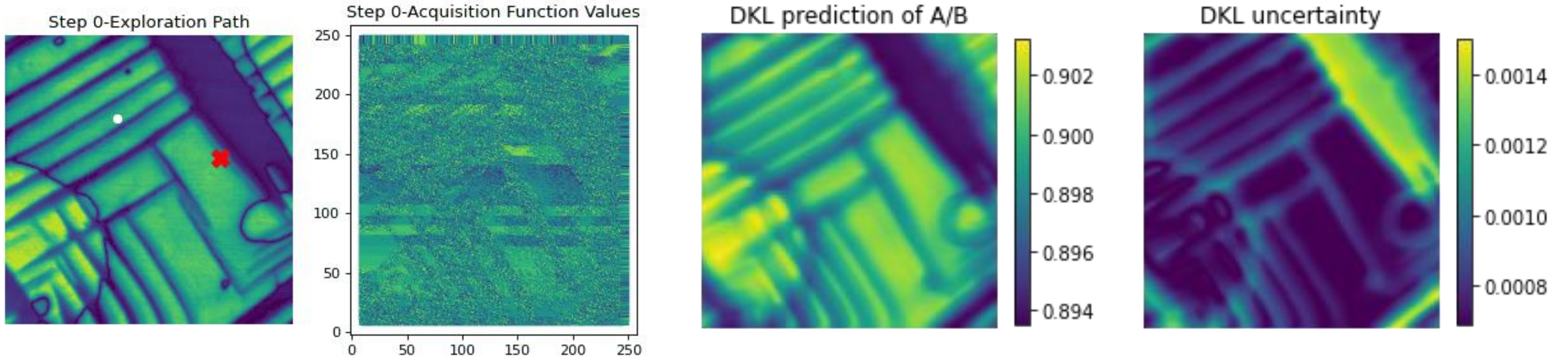
V_{AC} sweep curve at each location was fitted as $y = Ax^3 + Bx^2 + Cx$

A, B, C, and A/B were us as the target function to guide DKL-V_{AC} measurement.

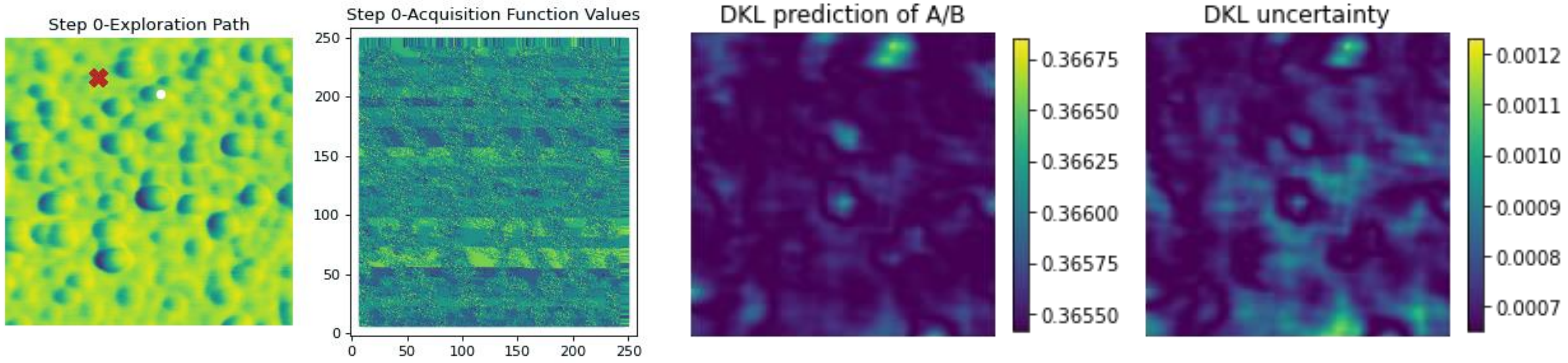
PTO and HZO thin films were studied.

- Shown are 200-step measurements of PTO and HZO thin films
- PFM amplitude was used as structure image; A/B was used to guide the measurement.

PTO experiment process and results



HZO experiment process and results

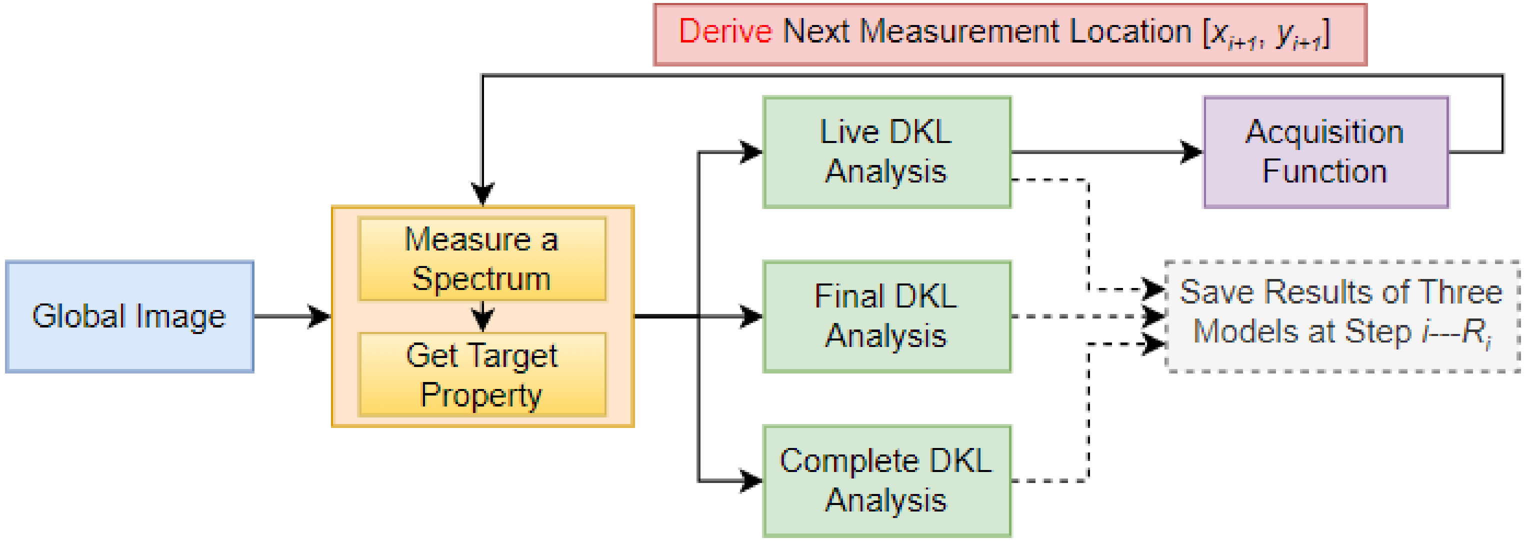


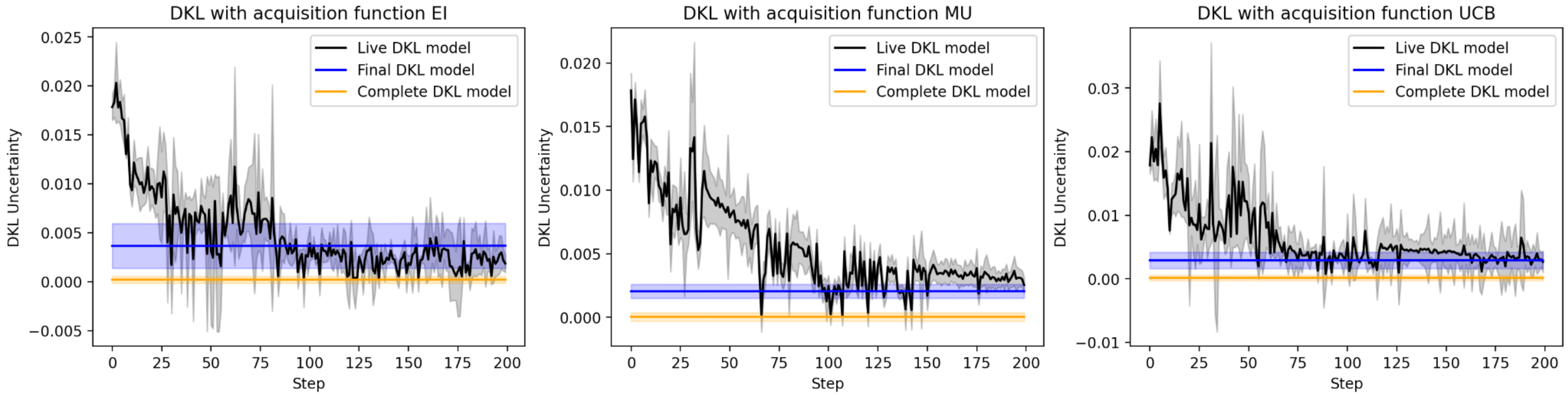
➢ So, how does it work and how can I control it?

- In conventional microscopy experiment, human runs everything directly – defines scan, positions the probe, defines measurement parameters.
- In AE SPM, the policies are defined before the experiment and do not change. Sometimes it works – but not always.
- How would we:
  - (a) explain the AE progression after the experiment and
  - (b) control it during the experiment ?

AE Forensics

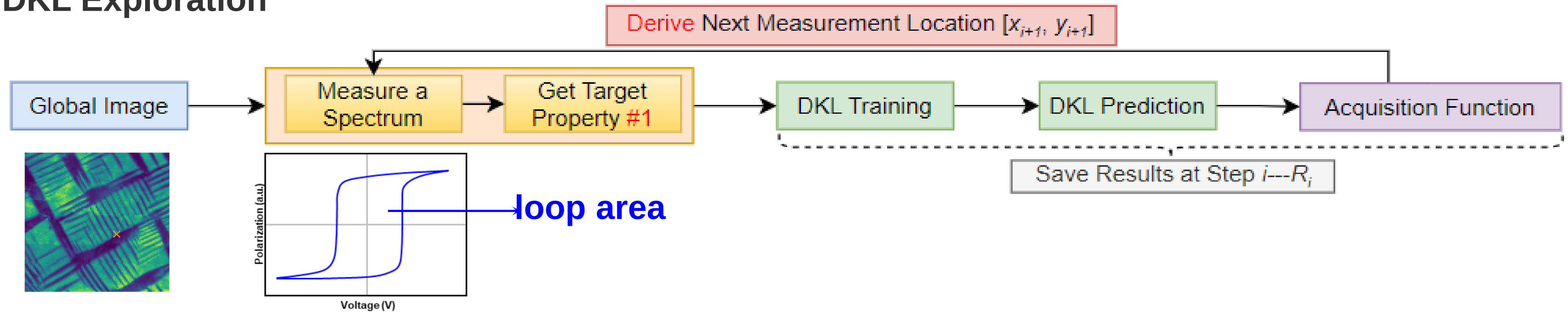
- During the AE, model learns structure-property relationships.
- What if we retrace the experimental steps – using the fully trained model?



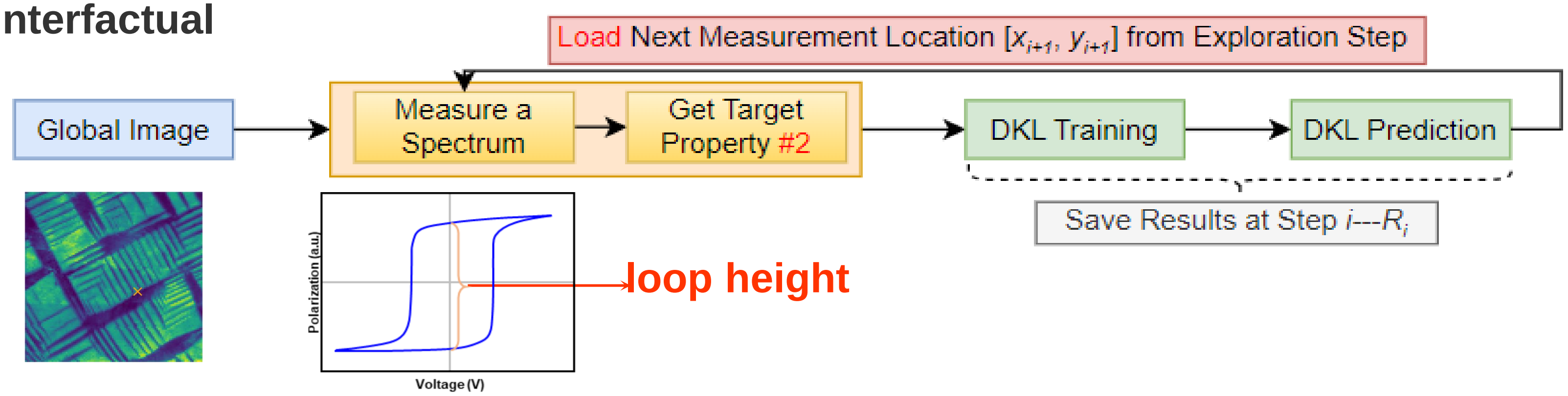


Counterfactual scalarizers

DKL Exploration



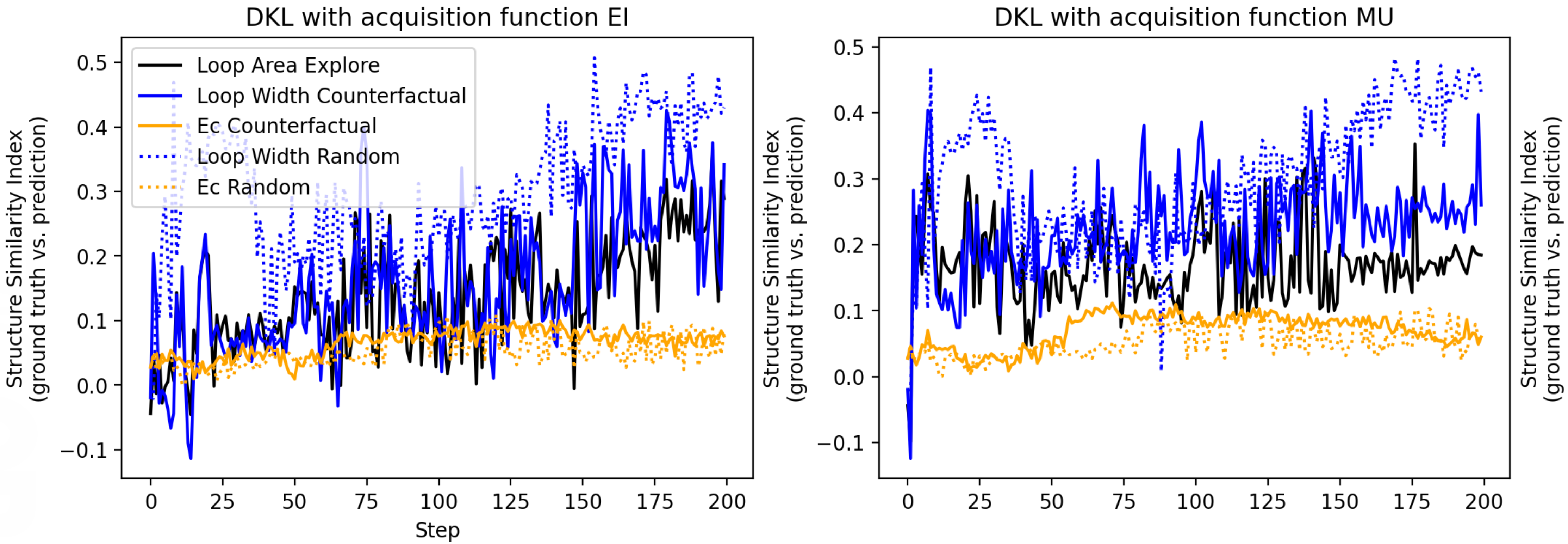
DKL Counterfactual



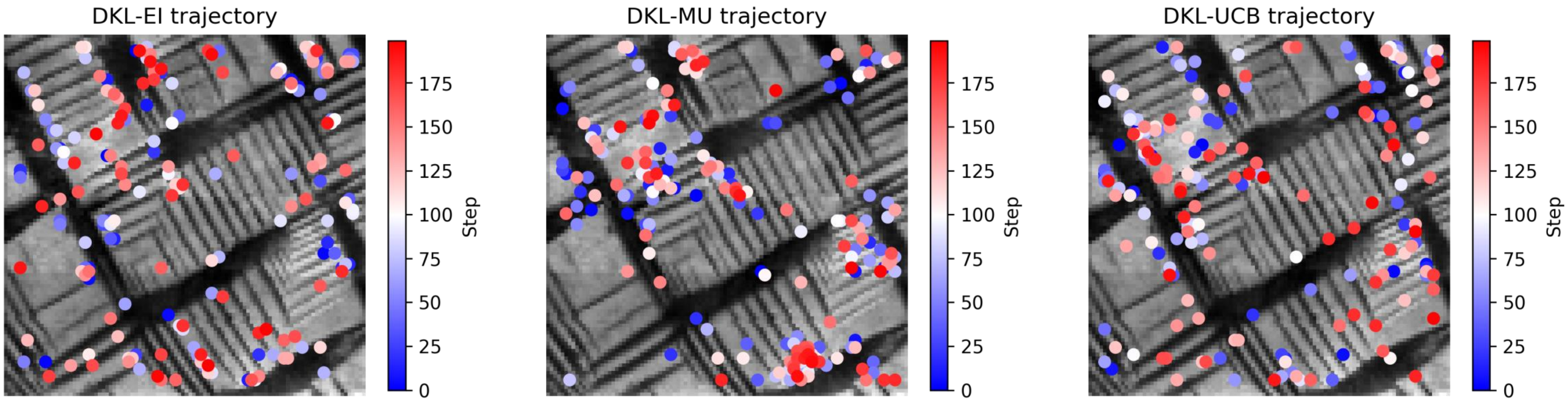
Target properties:

1. Loop Area
2. Loop Height
3. Coercive Field
4. …

- We save the full experimental trace
- What if we follow the actual experimental path – but calculate alternative (counterfactual) scalarizers?

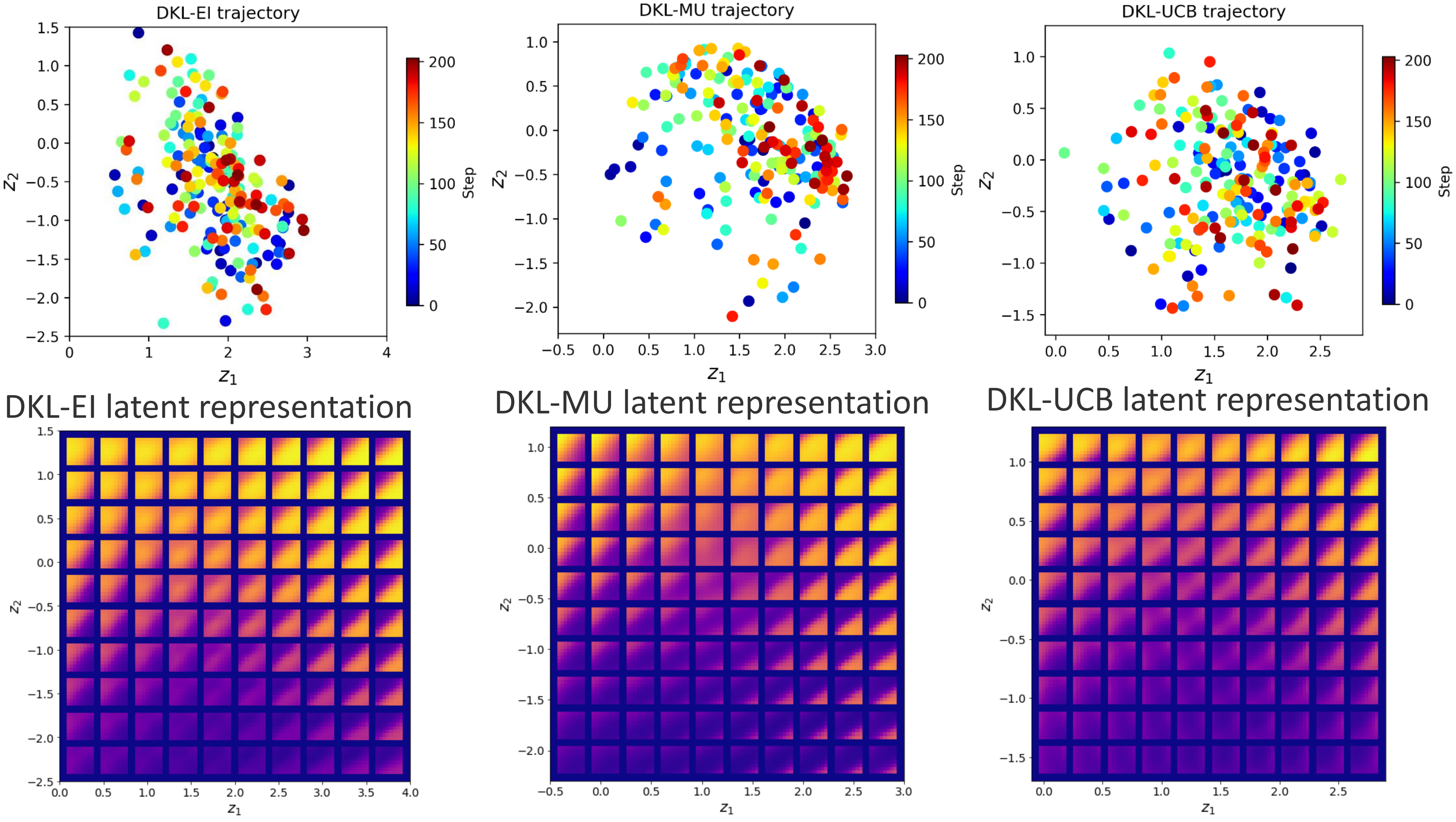

DKL with acquisition function EI
DKL with acquisition function MU
Loop Area Explore
Loop Width Counterfactual
Ec Counterfactual
Loop Width Random
Ec Random
Structure Similarity Index
(ground truth vs. prediction)
Step
0.5
0.4
0.3
0.2
0.1
0.0
−0.1
0
25
50
75
100
125
150
175
200

Monitoring the AE

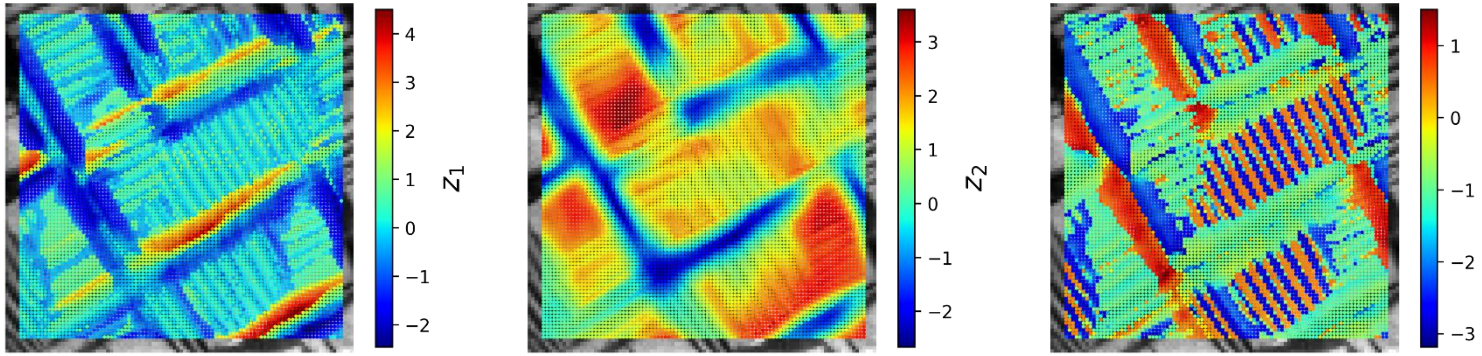


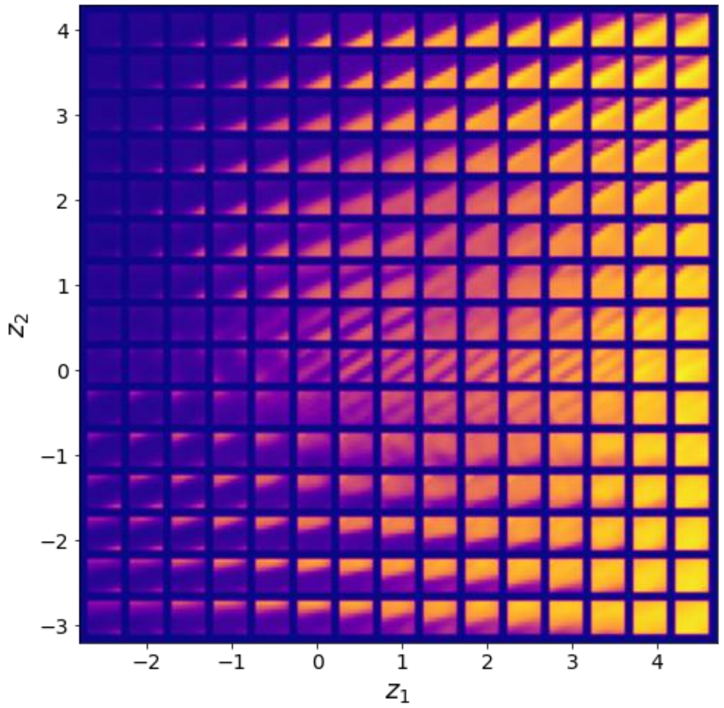
- Different acquisition functions (policies) give different experimental paths for AE
- Can we analyze what is special about points visited?

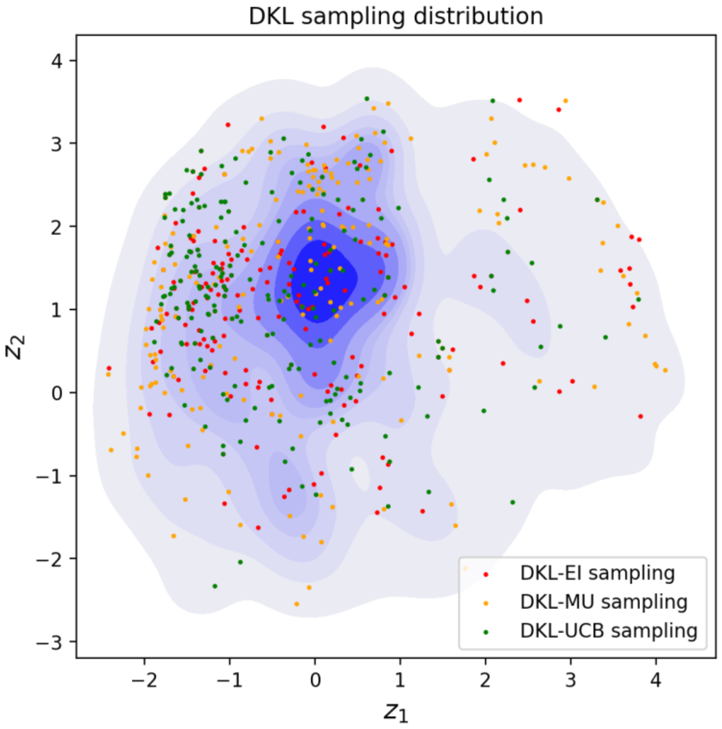
VAE approach: feature space of visited points



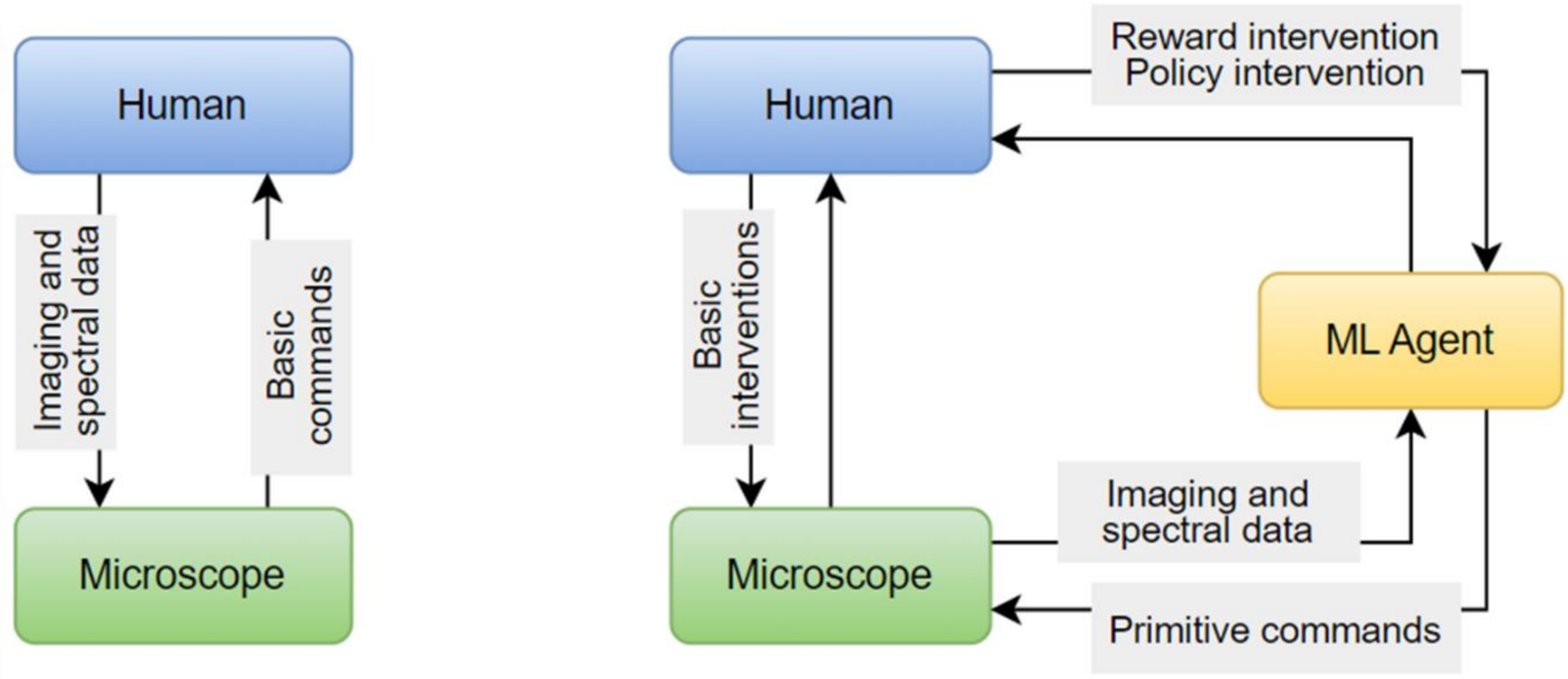
VAE approach: full feature space







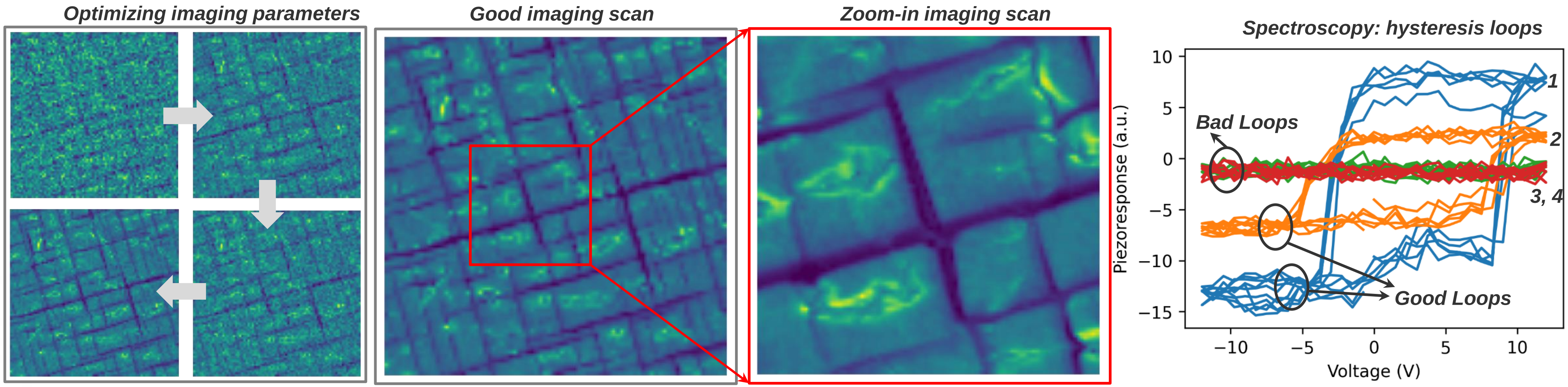
Human in the loop AE

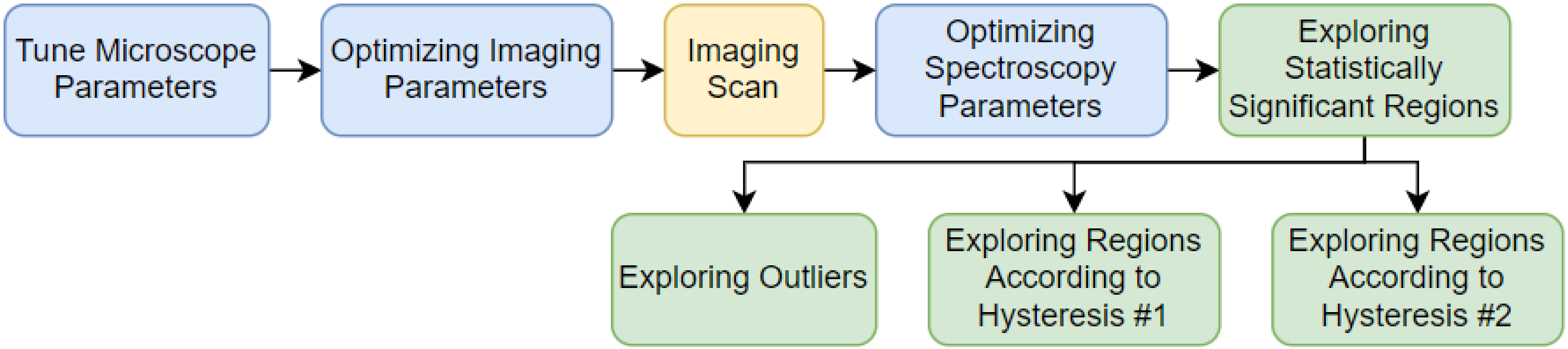


We can intervene on:

- Policies (acquisition functions): type and parameters
- Scalarizers: type and parameters
- Knowledge injection
- Direct operation

Future: full workflow optimization





Characteristic	**Definition**	**Availability**
Global image	Initial structural data set available before DKL experiment. Used to create patches for DKL training	Before
DKL latents	The latent variables encoding the structural information in the patches	During**
Scalarizer function	Function defining what characteristic of spectrum guides Bayesian Optimization	Before*
Acquisition function	Function combining DKL prediction and uncertainty of the scalarizer function	Before*
Policy	Principle for selection of next path. Simplest policy is maximization of acquisition function, but can be more complex including epsilon-greedy or switch between multiple scalarizers or acquisition functions. Human in the loop intervention tunes some aspect of the policy	Before*
Experimental trace	Collection of patches (and their coordinates) and spectra derived during experiment. Trace and global image are the results of AE SPM.	During

Characteristic	Definition	Availability
Live DKL model	DKL model in the state corresponding to the *n*-th experimental step	During
Final DKL model	DKL model in the state corresponding to the end of the experiment	After
Complete DKL model	DKL model trained on the full data set (if available from grid measurements, etc).	
Regret analysis	The difference between predictions of live DKL model and final DKL model after the whole experiment (i.e., after 200 steps in this work)	During** and After
Learning curve	Change of the DKL uncertainty (mean and deviation), indicative of the predictability of the patch-scalarizer relationship	During
Counterfactual scalarizer	The availability of full spectral data as a part of experimental trace allows to estimate what the BO step would be if scalarizer were chosen to be different	During
Trajectory analysis	Real-time trajectory of the probe that can be represented in the global image plane	During
Feature discovery	Analysis of the latent variables and latent representations of image patches and spectra in the trace. Here, we realize only patch analysis but extension to spectra is straightforward.	After
Latent trajectory analysis	Analysis of the experimental trajectory in the latent space of the full collection of the image patches derived from the global image	During**