THE UNIVERSITY of TENNESSEE KNOXVILLE

Rewards, Decisions, and Workflows

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Pacific Northwest
NATIONAL LABORATORY

Microscopy for nano- and atomic world

Asylum Cypher ES

Witec Alpha300 RS

Scanning probe microscopes:

- >100k worldwide
- Cost ~ 0.2 – 0.8 $M

Electron microscopes:

- >100k worldwide
- Can cost up to ~4-5$M

- The global SPM market: $765.2M in 2021 to $928.4M by 2026 at a CAGR of 7.2%
- The global EM market: $3.94B in 2022 to $8.67B by 2032 at CAGR of 8.4%
- Segments can grow much faster once downstream applications appear (Cryo-EM, e-cryst)

ML for Automated Microscopy?

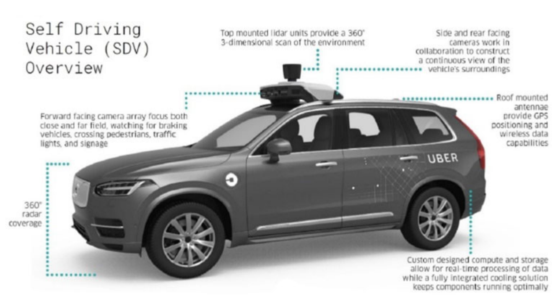
Microscopy today:

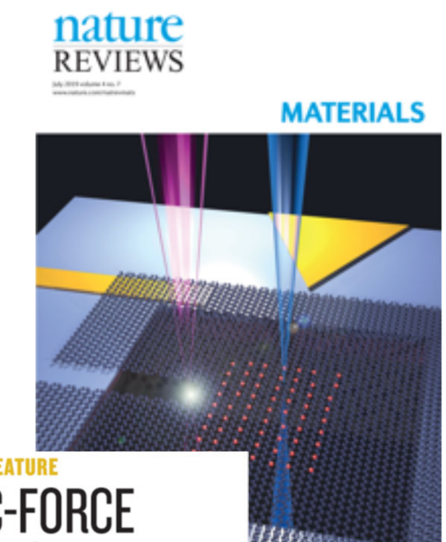
- Primary component of research in materials, physics and biology
- 1000s of high-end (S)TEM and SEM platforms, ~100,000 overall
- 1000s of high-end UHV SPMs, >100,000 ambient
- Chemical and mass-spectrometric imaging

What do microscopists do?

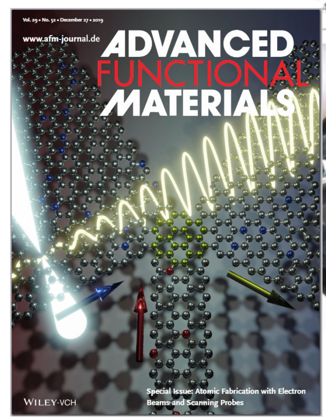
- Most of the time - sit alone in the dark room and turn knobs 😌
- Limited amount of collected data
- Case for automation: CryoEM

Unsurprisingly, inspired by autonomous cars, etc. – multiple proposals to make automated microscopes!



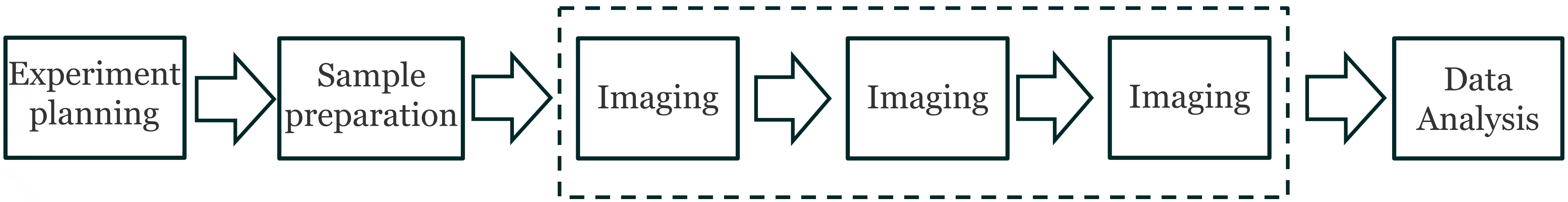


July 2019



Levels of ML in Microscopy

Level 4: Downstream Use of Microscopy Data:
Incorporates microscopy data into theory analysis pipelines, closing the synthesis-characterization-discovery loop.



Level 5: Upstream Planning:

ML is used for planning experiments, including sample selection and integrating microscopy with materials synthesis.

Level 2: Real-Time Analytics

- ML helps represent data in a form that is more understandable to humans.
- Decisions are still made and orchestrated by humans.

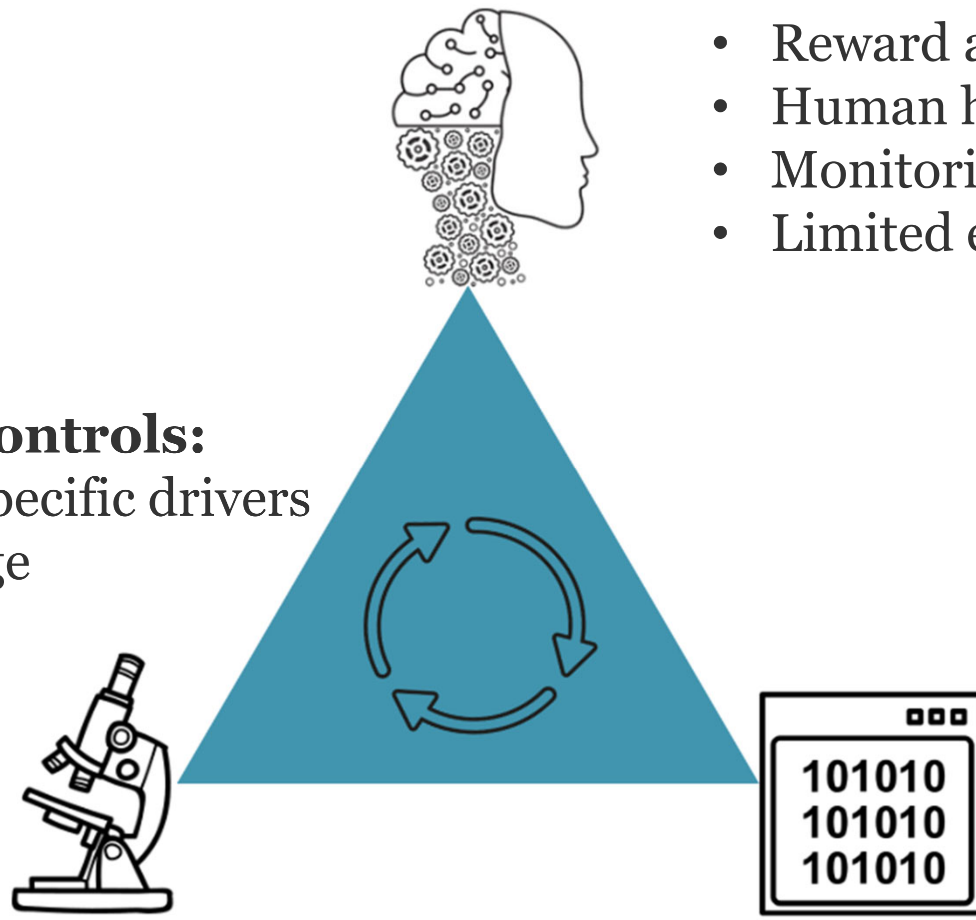
Level 3: ML Agent Introducing Decisions: automated microscopy

Level 1: Post-Acquisition Data Analysis

Challenges for the Automated Experiment

Workflow design:
- Reward and value functions
- Human heuristics
- Monitoring
- Limited experimental budget

Engineering controls:
- Instrument-specific drivers
- Hyperlanguage
- Python APIs



ML/AI

What is the Value of Microscopy?

How can we make microscopes better?

- (S)TEM
- SPM
- Both

Improve spatial resolution

Improve stability

Improve energy resolution

Increase modalities

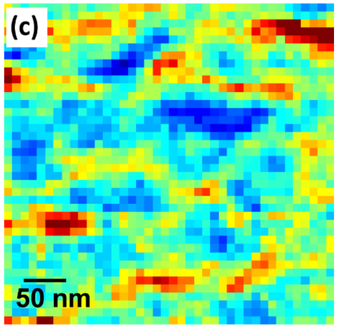
Minimize beam damage

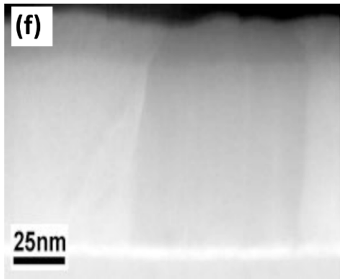
Minimize probe damage

But for customer, the value is different!

Ultimately, we run microscopy experiments to solve real world problems:

- Make better material for nuclear reactors
- Improve materials for batteries
- Find materials for direct air capture
- Remove methane from atmosphere
- Reduce corrosion in steels
- … and so on





These can be specific immediate goals (corrosion, battery materials) or fundamental discovery

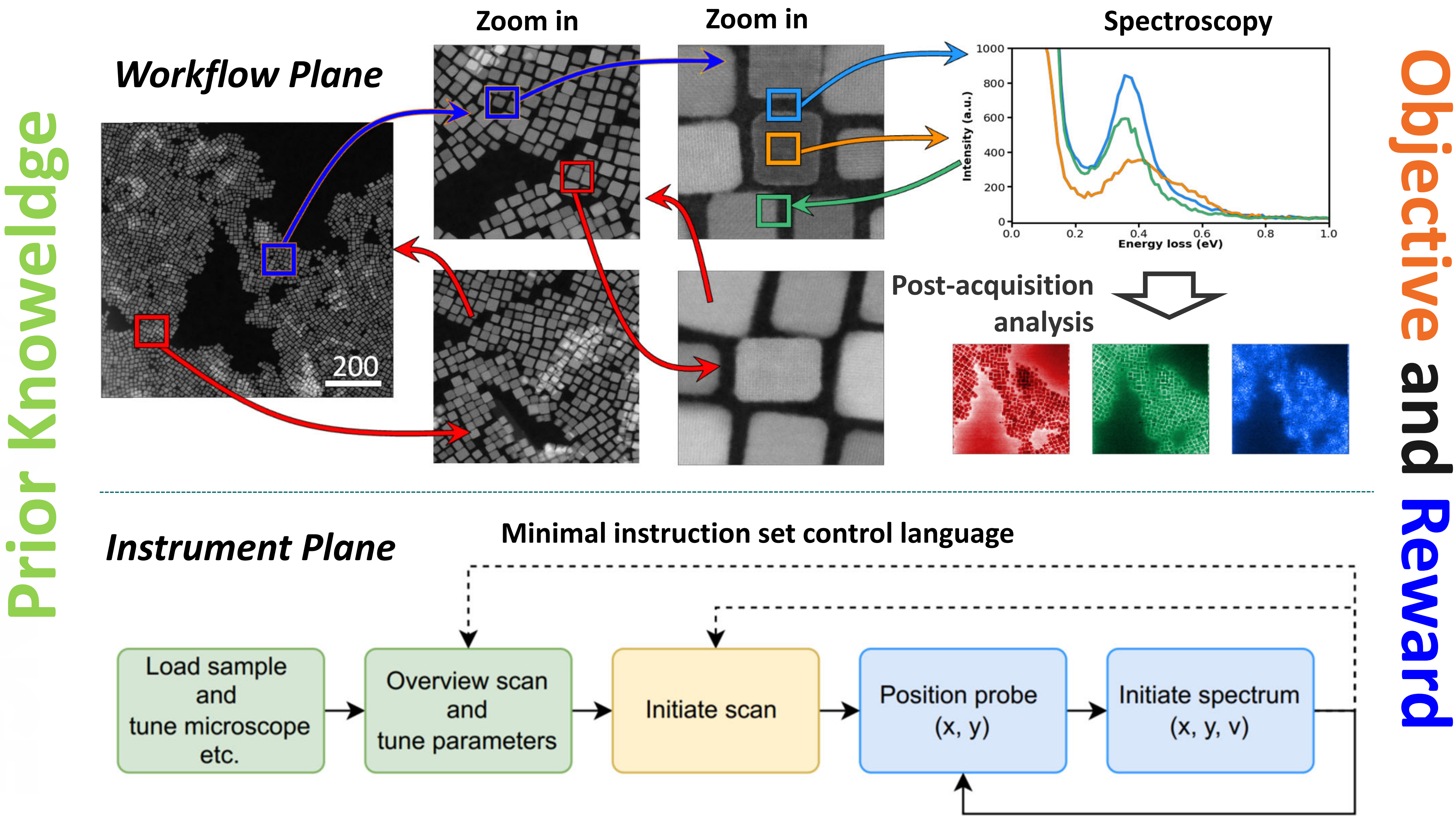
Objectives and rewards

- Objective 1: reduce global warming
- Objective 2: make cheap materials for grid energy storage
- Objective 3: understand mechanisms for material degradation
- …
- Objective n: run electrochemical reaction *in-situ* in STEM and observe crack propagation

With this knowledge, we can design a better binder for batteries – a small step towards our Objective 1. But this knowledge is also useful in other contexts

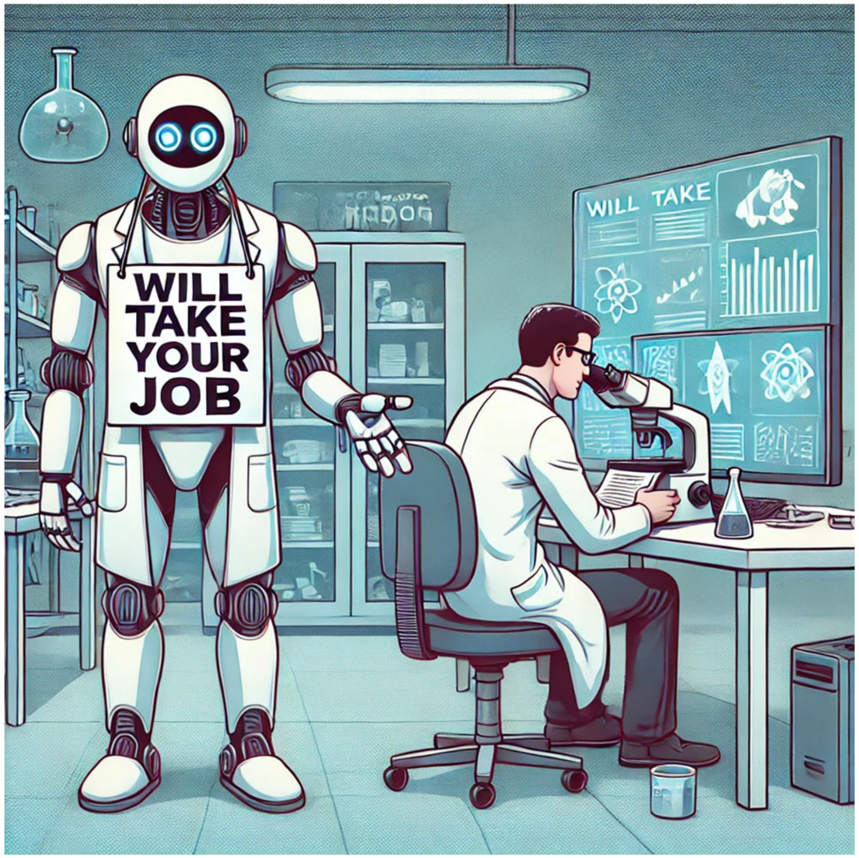
The problem: each customer plans experiment based on combination of objective and informed by prior knowledge, past experience, and intuition

Workflows in STEM



Can Machine Learning Help?

The Hype, The Reality, and The Opportunity



AI was supposed to change everything… but has it?

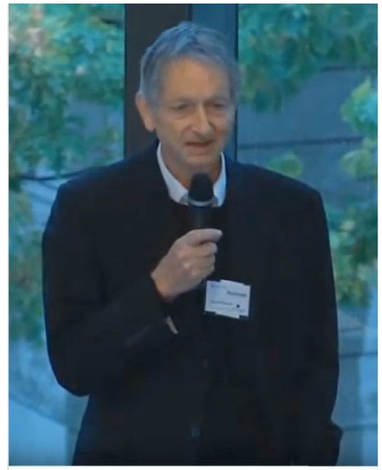
Taking the Human Out of the Loop: A Review of Bayesian Optimization

Citation

Shahriari, Bobak, Kevin Swersky, Ziyu Wang, Ryan P. Adams, and Nando de Freitas. 2016. "Taking the Human Out of the Loop: A Review of Bayesian Optimization." Proc. IEEE 104 (1) (January): 148–175. doi:10.1109/jproc.2015.2494218.

Published Version

doi:10.1109/JPROC.2015.2494218



"I think that if you work as a radiologist, you are like Wile E. Coyote in the cartoon. You're already over the edge of the cliff, but you haven't yet looked down. There's no ground underneath. People should stop training radiologists now. It's just completely obvious that in five years deep learning is going to do better than radiologists."

Nov 24, 2016

https://www.reddit.com/r/singularity/comments/13c3n36/geoffrey_hinton_said_radiologists_would_be/

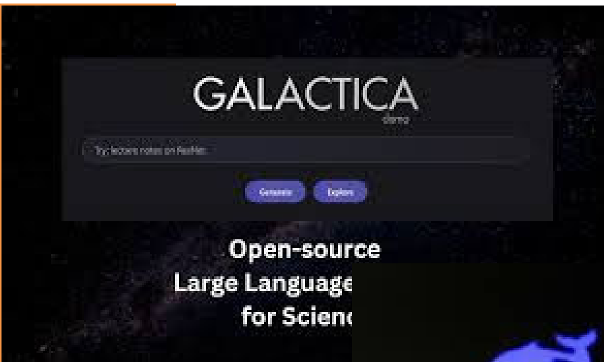
Credit: Mimi Phan / Cole Burston via Getty Images

IDEAS MADE TO MATTER | ARTIFICIAL INTELLIGENCE

Why neural net pioneer Geoffrey Hinton is sounding the alarm on AI

https://mitsloan.mit.edu/ideas-made-to-matter/why-neural-net-pioneer-geoffrey-hinton-sounding-alarm-ai

https://insideevs.com/news/717533/tesla-musk-self-driving-promises/



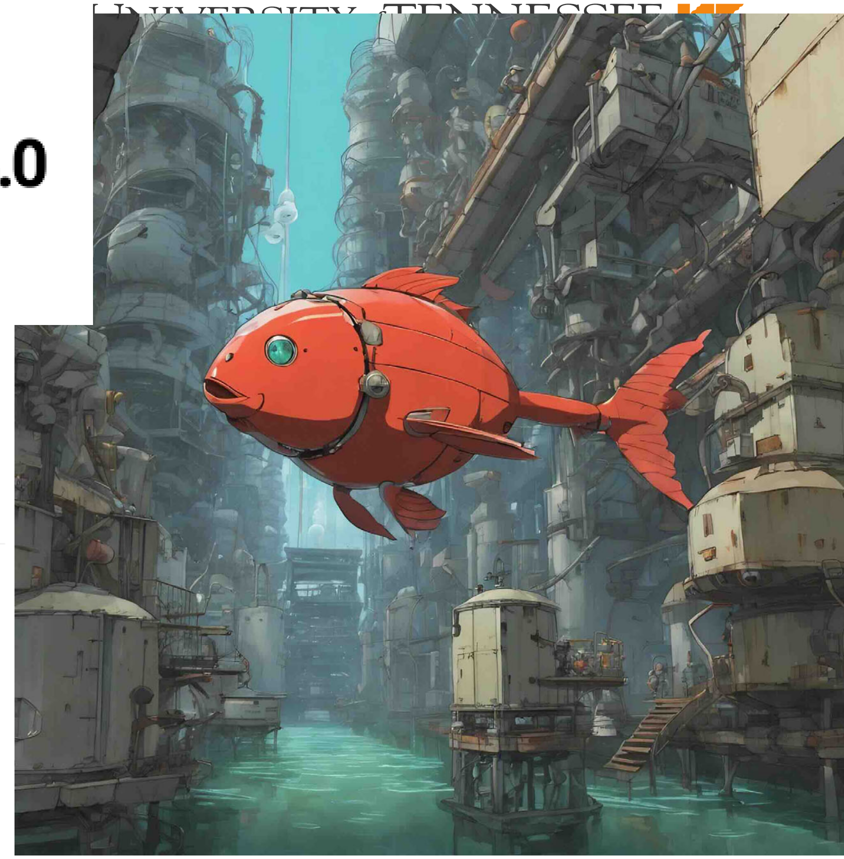
OpenAI
ChatGPT 4.0

The KBS Chronicle

Google Suspends Gemini AI's Image Generation Amidst Accuracy Concerns

Some of the results returned and images generated were bordering on the absurd.

KBS SIDHU
FEB 23, 2024



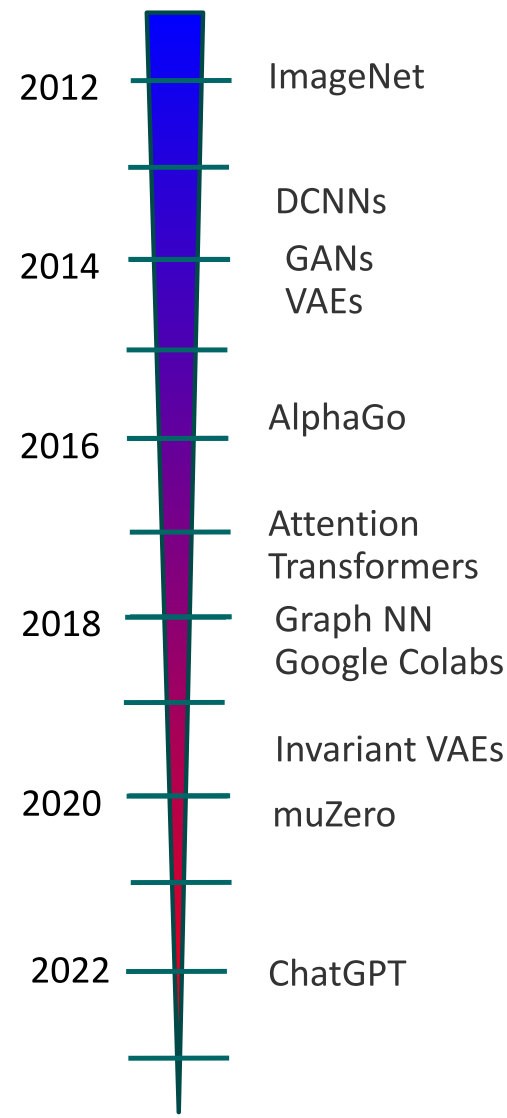
The AI Scientist is designed to be compute efficient. Each idea is implemented and developed into a full paper at a cost of approximately $15 per paper. While there are still occasional flaws in the papers produced by this first version (discussed below and in the report), this cost and the promise the system shows so far illustrate the potential of The AI Scientist to democratize research and significantly accelerate scientific progress. https://sakana.ai/ai-scientist/

Why Machine Learning?

- Last decade has experienced an explosive growth of machine learning and artificial intelligence applications
- These developments have spanned areas from computer vision to medicine to autonomous systems and games
- However, the progress and impact as applied to experimental physical sciences has been minimal….

Why is it difficult?

- Requires domain expertise and domain-specific goals
- Deeply causal and hypothesis drive nature of domain sciences
- No single answer: culture, not a method
- Infrastructure, open code, open data
- **Most important:** active nature of scientific process



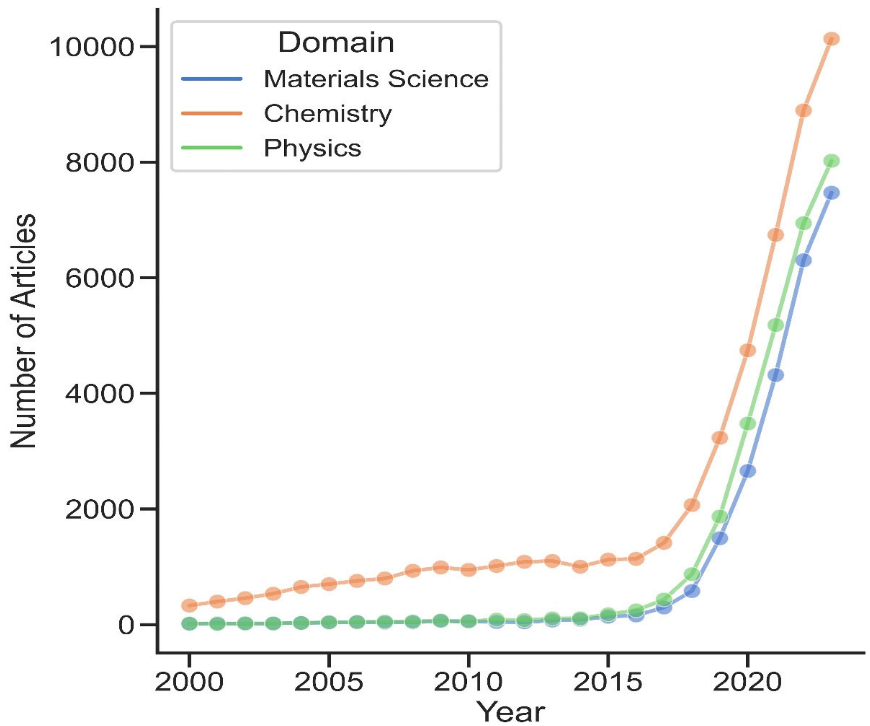
“Eras” of ML in Industry

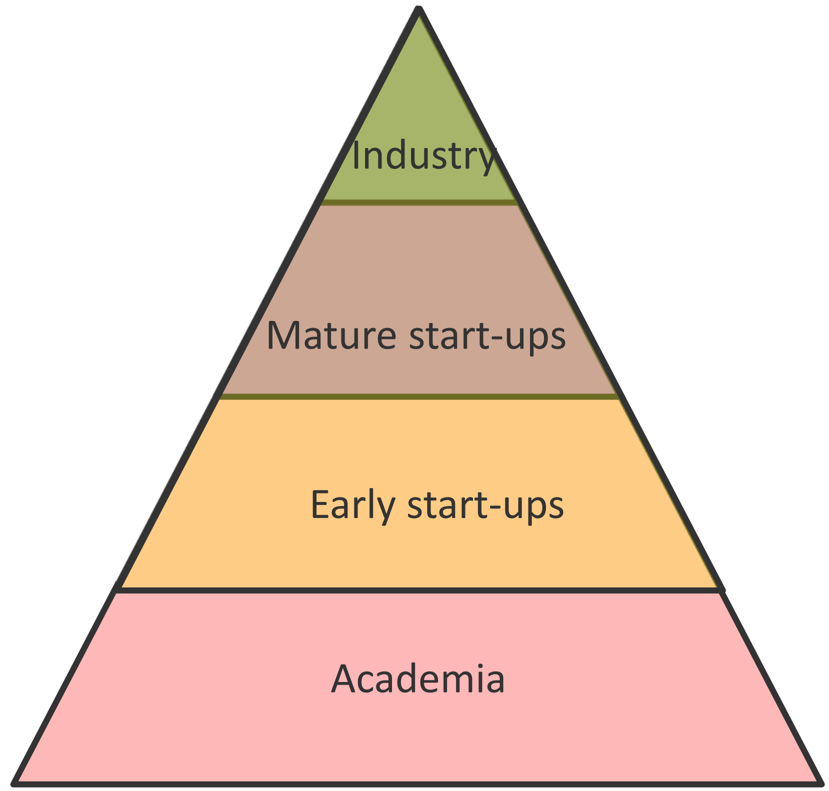
- **Before 2002:** It’s all about IT (dotcoms, Amazon, etc)
- **2002 - 2012:** It’s all about collecting and searching data (Facebook, Google, Uber)
- **2012 – 2022:** What do we learn from data (correlative era)
- **2022 – now:** LLMs and Reasoning; Physics based ML

Microsoft: GitHub
Meta: Open Catalyst,
Meta: Papers with Code
Toyota: TRI
Google: AlphaFold
NVIDIA: protein folding

- Classical machine learning is underpinned by the existence of the static data sets – from MNIST to medical, bio, faces, etc.
- Real world problems are associated with the large distribution shifts, small data sets, and presence of uncontrollable exogenous factors
- Real world problems are often active learning: we interrogate the data generation process and provide feedback
- However, we often have extensive prior knowledge of past data, physical laws generalizing them, and strong set of inferential biases

ML in Domain Sciences





Analysis by B. Blaiszik, Argonne

- The rapid adoption of ML in domain sciences and industrial R&D is a very recent trend
- Technologies and workforce emerge from academia into industry
- We can estimate potential growth rates comparing to cloud computing 15 - 20 years ago

How can we cut through hype?

How we make decisions:
human + AI

How we execute decisions:
human + (automated) instrumentation

Making it real:

- What decisions can be executed?
- How fast can decisions be made?
- How fast can decisions be executed?
- How do we improve decisions?

Each hypothesis requires defining experimental action space

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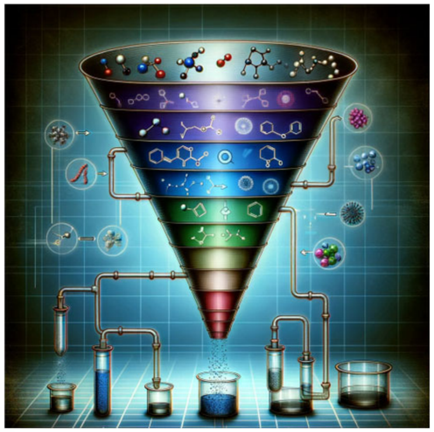
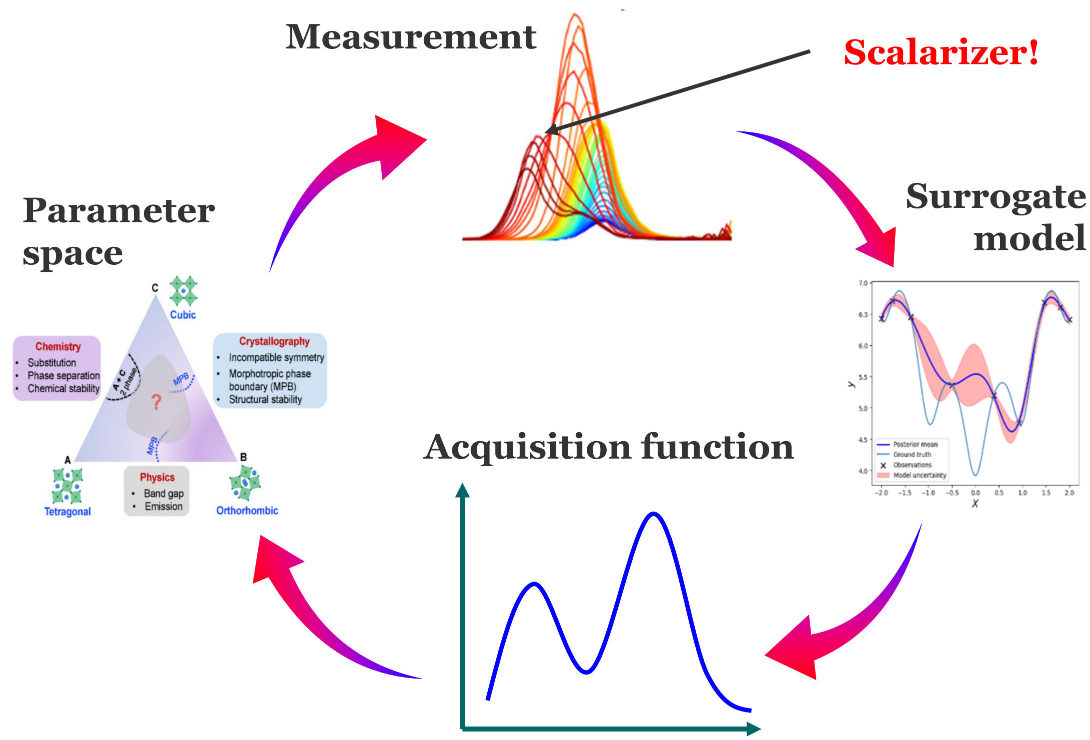
Microscopy starts in the materials lab!

How can we bring ML to real world?

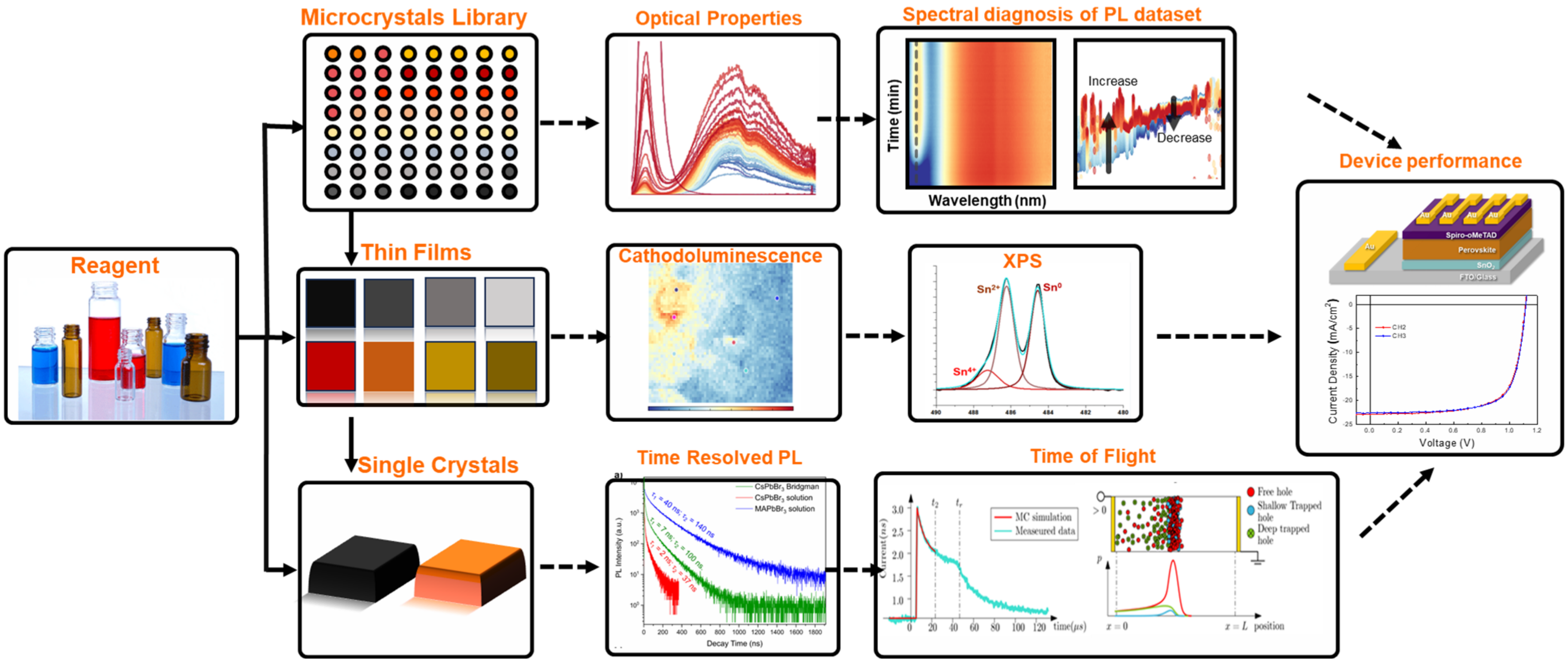


Theory workflows
- Established field with active industry and academic presence
- Based on "funnel" workflows for prediction.
- Need experimental validation
- Can we learn from experiment?

Experiment workflows
- Based on myopic optimization
- Limited use of proxies via multifidelity schemes
- Requires well-defined optimization (aka utility) functions
- What is the real (economic) value?



Decision science of workflows (Ahmadi Lab)

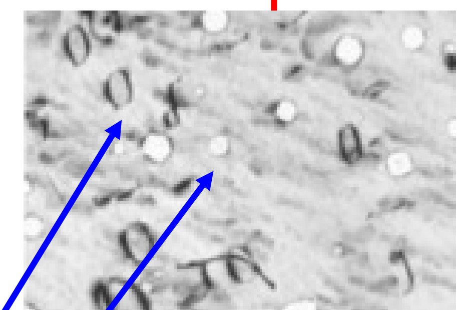


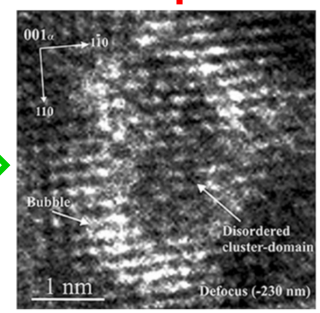
- Multiple levels of decision making based on perceived gain, latencies, and costs
- Iterative cycles between low-cost and expensive measurements
- Learning **basic science/models** as a strategy to minimize cost and answer interventional and counterfactual questions

Workflows for Nuclear Materials Design

Traditional experiment:
1. Always based on workflows
2. Ideated, orchestrated, and implemented by humans
3. The "gain of value" during the workflow implementation is uncertain

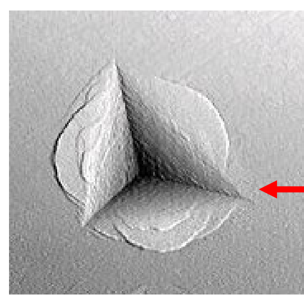
Materials selection





Prior knowledge

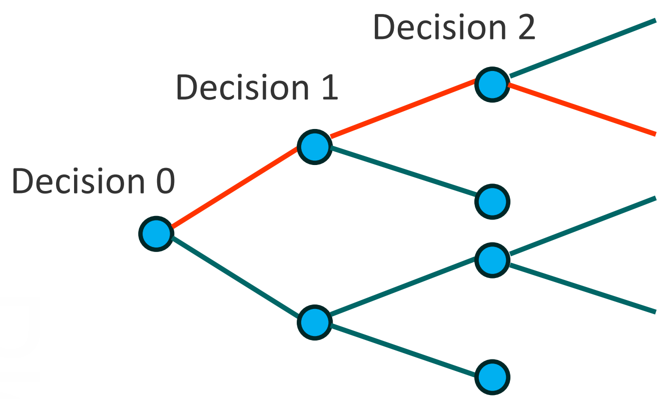
Operator curiosity

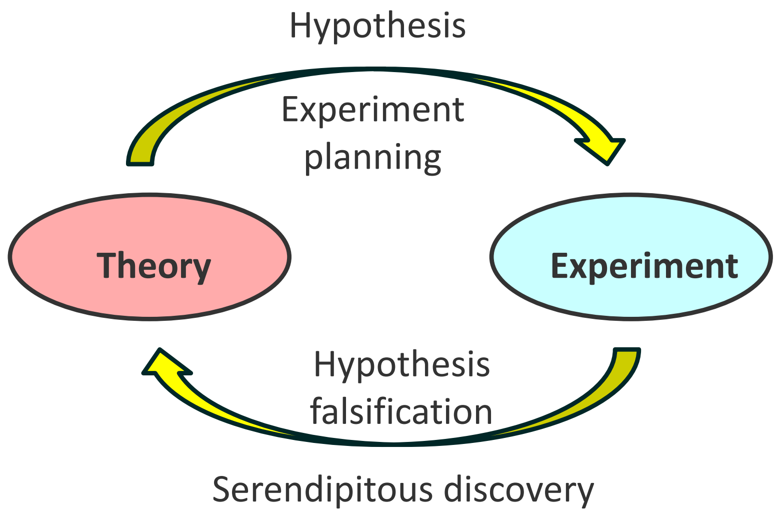


Value

Value of the step is key element:
- Either based on prior knowledge
- Or defined in a sense of the reinforcement learning Q-function

Decision science of workflows

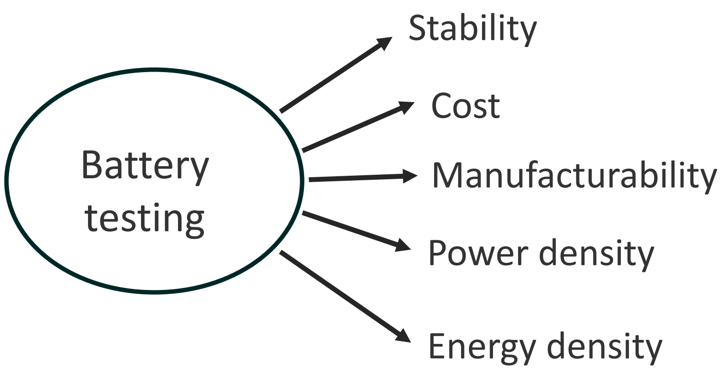


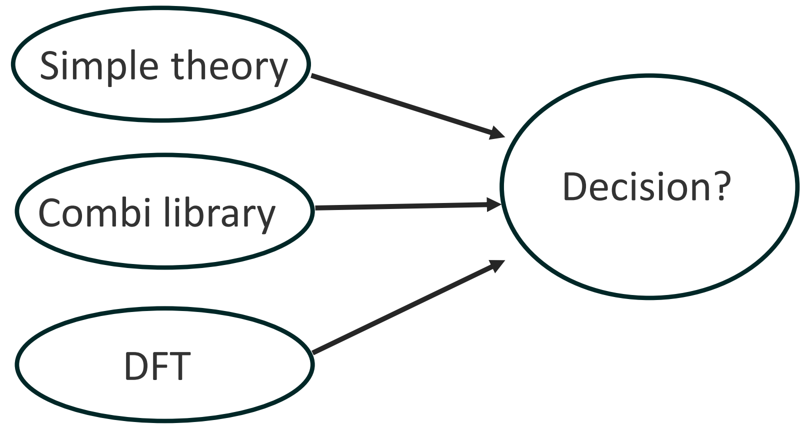


- **Experiment is a combinatorial space of opportunities:**
  → Investing only in scaling of throughput is only a linear improvement
- **Knowledge of physics often allows to reduce complexity: combinatorial to linear**:
  → Basic science pays off (with time)!
- **Science is a cycle between theory-driven hypothesis generation and experiment**:
  → We need to accelerate all elements of the cycle
- **Experimental and computational tool development:**
  → Currently constrained by human paradigm

If the part of a workflow is automated, our autonomous decision-making ability should match the level of autonomy!

Decision science of workflows

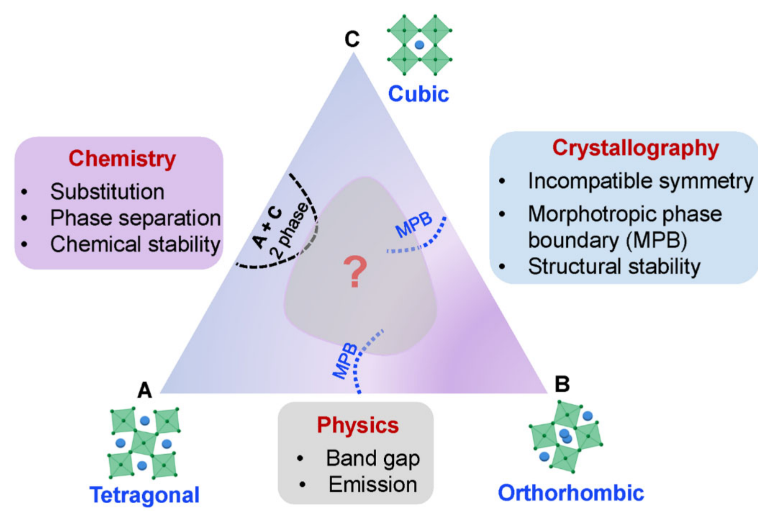


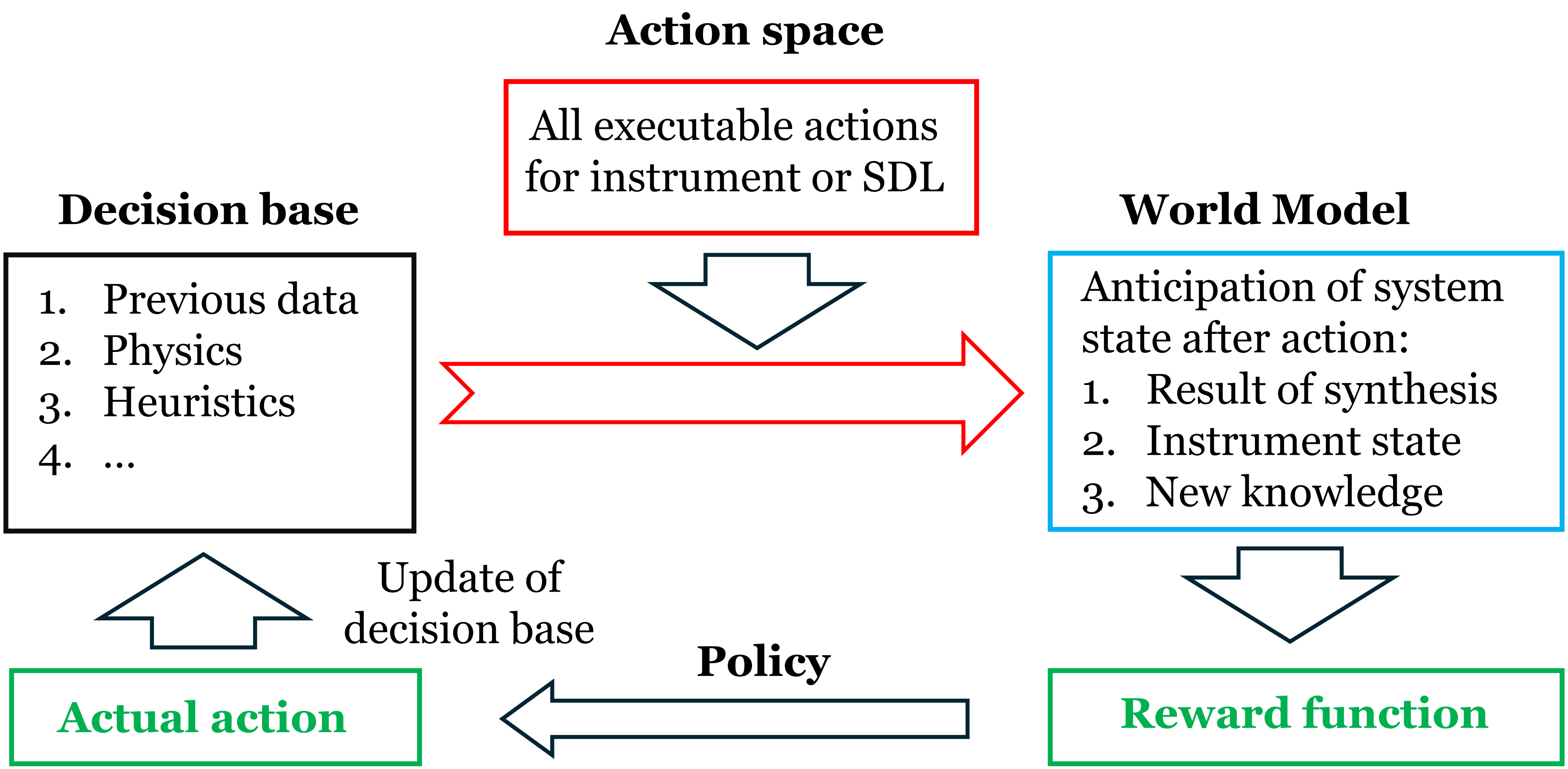


1. We need to balance multiple functionalities
2. Integrate multiple sources of data
3. Make decisions considering costs, latencies, physical inferential biases, and beliefs

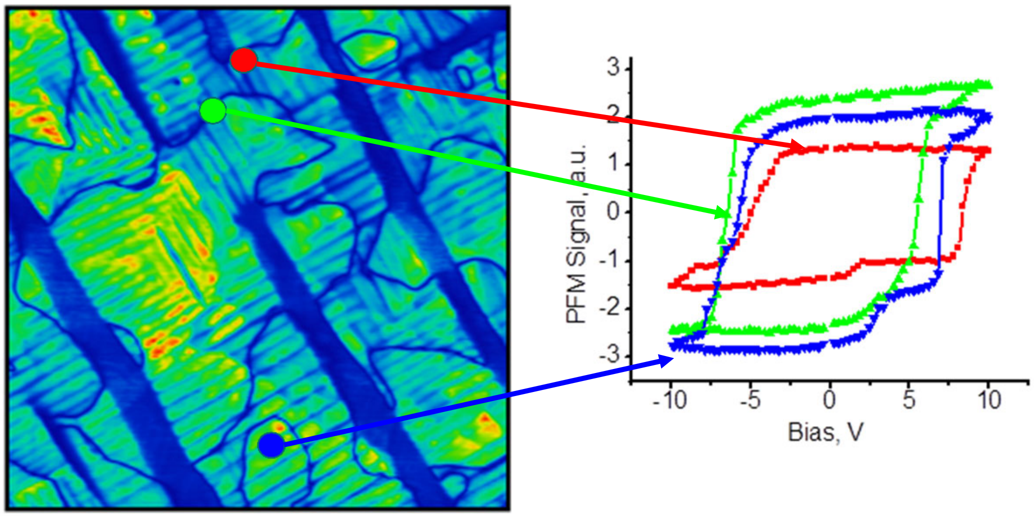
Key consideration: reward function

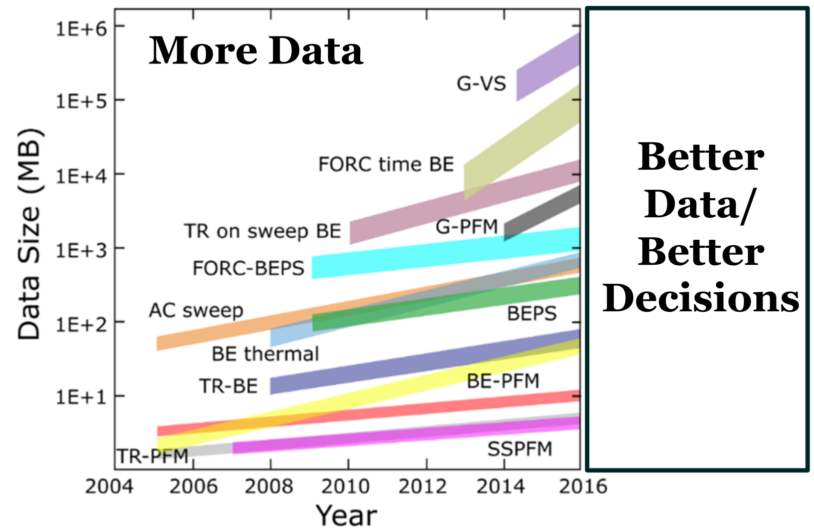
1. Pure physical discovery (symbolic laws)
2. Data-driven exploration
3. Materials optimization
4. …




Action space
All executable actions for instrument or SDL
Decision base
1. Previous data
2. Physics
3. Heuristics
4. ...
World Model
Anticipation of system state after action:
1. Result of synthesis
2. Instrument state
3. New knowledge
Update of decision base
Policy
Actual action
Reward function

Why do we do experiments?



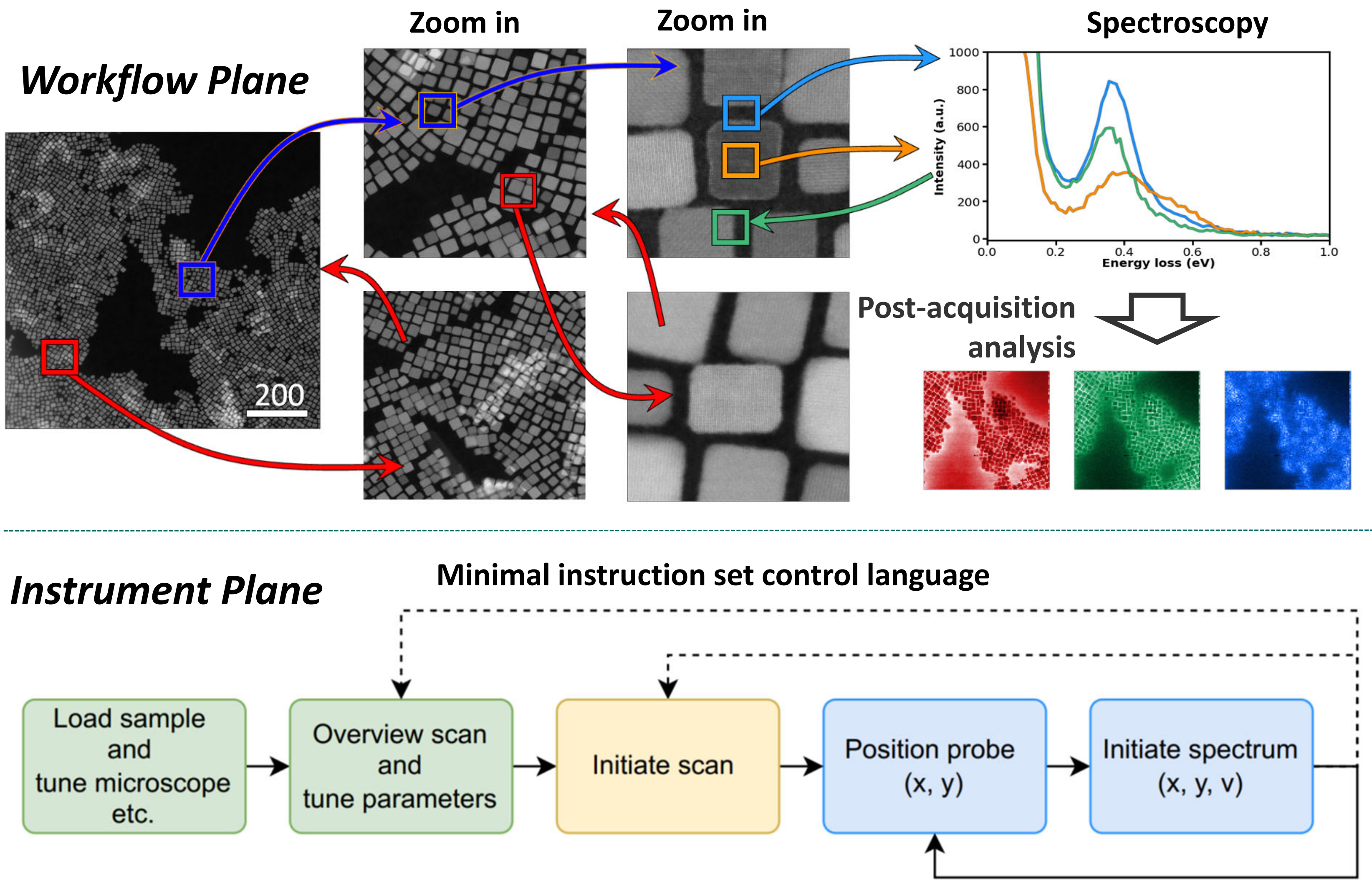


- Structure-property measurements (SPM, STEM-EELS, SEM-nanoindentation)
- Equivalent problem to molecular and property discovery
- Interesting functionalities are expected at the certain elements of domain structure
- We can guess some; we have to discover others

- **Experimental objectives → ML Rewards**
  - Microscope optimization
  - Properties of a priori known regions of interest
  - Discovery of regions with interesting properties
  - Physical theory falsification - - - - - - - - - - - - - - → **Objective**

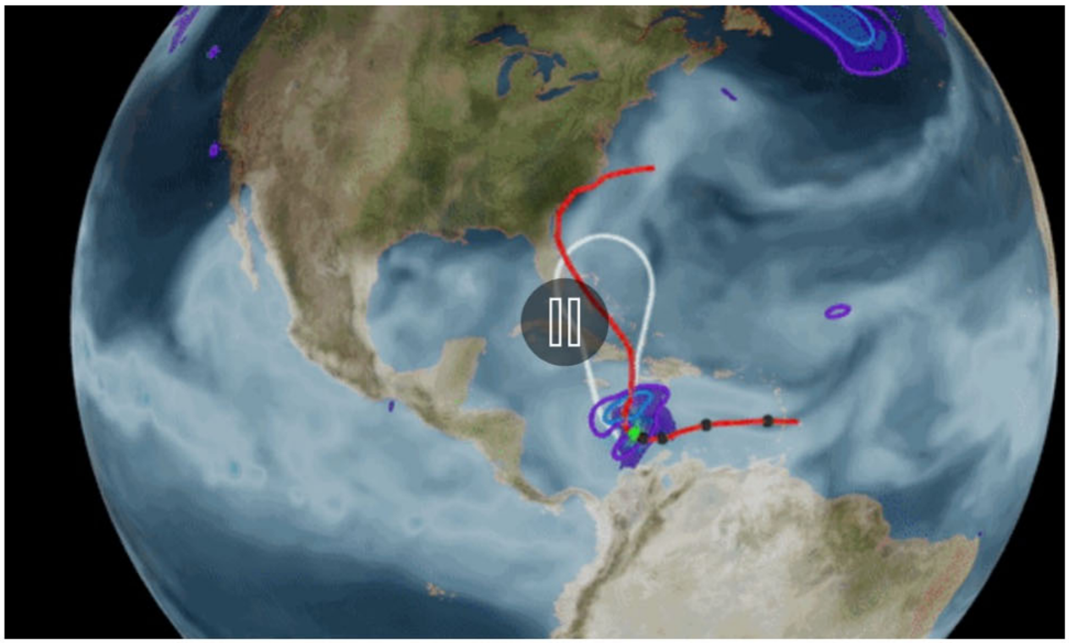
Workflows in STEM

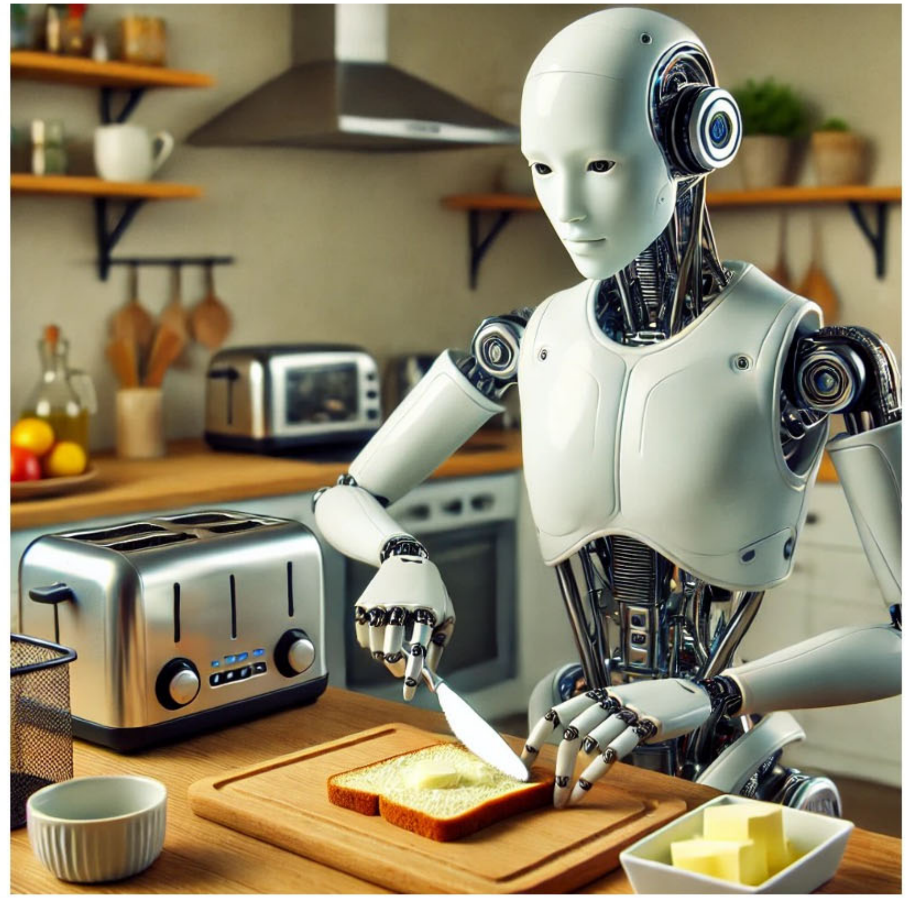
Prior Knoweldge



Objective and Reward

AI can solve calculus, but struggles with buttering toast

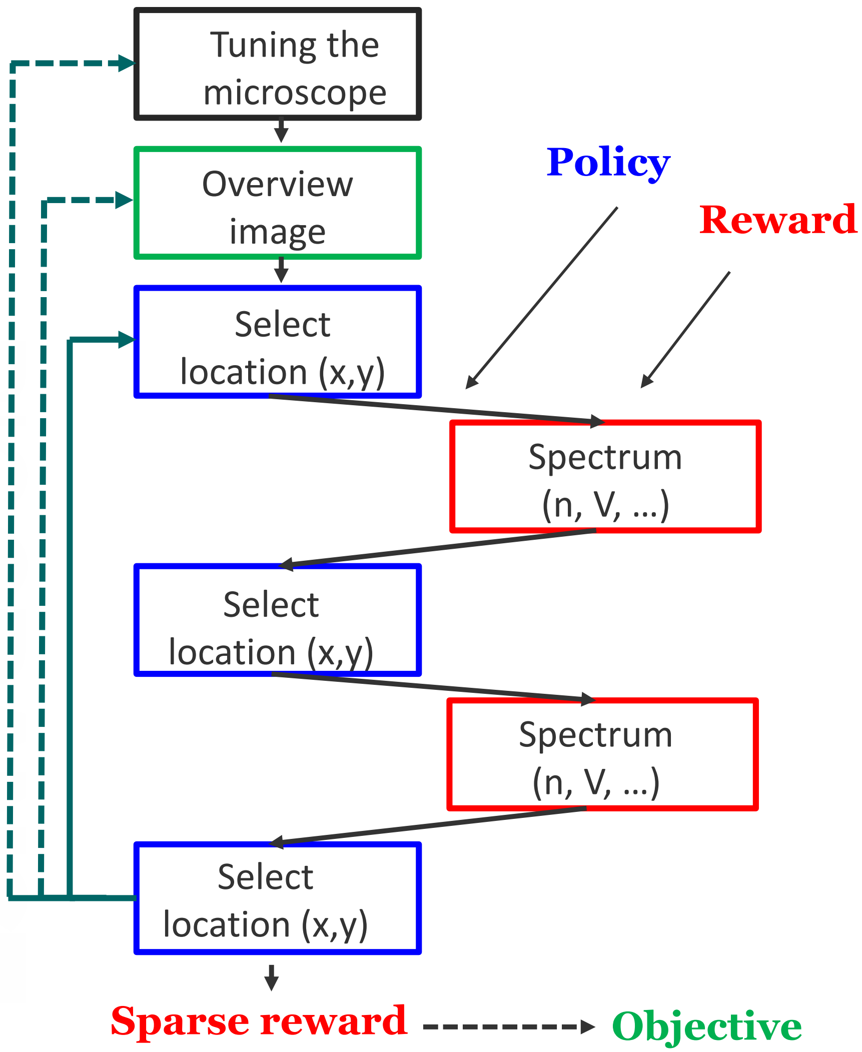




https://zongyi-li.github.io/neural-operator/

But the real issue isn't just precision—it's rewards. The robot doesn't need toast. I do. And I need to explain what I need before it can make it.

Workflows in Microscopy



To implement the ML workflows, we start from emulating the human operations:

- Well defined and explainable commands
- Extensive domain expertise
- Potentially available data from experiments

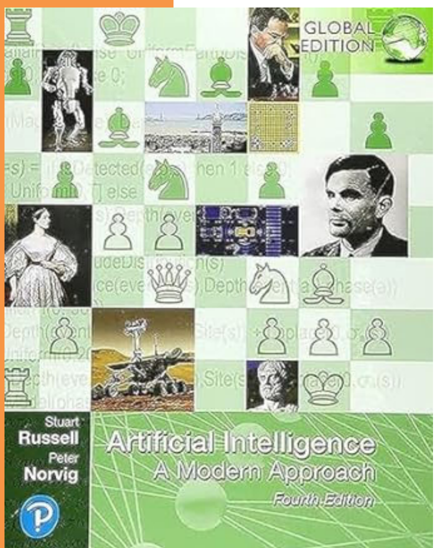
Development of ML workflows can give rise to more complex imaging modalities

- Data volumes and dimensionalities above human level
- More complex modes of sampling
- “Guardian angel” modules

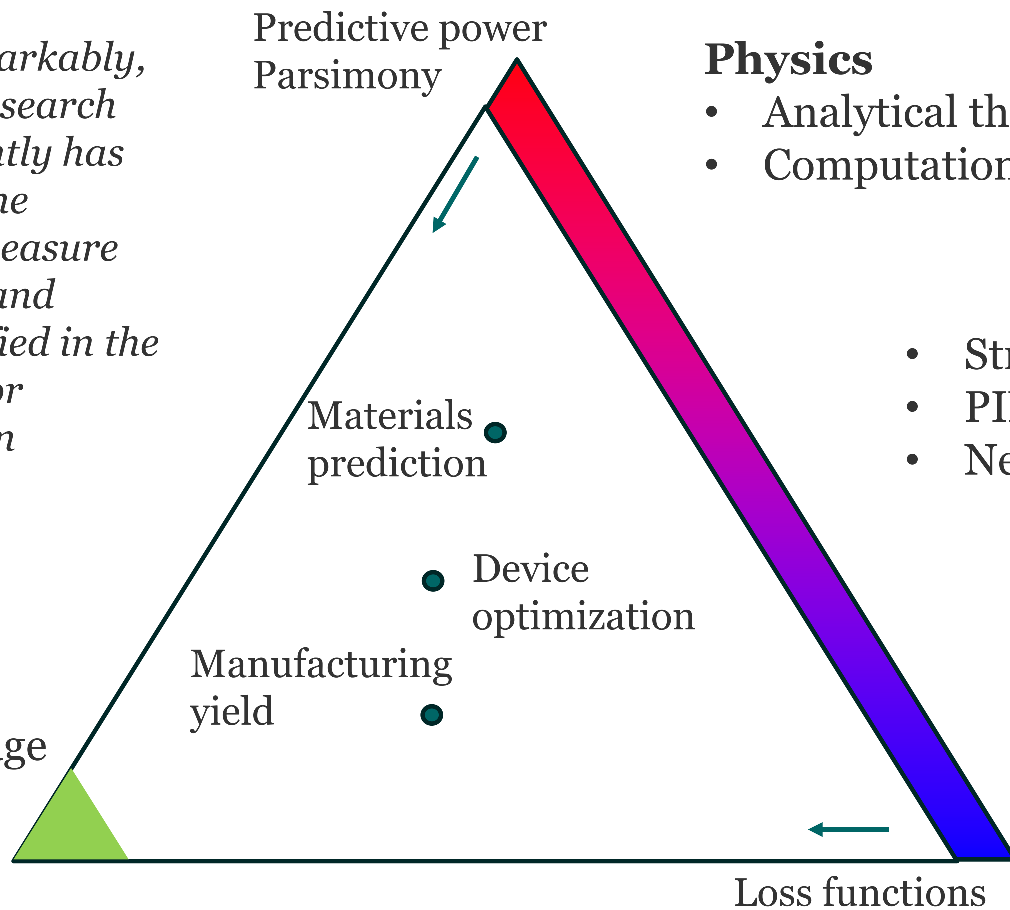
However, we always have to think about

- Reward function(s) for imaging problem
- Reward functions for materials problem
- Overall objective

Is Machine Learning and Physics Enough?



Somewhat remarkably, almost all AI research until very recently has assumed that the performance measure can be exactly and correctly specified in the form of utility or reward function



Physics
- Analytical theory
- Computational experiments

- Structured GPs
- PINNs
- Neural operators

Rewards
- Energy generation
- Better storage materials
- …

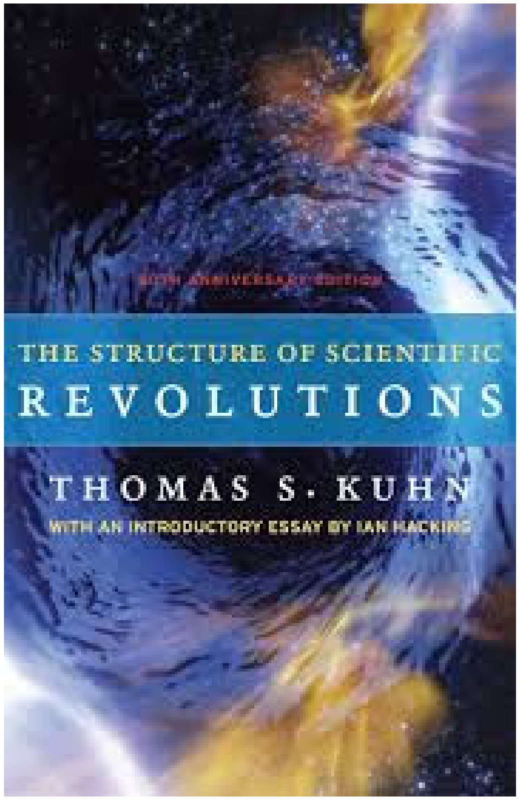
Data:
- DCNNs
- LLMs
- And so on

With defined reward function, any problem is optimization problem – and we know how to solve optimization problems!

What if rewards are “all we need”?

The new approach should:

- Explain previous data and incorporate past theories as special cases
- Allow to do new things: predict new phenomena, build workflows, etc.



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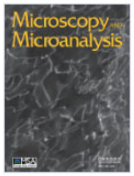

JOURNAL ARTICLE

Towards the Thinking Microscope

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OS Ovchinnikov, S Jesse, SV Kalinin, HJ Chang, SJ Pennycook, AY Borisevich

Microscopy and Microanalysis, Volume 16, Issue S2, 1 July 2010, Pages 160–161,
https://doi.org/10.1017/S1431927610062720
Published: 01 August 2010

Functional recognition imaging using artificial neural networks: applications to rapid cellular identification via broadband electromechanical response

M P Nikiforov[1], V V Reukov[2], G L Thompson[2], A A Vertegel[2], S Guo[1], S V Kalinin[1] and S Jesse[1]

Published 14 September 2009 • IOP Publishing Ltd
Nanotechnology, Volume 20, Number 40

Disorder Identification in Hysteresis Data: Recognition Analysis of the Random-Bond–Random-Field Ising Model

O. S. Ovchinnikov, S. Jesse, P. Bintacchit, S. Trolier-McKinstry, and S. V. Kalinin
Phys. Rev. Lett. **103**, 157203 – Published 9 October 2009

ACS Nano > Vol 15/Issue 8 > Article

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REVIEW | July 16, 2021

Automated and Autonomous Experiments in Electron and Scanning Probe Microscopy

Sergei V. Kalinin*, Maxim Ziatdinov, Jacob Hinkle, Stephen Jesse, Ayana Ghosh, Kyle P. Kelley, Andrew R. Lupini, Bobby G. Sumpter, and Rama K. Vasudevan

nature > nature materials > progress article > article

Progress Article | Published: 23 September 2015

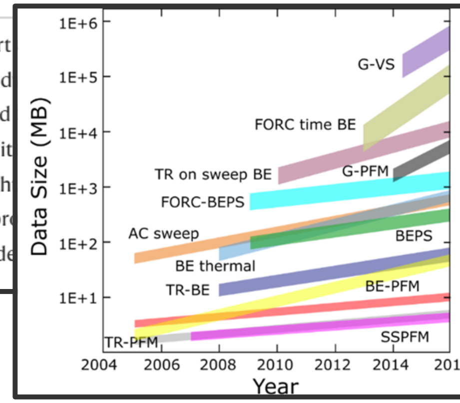
Big-deep-smart data in imaging for guiding materials design

Sergei V. Kalinin, Bobby G. Sumpter & Richard K. Archibald

Nature Materials **14**, 973–980 (2015) | Cite this article

Abstract

Harnessing big data, deep data, and smart
accelerate the design and realization of ad
opportunities in materials design enabled
analytics approaches, including their limit
specifically focus on how these tools migh
Such methodologies are particularly appr
improvements in atomistic imaging, mode



Machine learning for automated experimentation in scanning transmission electron microscopy

Sergei V. Kalinin, Debangshu Mukherjee, Kevin Roccapriore, Benjamin J. Blaiszik, Ayana Ghosh, Maxim A. Ziatdinov, Anees Al-Najjar, Christina Doty, Sarah Akers, Nageswara S. Rao, Joshua C. Agar & Steven R. Spurgeon

npj Computational Materials **9**, Article number: 227 (2023) | Cite this article

The dance of policies and rewards

Rewards and objectives:

- What is our (hierarchical) objective?
- Can we define reward(s)?

Inferential biases:

- What do we know before the experiment?
- What do we (hope to) learn after the experiment?

Experiment planning – policies and values

- How do we plan experiment in advance (policies or values based on rewards)?
- Can we ascribe value to certain steps?
- Do we change our policies during experiment?

Reward functions in imaging

Imaging Optimization

Physical laws discovery

Image-based reward functions
- Human selected objects (DCNNs)
- Equal sampling of feature space
- Equal sampling of parameter space (combi library)

Structure property relationship
- Reward definition (with cost)
- Tuning curiosity
- Human in the loop DKL

Co-orchestration multiple tools
Co-navigation theory and experiment

Article | Published: 04 April 2022

Experimental discovery of structure–property relationships in ferroelectric materials via active learning

Yongtao Liu, Kyle P. Kelley, Rama K. Vasudevan, Hiroshi Funakubo, Maxim A. Ziatdinov & Sergei V. Kalinin

Nature Machine Intelligence 4, 341–350 (2022) | Cite this article

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RESEARCH ARTICLE | CONDENSED MATTER PHYSICS

Dynamic STEM-EELS for single-atom and defect measurement during electron beam transformations

KEVIN M. ROCCAPRIORE, RICCARDO TORSI, JOSHUA ROBINSON, SERGEI KALININ, AND MAXIM ZIATDINOV Authors Info & Affiliations

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ARTICLE · Volume 4, Issue 3, 100704, March 10, 2023 · Open Access Download Full Issue

Autonomous scanning probe microscopy with hypothesis learning: Exploring the physics of domain switching in ferroelectric materials

Yongtao Liu [1,5] · Anna N. Morozovska [2] · Eugene A. Eliseev [2,3] · Kyle P. Kelley [1] · Rama Vasudevan [1] · Maxim Ziatdinov [1,4] · Sergei V. Kalinin [1] Show less

Fixed Policy Experiments


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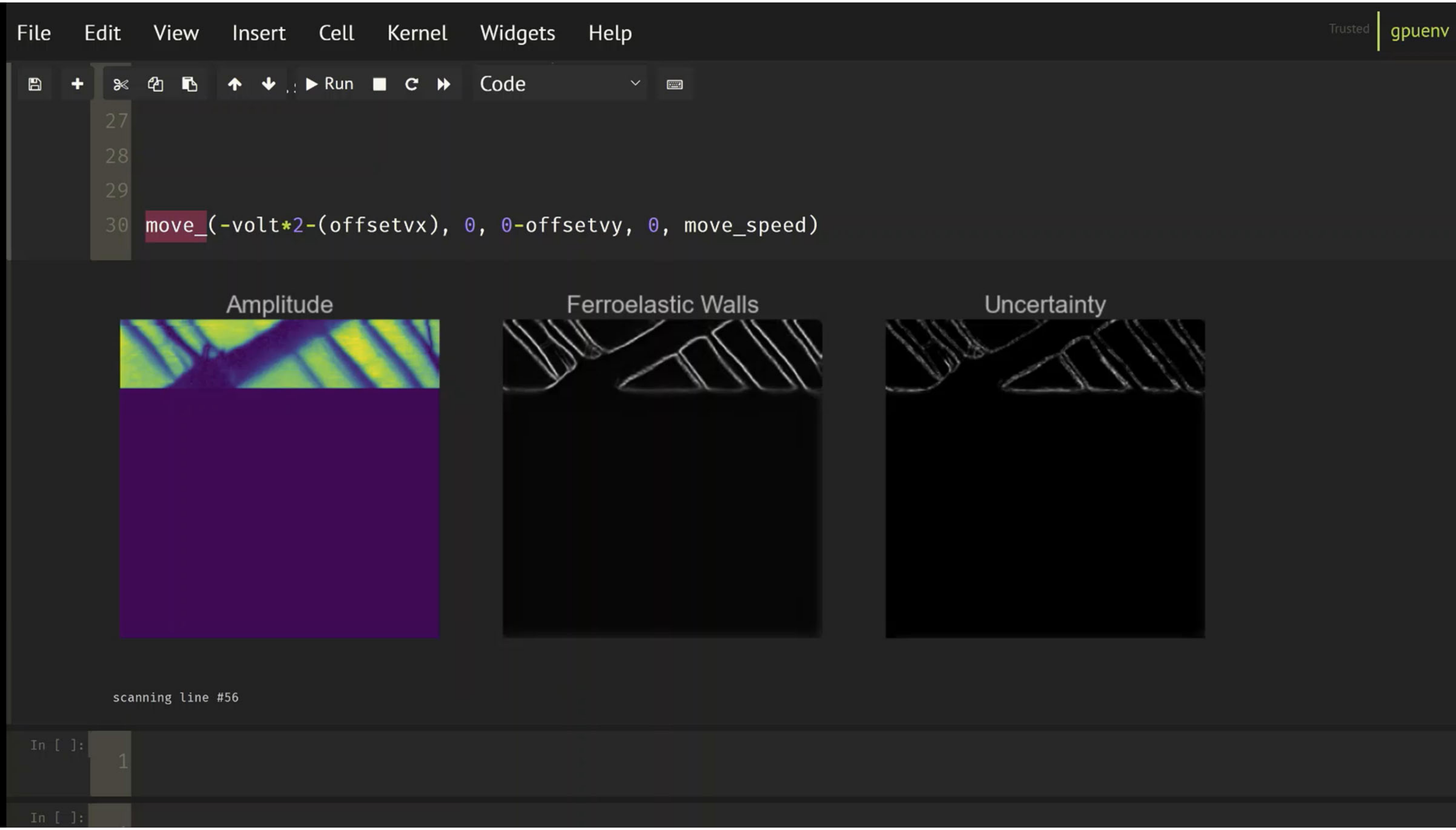
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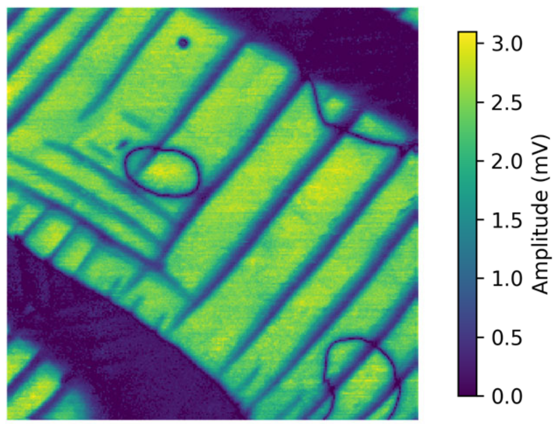
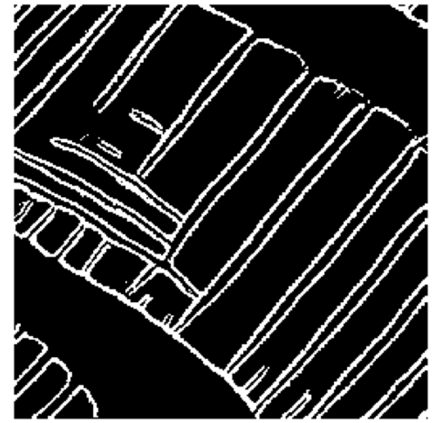
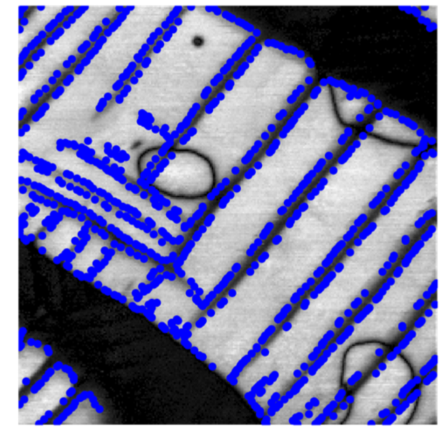
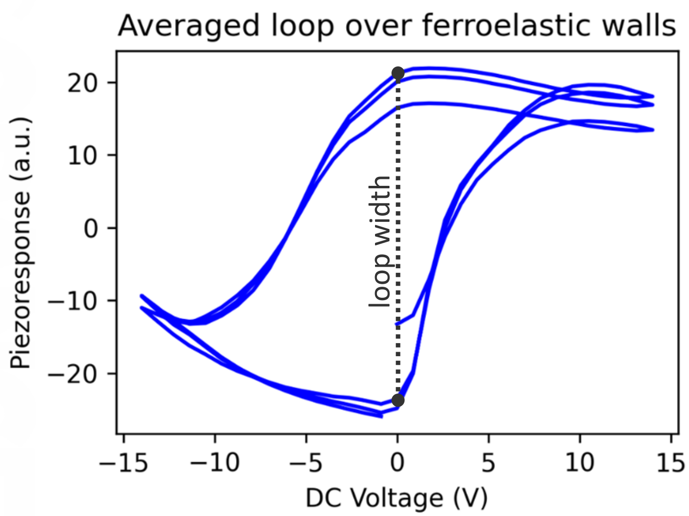
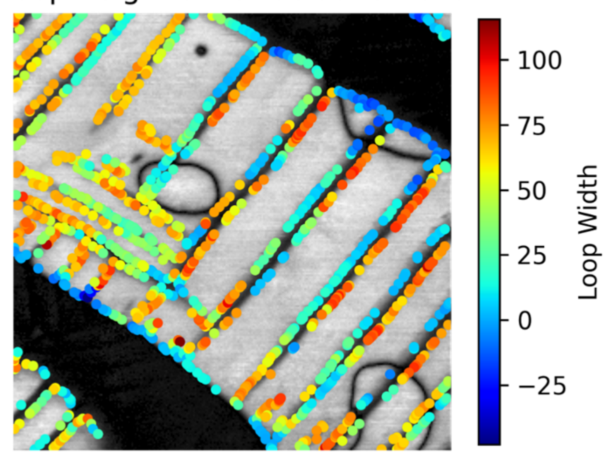
Mapping Activity of Domain Walls

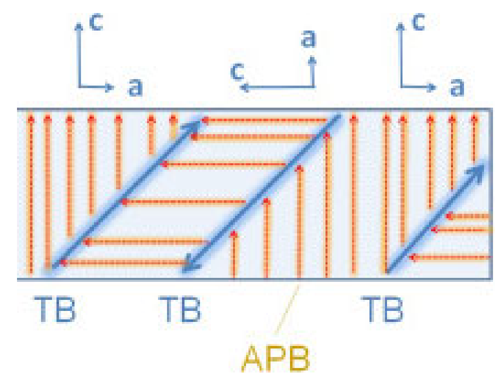






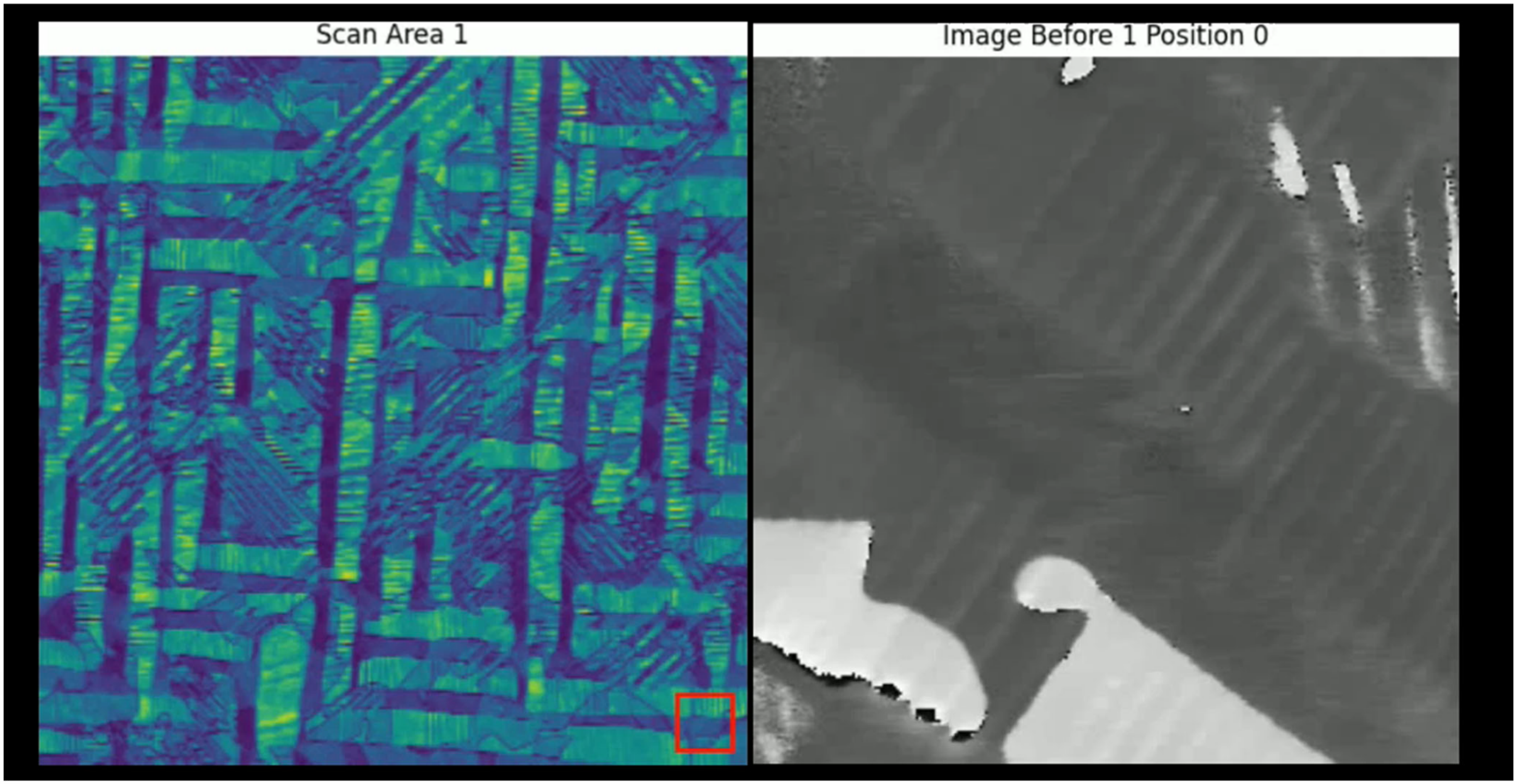






Liu, Y., Kelley, K.P., Funakubo, H., Kalinin, S.V., Ziatdinov, M., Arxiv, submitted

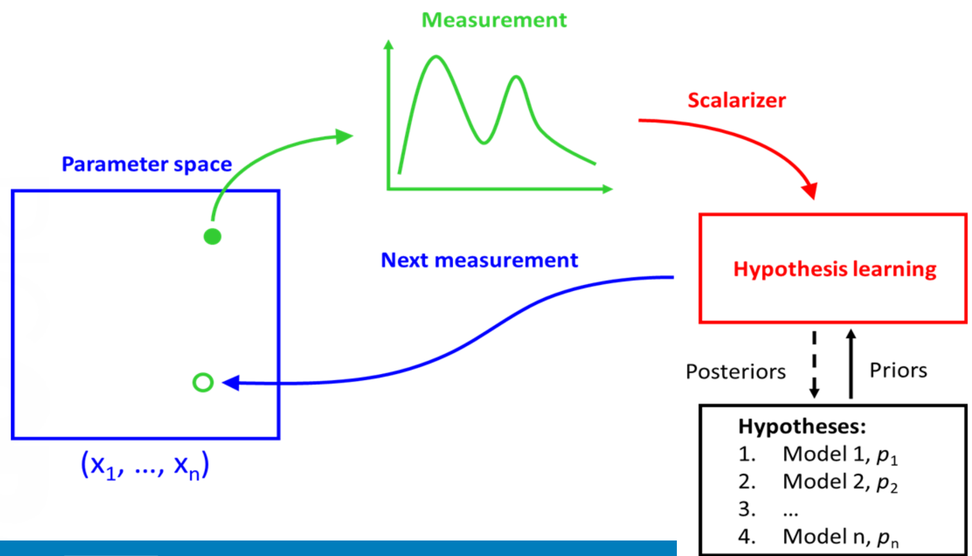
Material Discovery with AE-SPM

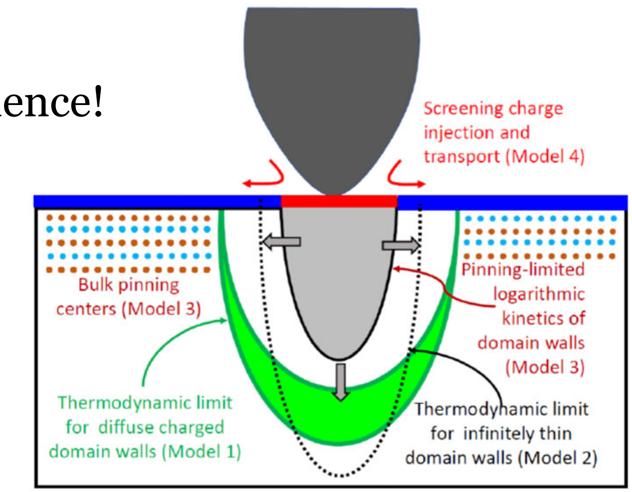


Reward: Physics Discovery

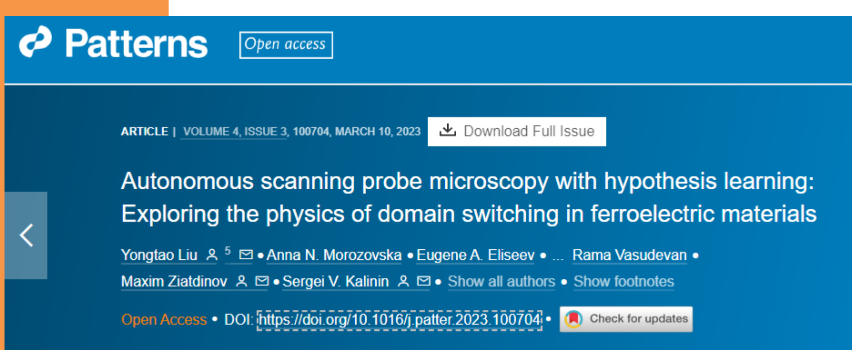
Hypothesis Learning

- Can ML algorithm think like a scientist?
- Yes – automated experiment can pursue hypothesis-driven science!





		Model Equation
Thermodynamic 1	**Model I**	$r(V) = r_{cr} + r_0\sqrt{\left(\frac{V}{V_c}\right)^{2/3} - 1}$
Thermodynamic 2	**Model II**	$r(V) = r_{cr} + r_0\sqrt[3]{\left(\frac{V}{V_c}\right)^{2} - 1}$
Wall pinning	**Model III**	$r(V,t) = V^{\alpha}\log\tau$
Charge injection	**Model IV**	$r(V,t) = V^{\alpha}\tau^{\beta}$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Autonomous scanning probe microscopy with hypothesis learning: Exploring the physics of domain switching in ferroelectric materials

Yongtao Liu • Anna N. Morozovska • Eugene A. Eliseev • ... Rama Vasudevan • Maxim Ziatdinov • Sergei V. Kalinin • Show all authors • Show footnotes

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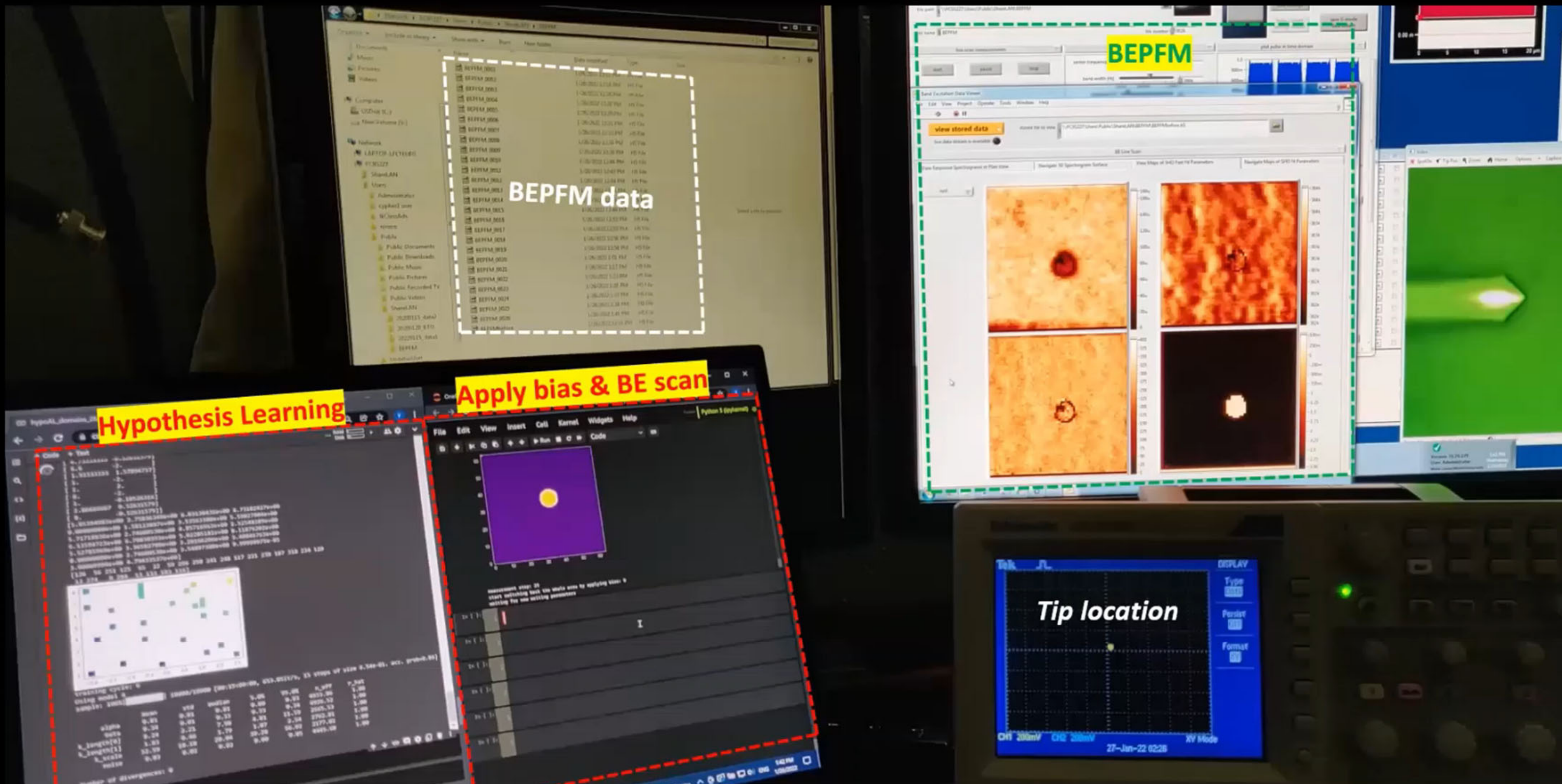
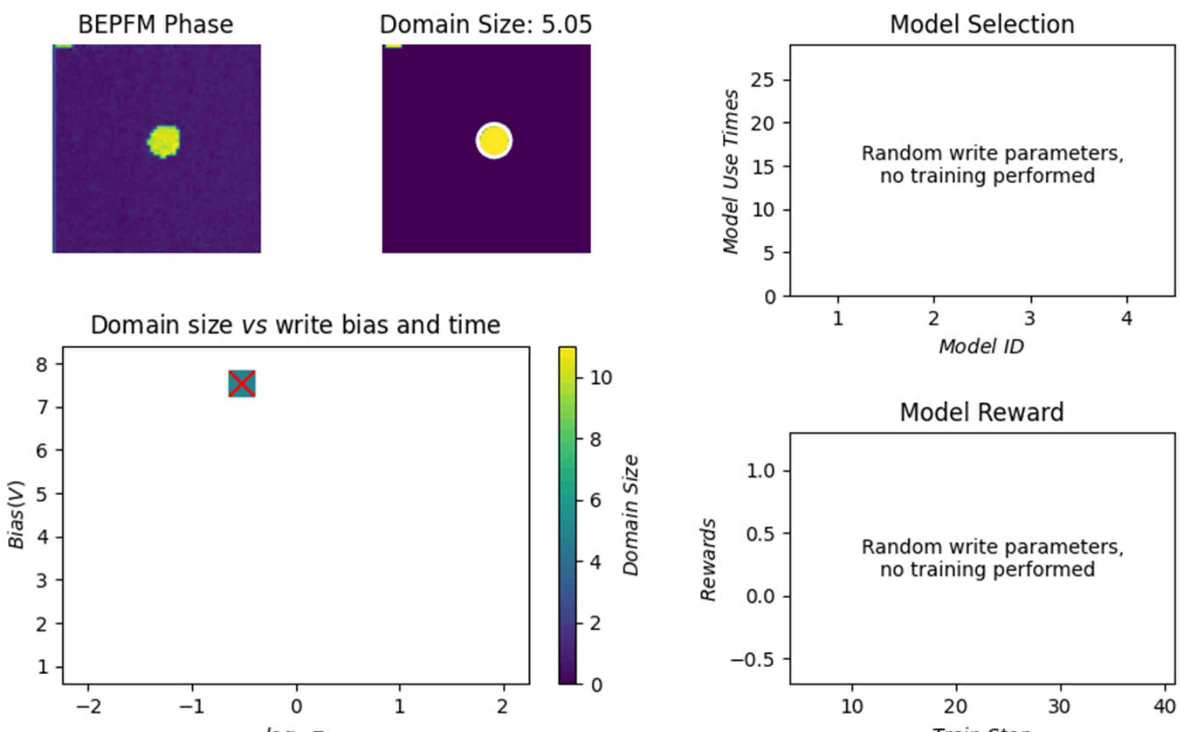

BEPFM data
BEPFM
Hypothesis Learning
Apply bias & BE scan
Tip location

Hypothesis learning in action



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Autonomous scanning probe microscopy with hypothesis learning: Exploring the physics of domain switching in ferroelectric materials

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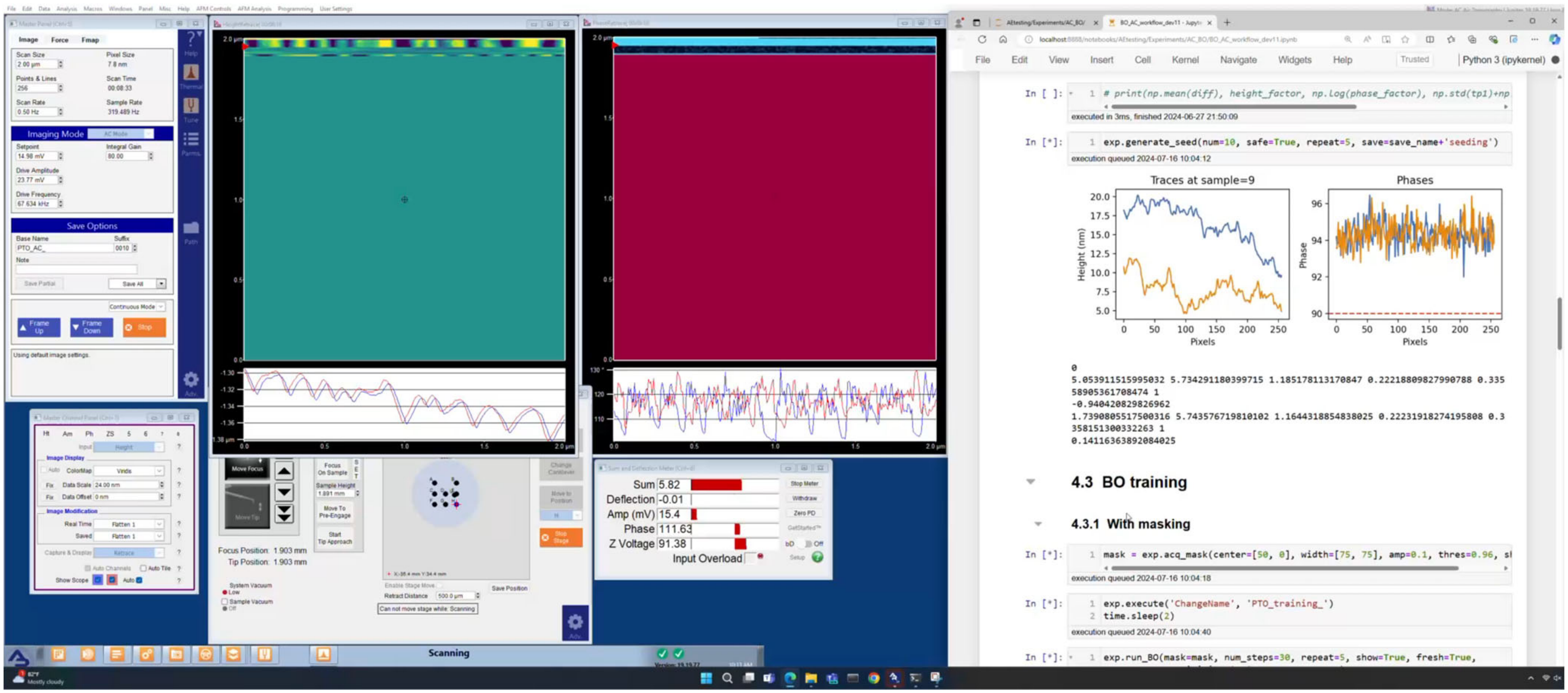
- ML algorithm has 4 competing hypothesis on domain switching mechanisms
- These hypothesis represent full set of possibilities for this system
- The microscope chooses experimental parameters in such a way as to establish which hypothesis is correct fastest
- Important: the same approach can be implemented in synthesis and electrical characterization
- Machine learning meets hypothesis-driven scientific discovery!

Reward: Image Optimization

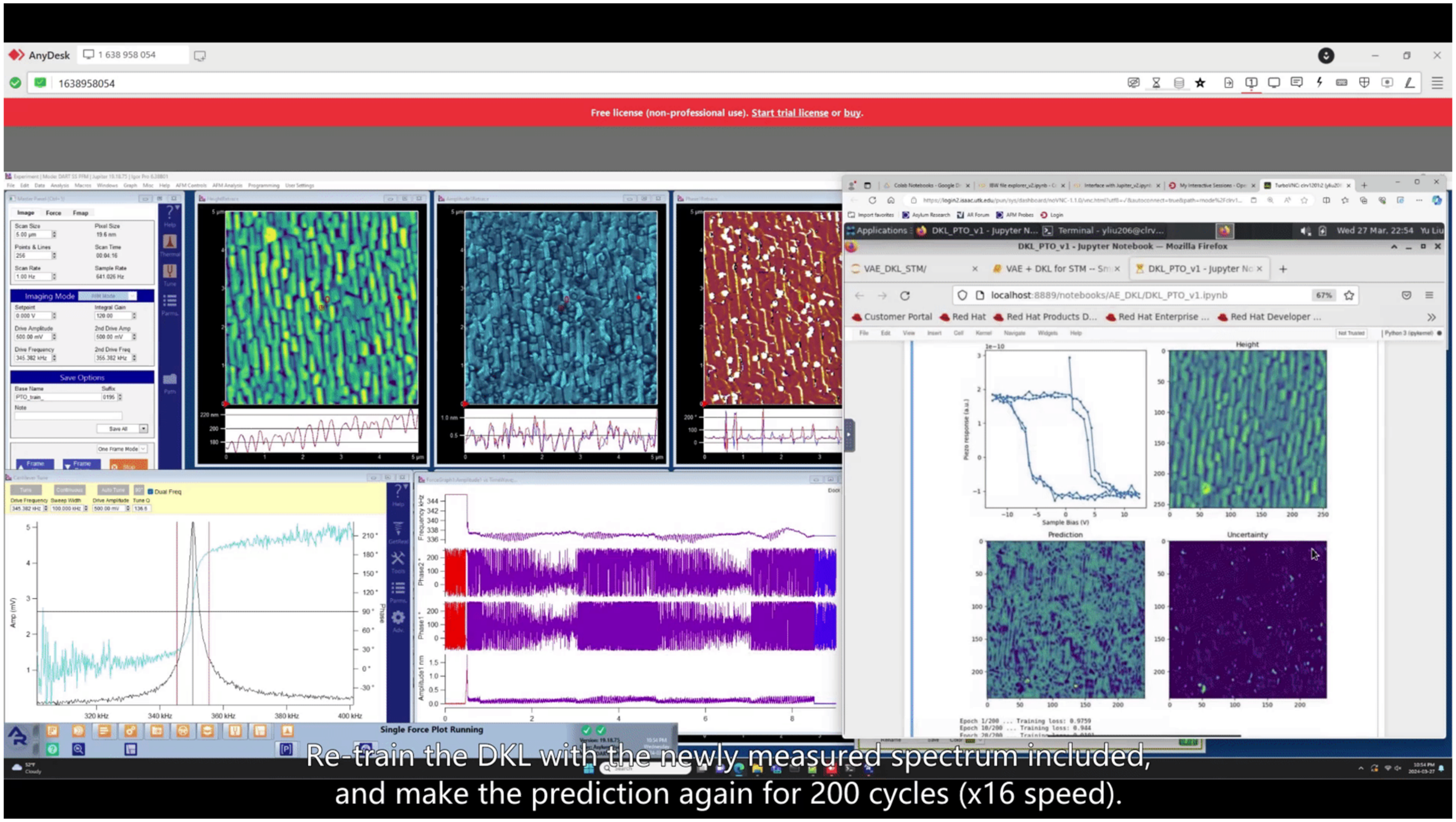
Automated Tuning of SPM



THE UNIVERSITY of TENNESSEE KNOXVILLE

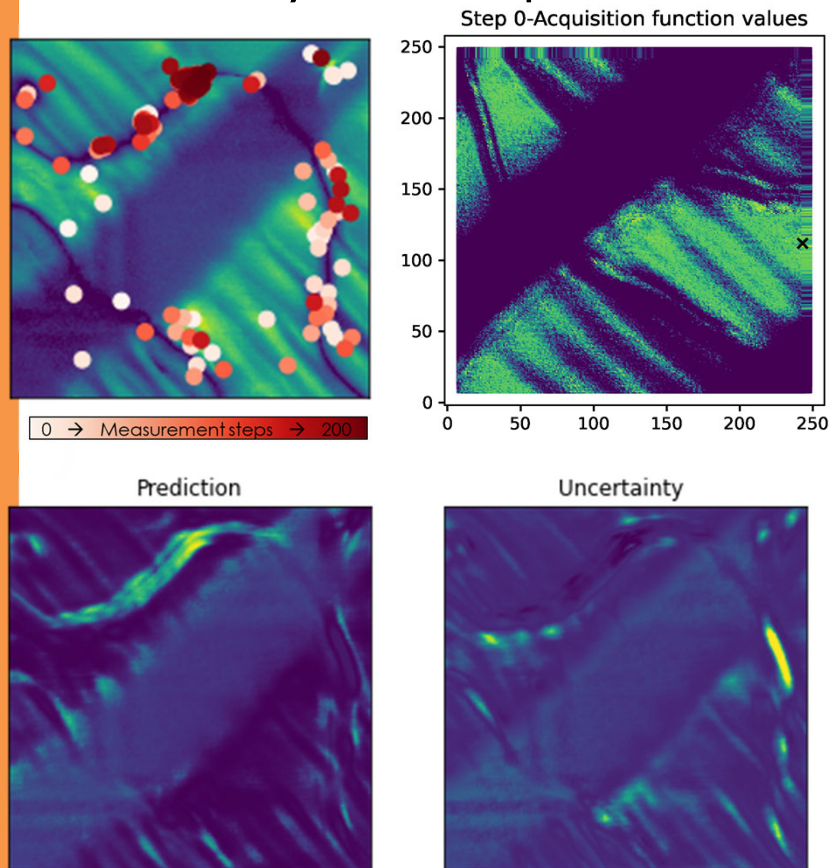
Reward: Structure-Property Discovery

Material Discovery with AE-SPM

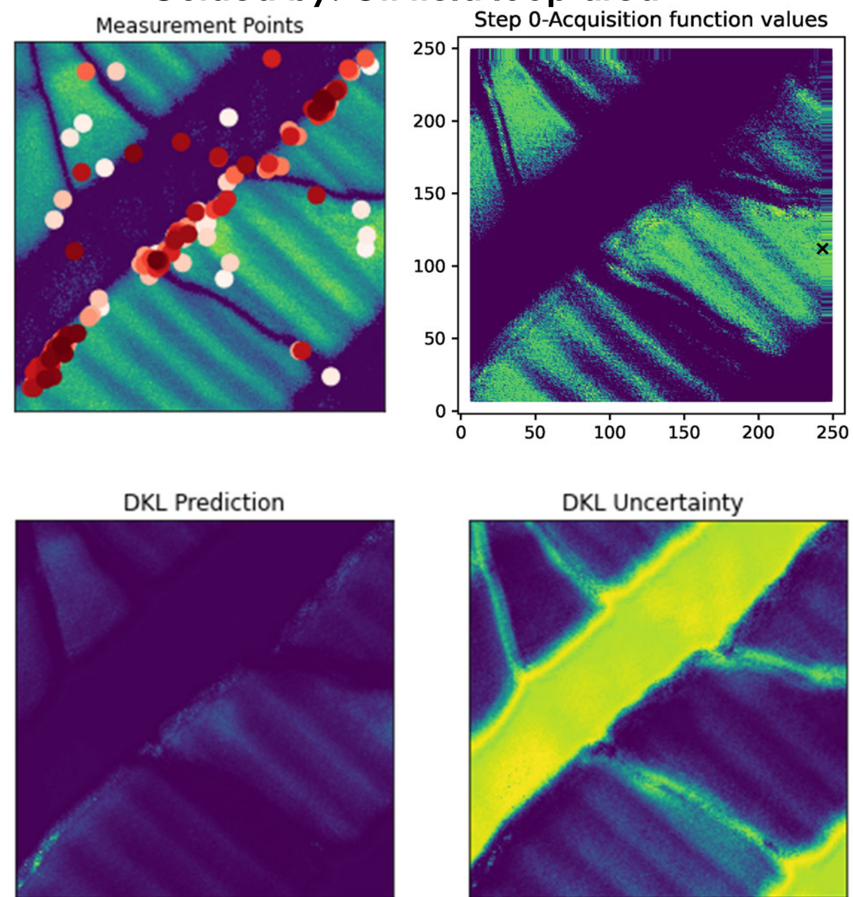


Deep Kernel Learning SPM

Guided by: On field loop area



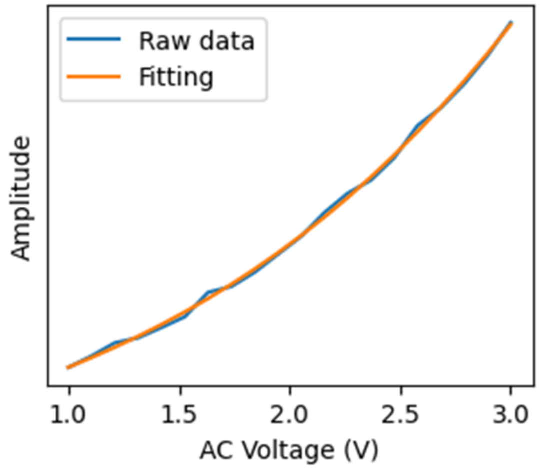
Guided by: Off field loop area

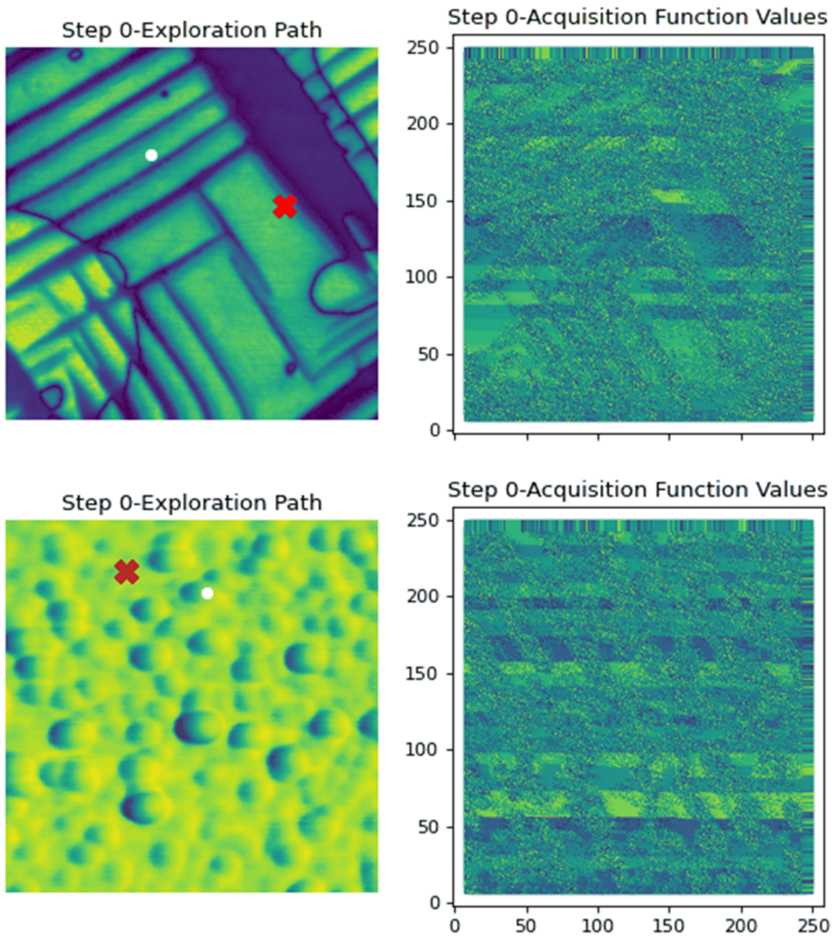


- ➢ Large loop opening corresponding 180^o domain walls
- ➢ This behavior can be attributed to the large polarization mobility of 180^o walls

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

Why human in the loop?



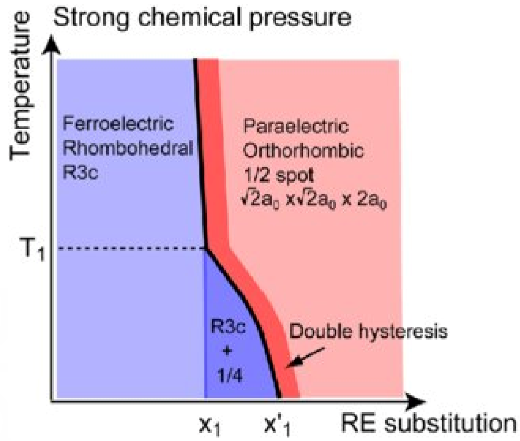


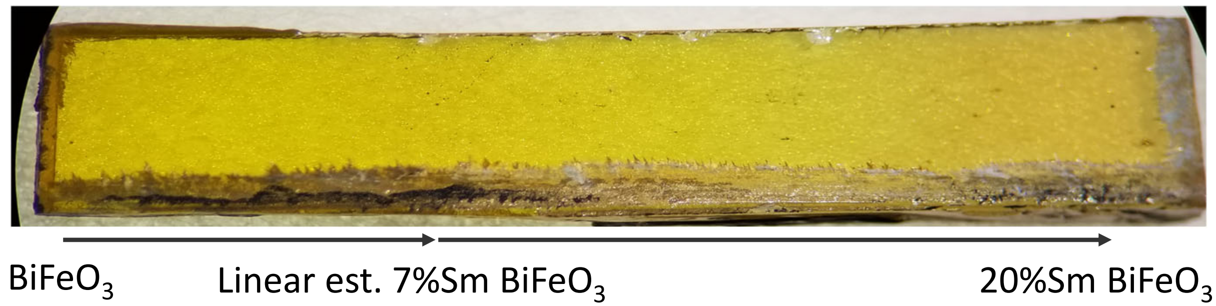
- 200-step automated experiment
- PFM amplitude was used as structure ima
- V_{AC} sweep curve at each location was fitte
  $y = Ax^3 + Bx^2 + Cx$
- A, B, C, and A/B were used as the target function to guide DKL-V_{AC} measurement.

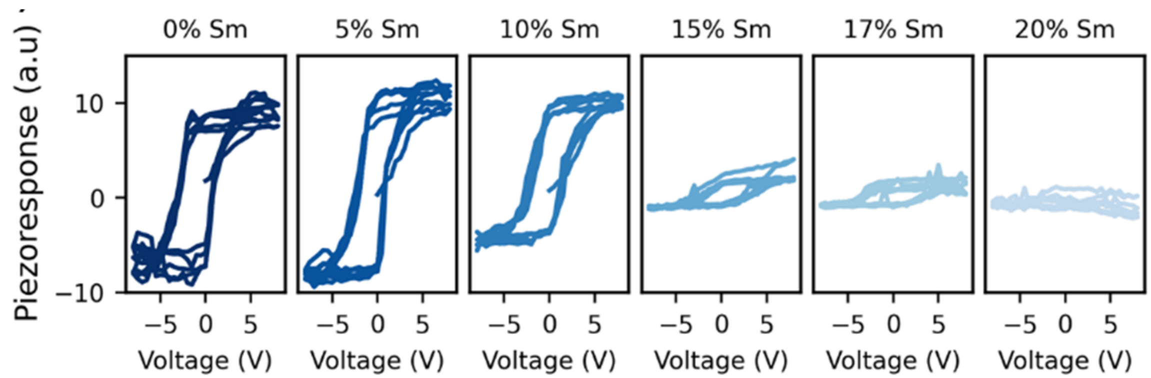
The methodologies of classical ML (hyperparameter optimization, cross-validation) are rarely applicable for active learning!

Reward: Materials Optimization

Combinatorial Library



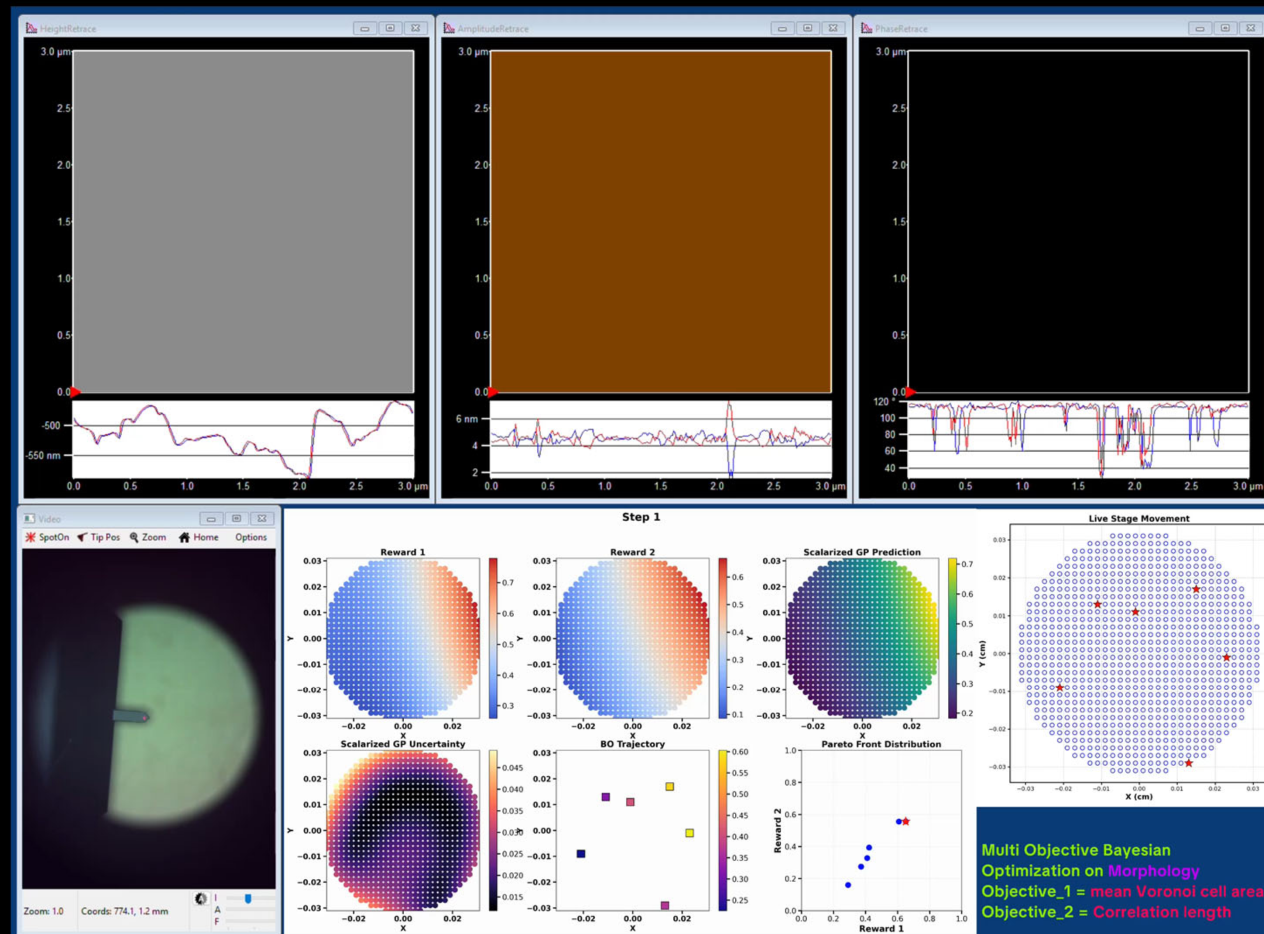




Exploration target

- Minimize the uncertainty in the composition – loop height relation
- Find the composition that gives the largest/smallest loop height


OXFORD INSTRUMENTS
Jupiter XR
Asylum Research AFM
High Voltage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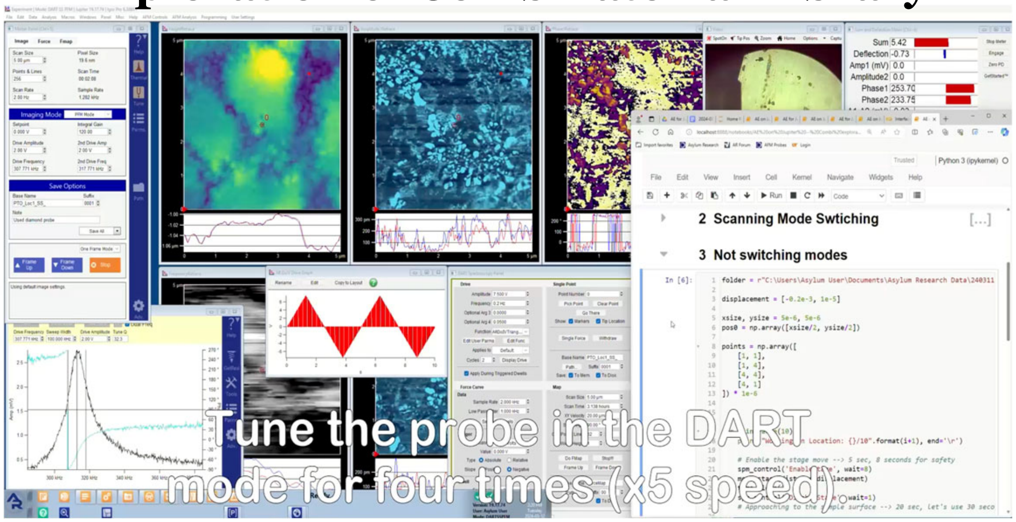
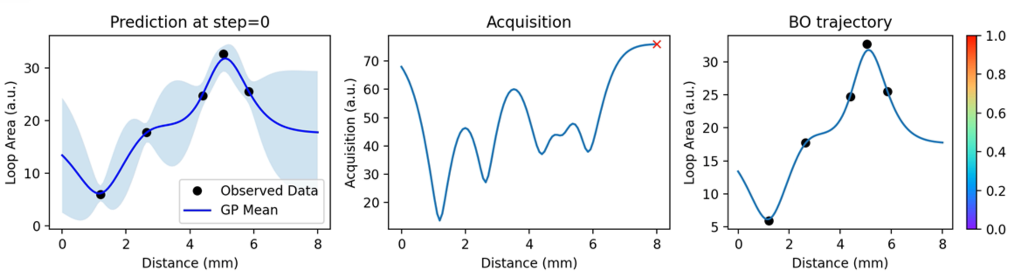
Reward 1
Reward 2
Scalarized GP Prediction
Scalarized GP Uncertainty
BO Trajectory
Pareto Front Distribution
Live Stage Movement
Multi Objective Bayesian
Optimization on Morphology
Objective_1 = mean Voronoi cell area
Objective_2 = Correlation length

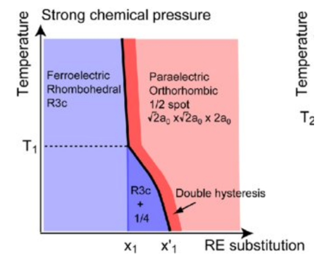
Combinatorial Library Exploration

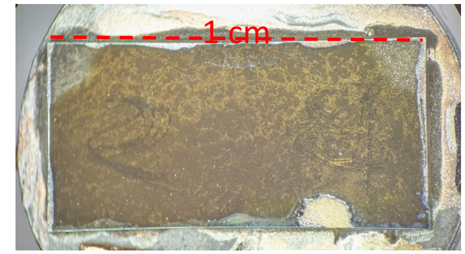
Exploration of Combinatorial Library



Each point is experimental measurement







Automated multiple steps of microscope operation:

- Reward based optimization of imaging conditions
- Reward-based optimization of ferroelectric hysteresis loop measurements
- Exploration of combinatorial libraries (large-scale stage motion)
- Identification of real space features and spectroscopy of selected locations
- **All integrated into ML-driven multistep automated experiments**

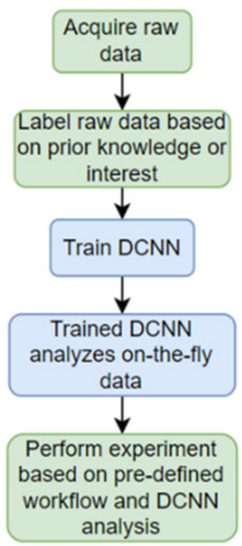
Combinatorial library of Sm-BFO

- Phase transition from ferroelectric to non-ferroelectric endmember
- Morphotropic phase boundary
- Simple and structured Gaussian Process with constant, measured, and heteroscedastic noise

Summary: Workflow Building Blocks

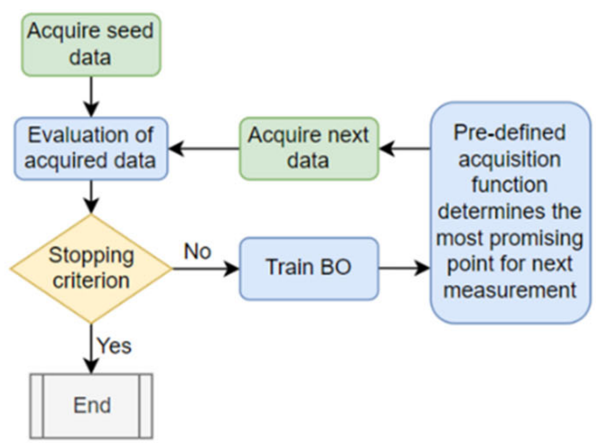
Types of automated experiment

Direct



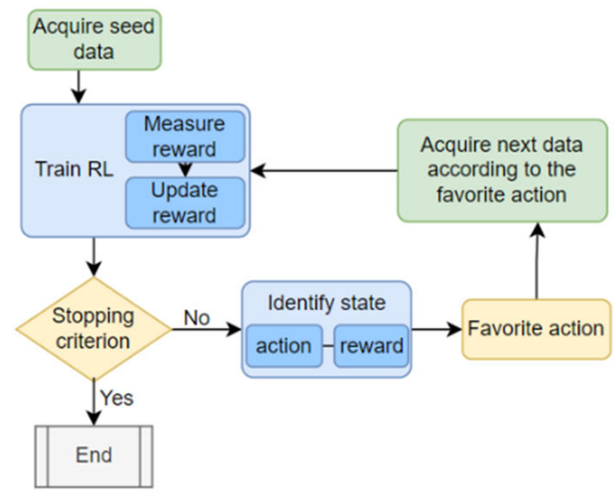
- Fixed policies
- Need DCNNs stable wrt. out of distribution shift

Myopic discovery



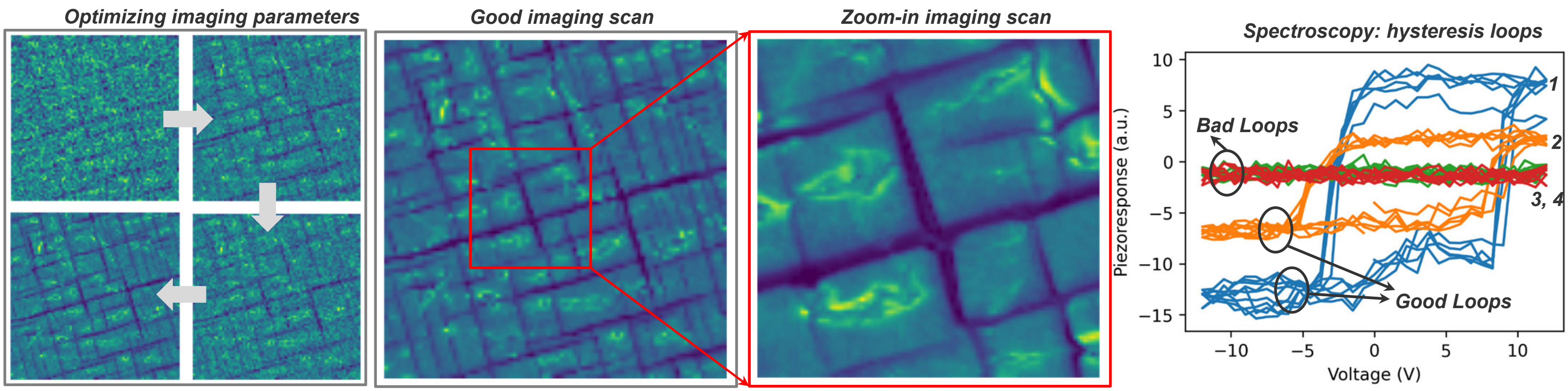
- Adjustable policies
- One step planning
- Can be implemented via Bayesian workflows
- Can be human in the loop

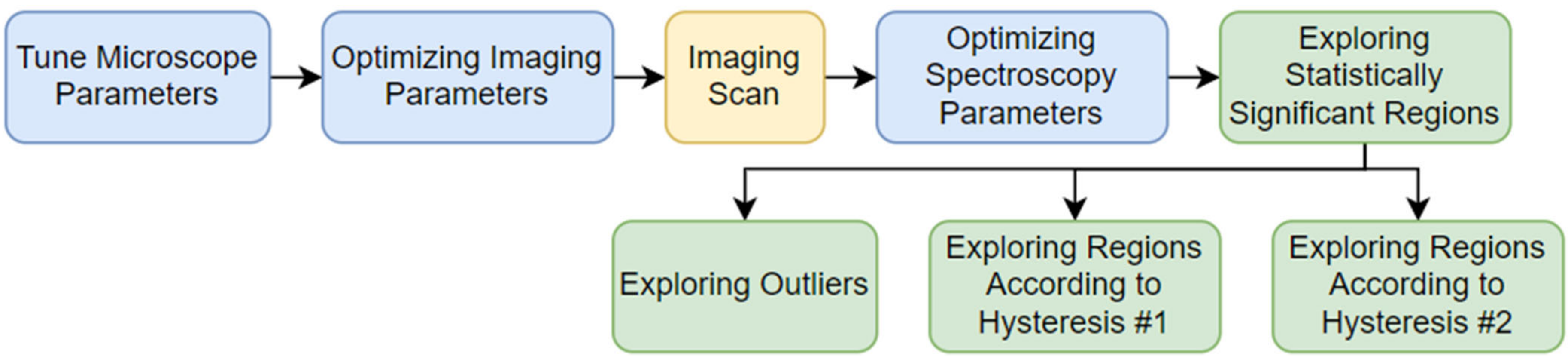
Multistage discovery



- Adjustable policies
- Multi-step planning
- Requires heuristic to start
- Requires **reward function**

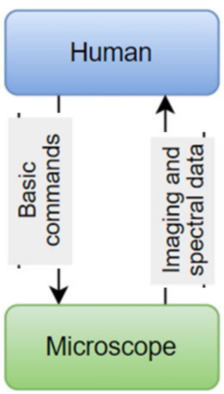
Future: full workflow optimization



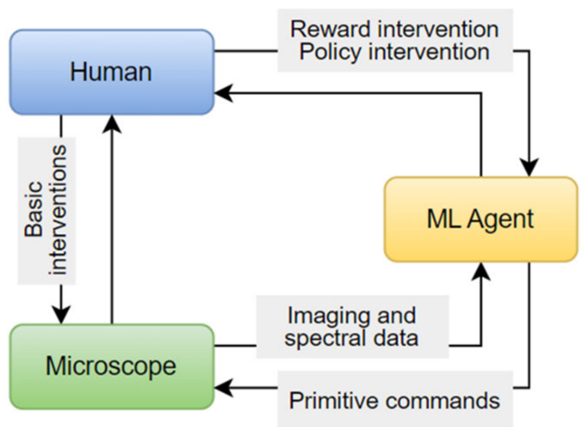


Human in the loop AE

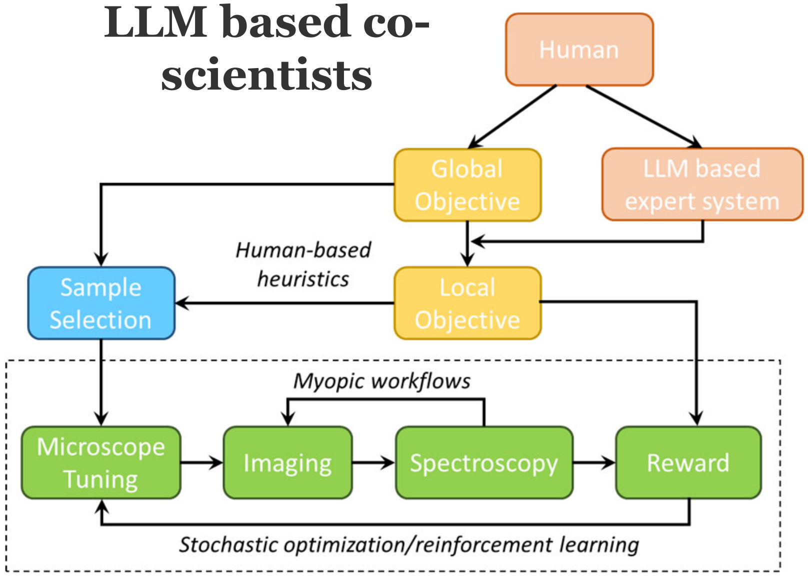
Current generation of tools



The tools we are building



LLM based co-scientists



We can intervene on:

- Policies (acquisition functions)
- Scalarizers (physics descriptors)
- Moving on Pareto fronts for rewards
- Knowledge injection
- Direct operation

From ML to co-Scientists:

- Probabilistic reward functions
- Community of experts
- Theory in the loop

From One to Many

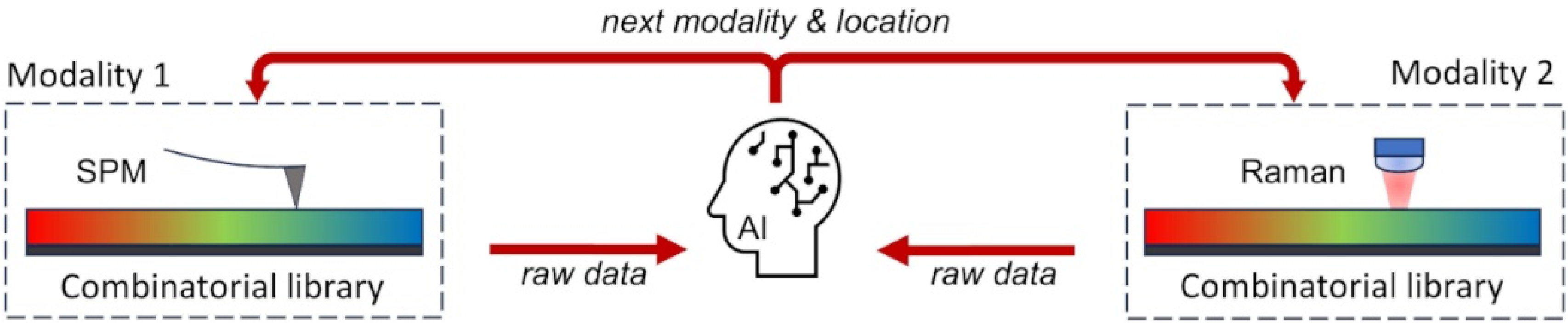
Four eras of automated labs

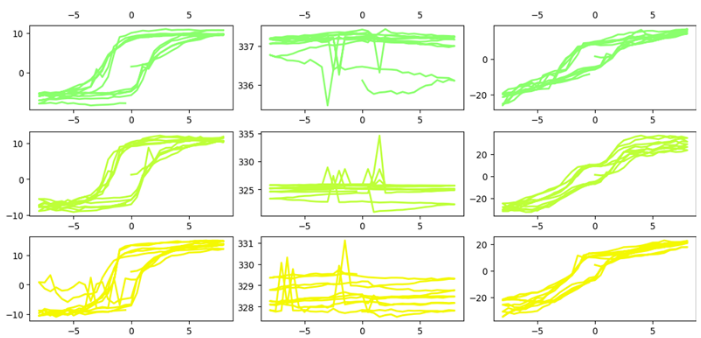
- **Before 2015:** Small number of enthusiasts in academic community, industry efforts
- **2015 - 2020:** Engineering developments
- **2020 – 2025:** Broad adoption of the commercial tools, modification of commercial platforms
- **2025 :** Workflows design?

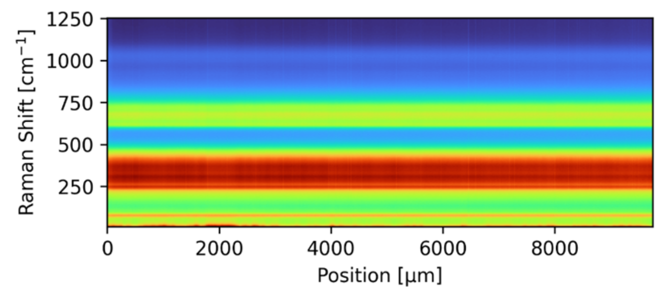
Elements of realistic workflow design

- Co-orchestration of multiple measurement modalities
- Building theory in the loop
- Integration between multiple domains

From one (scalar) to many (vectors)



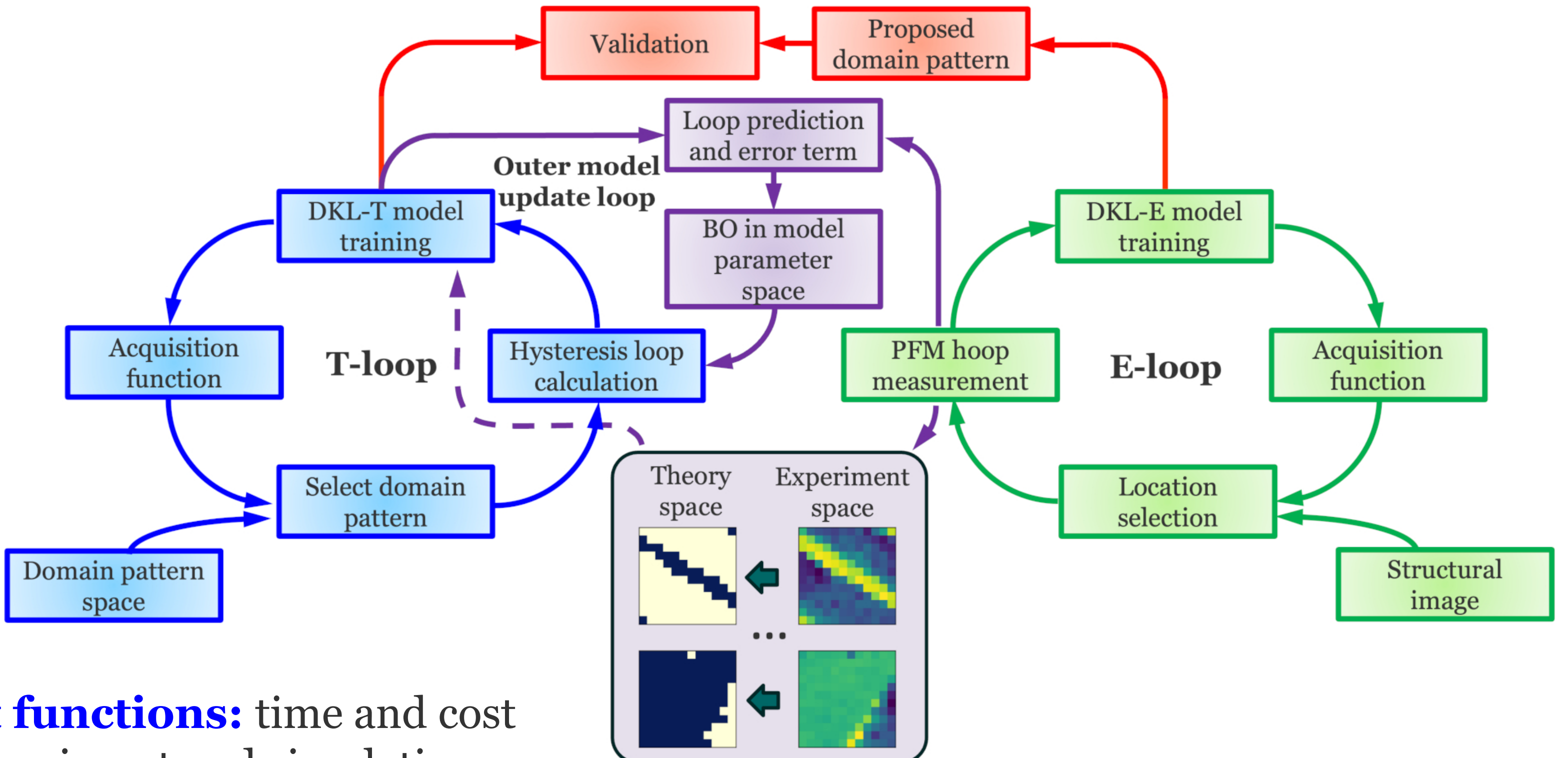




- Characterization data is usually high-D (images and spectra)
- How can we co-orchestrate the operation of several characterization tools
- And access the gains?

Building Active Digital Twins

- Continuous training of the surrogate model for theory (T-loop)
- Co-training surrogate model for experiment (E-loop)
- Theory update based on error function over support of interest (Outer theory update loop)



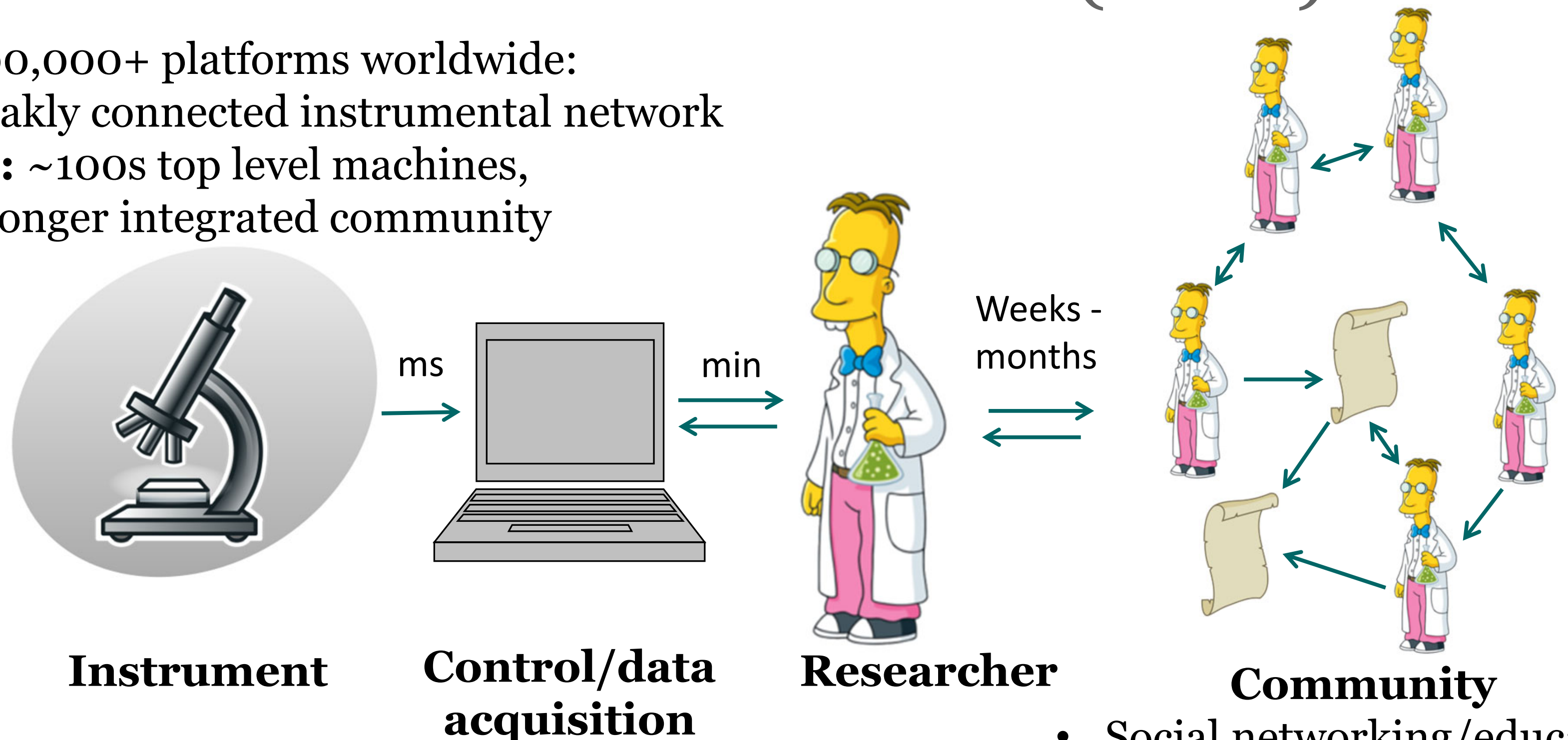
- **Cost functions:** time and cost of experiment and simulation
- **Gain:** predictive uncertainty

https://arxiv.org/abs/2404.12899

The Time of Integration

Classical Instrumental Research (2016)

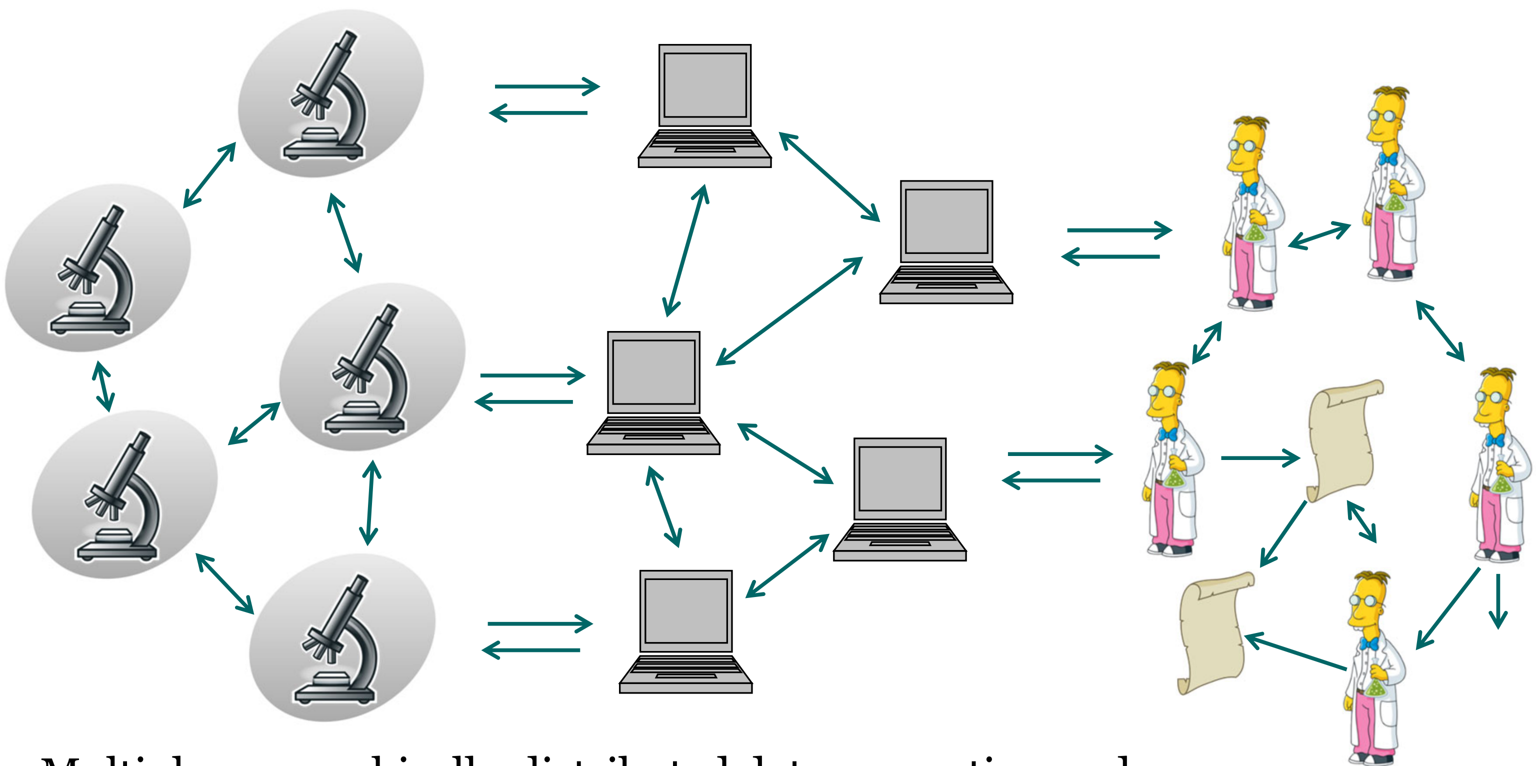
SPM: 100,000+ platforms worldwide:
Large weakly connected instrumental network
(S)TEM: ~100s top level machines,
much stronger integrated community



- Social networking/education
- Publications/citations

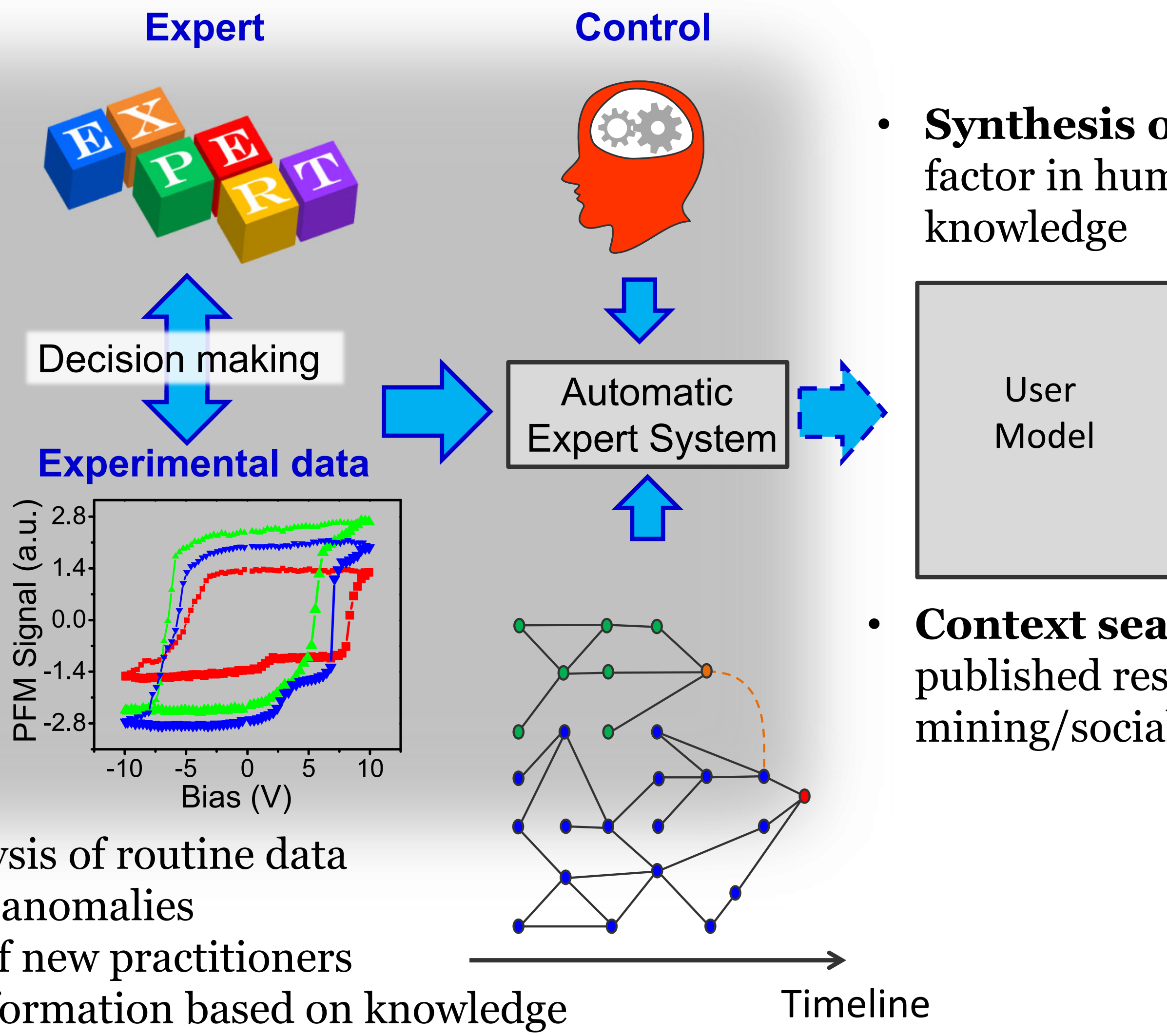
1. Only small fraction of data stream from the instrumentation is captured
2. Only small fraction of captured data is analyzed, interpreted, and put in the context
3. Human-machine interaction during acquisition is often slow and can be non-optimal
4. Human interpretation of data is limited: bias and ignoring serendipity
5. Information propagation and concept evolution in scientific community is slow

Step 1: Cloud Integration (2016)



1. Multiple geographically-distributed data generation node
2. Full capture of instrumental data stream /compression/curation
3. Coordination of protocols and data/metadata across the cloud
4. Cloud-based processing and dimensionality reduction
5. Community-wide analytics

Step 2: Cloud Analytics (2016)

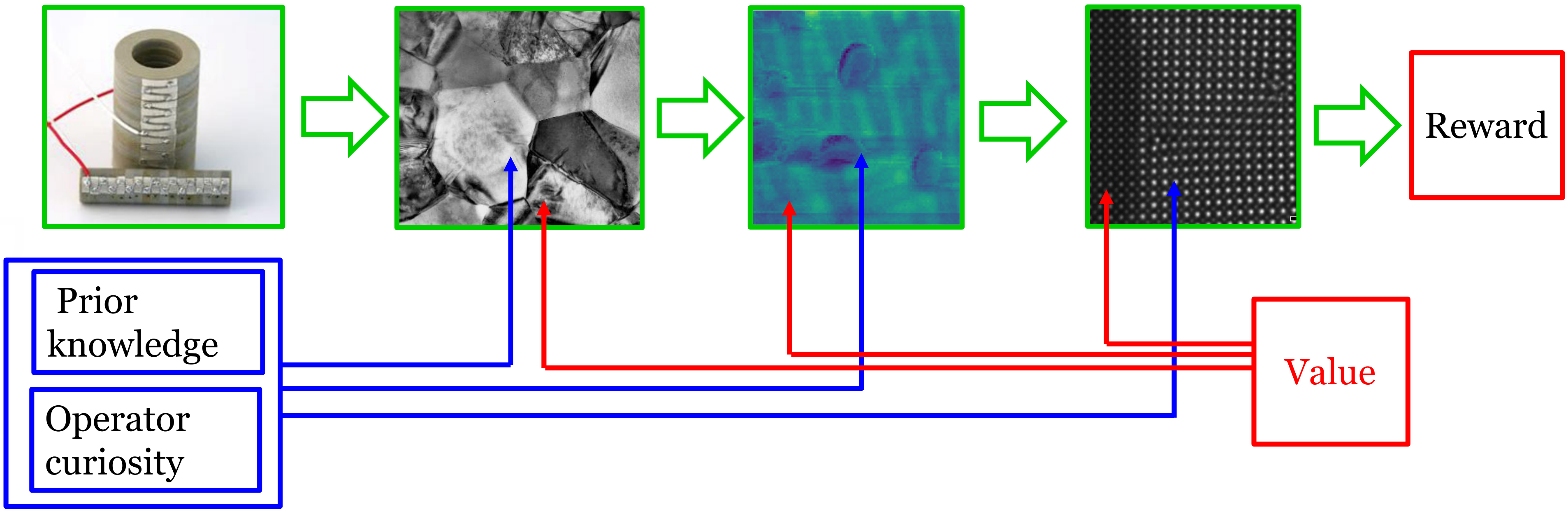


- **Synthesis of expertise:** factor in human expert knowledge
- **Context search:** published results data mining/social networks

Future:

- Automated analysis of routine data
- Identification of anomalies
- Initial training of new practitioners
- Data centers: information based on knowledge

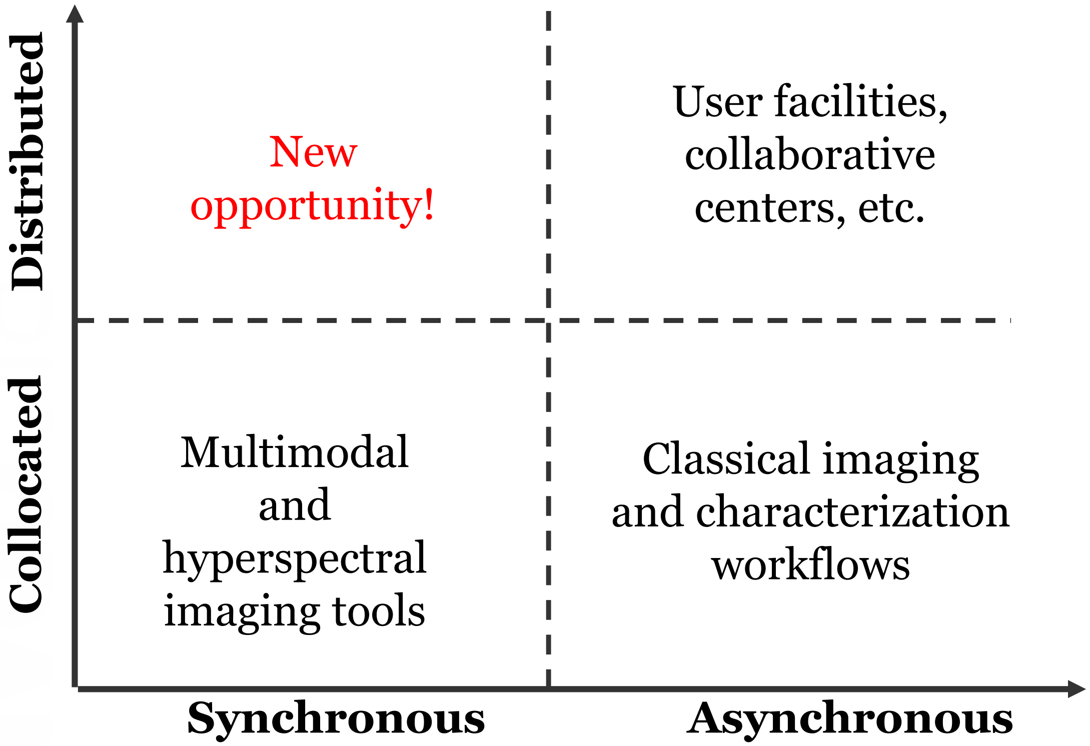
Step 3: Workflow Design (2022)



Traditional experiment:
1. Always based on workflows
2. Ideated, orchestrated, and implemented by humans
3. The "gain of value" during the workflow implementation is uncertain

Value of the step is key element:
- Either based on prior knowledge
- Or defined in a sense of the reinforcement learning Q-function

Cloud Labs: Facilities of the Future



Emerald Cloud Lab, SF and CMU

1. Combined human-machine workflow implementation
2. Computer orchestrating agent
3. How would beyond human workflows be ideated?

Reward Driven Workflow Design

1. Development of the labs capable of orchestrating predefined workflows based on human and robotic agents.

2. Workflow design based on AI and human decision making, meaning specific series of synthesis and characterization steps described via executable hyperlanguage.

3. Defining domain-specific reward functions. Why are we running experiments? Ultimately, we need to quantify (in the style of Bell's equation) what is the benefit of the specific step in the workflow, and how does it accomplish or affects exploration and exploitation goals.

4. Integration of reward functions from dissimilar domains. For example, how does better microscope help us learn physics of specific material? Why would the specific DFT calculation help us understand experimental data?

5. Creating experimentally falsifiable hypothesis from the domain specific body of knowledge that can be incorporated in the exploratory part of automated workflows.

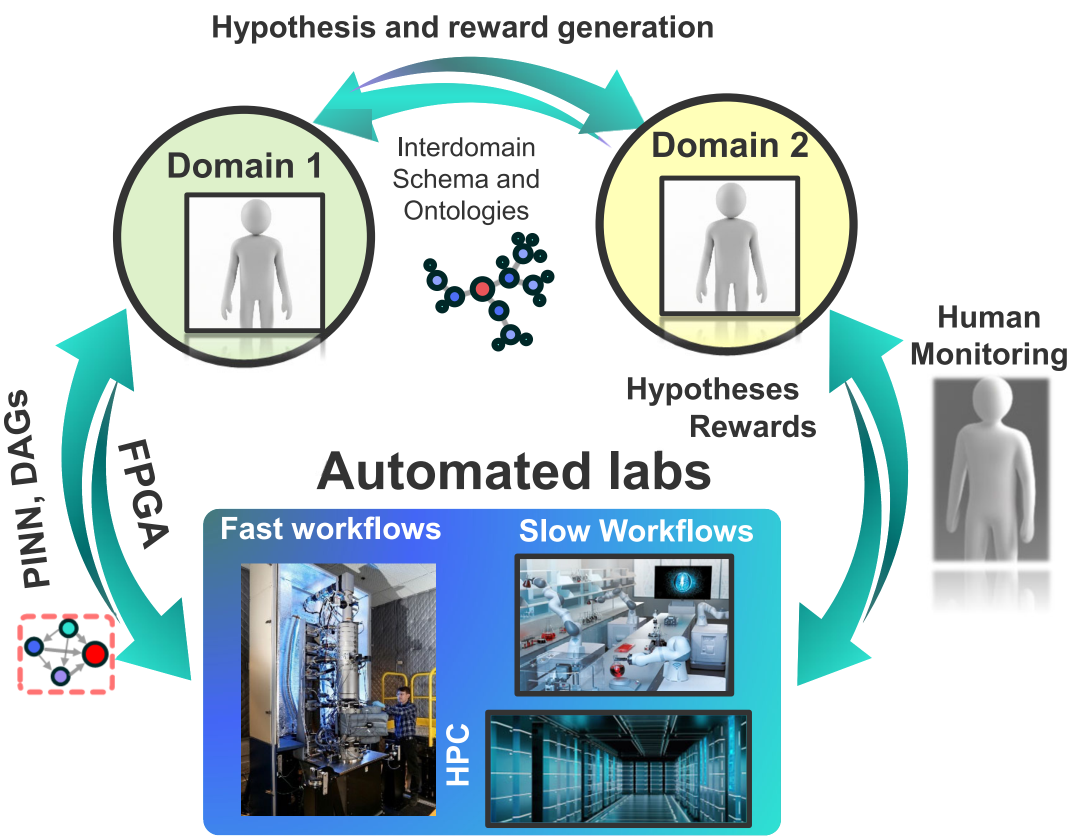
6. Hypothesis generation beyond human (an AGI question).

Integration across human domains

Simple GP-BO, structured GP with probabilistic physical models, and multifidelity GP can be used for fully autonomous workflows and account for real times/costs of experiments.

Multi-task GP-BO, multifidelity sGP-BO, and more complex methods require human intervention:

- **All metods:** reward and objective functions
- **Interactive BO:** balanceof exploration-exploitation and strength of fidelity- and physics priors
- **Asymmetric MF BO:** belief in parameters, causal structure between observables
- **A* and Decision trees:** human heuristics for roll-outs
- **Experiment planning:** hypotheses making



Homo Ludens: Gamification of SDLs

- Collaborative Environment between humans and NPCs
- Role Specialization
- Quests and Objectives
- Dynamic Interaction and Adaptation:
- Skill and Experience Growth
- Real-time Decision
- Interactive World
- Automated Tasks and Challenges
- Resource Management
- Progress Tracking and Rewards