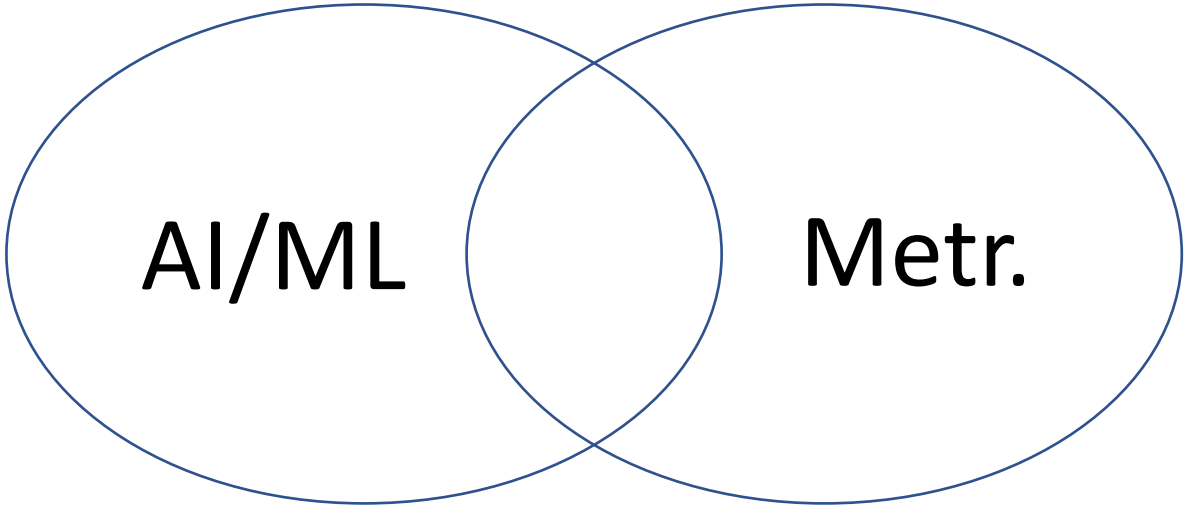
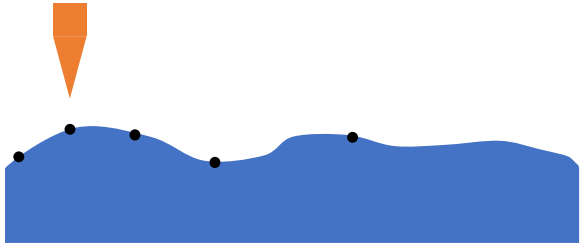
Autonomous Metrology

A. Gilad Kusne, aaron.kusne@nist.gov

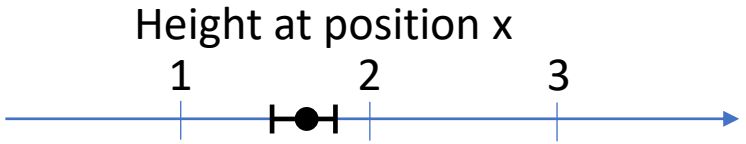
Autonomous Metrology



- Current Measurement:

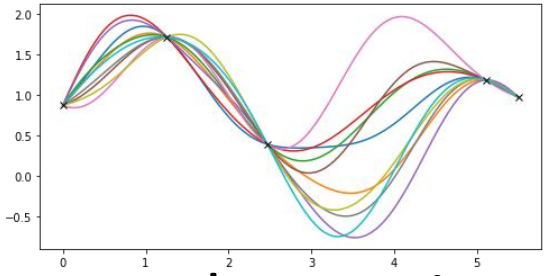


Measurand: Point value

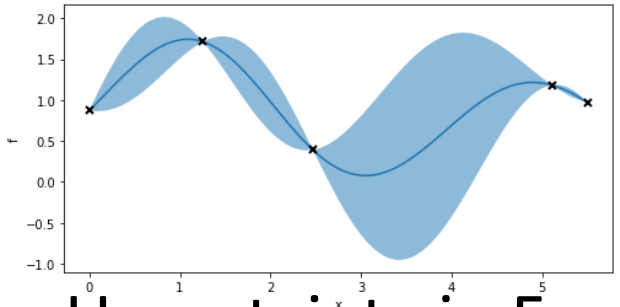


Uncertainty

- Autonomous Measurement

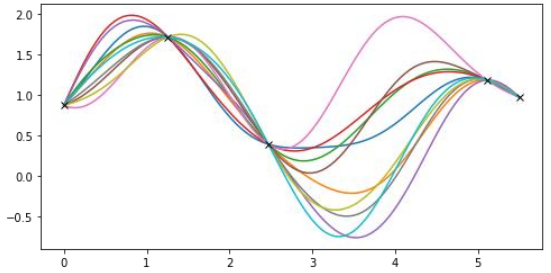


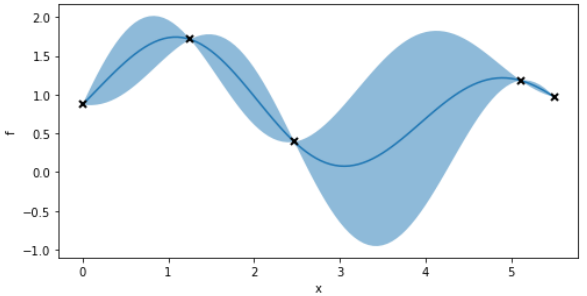
Measurand: Function



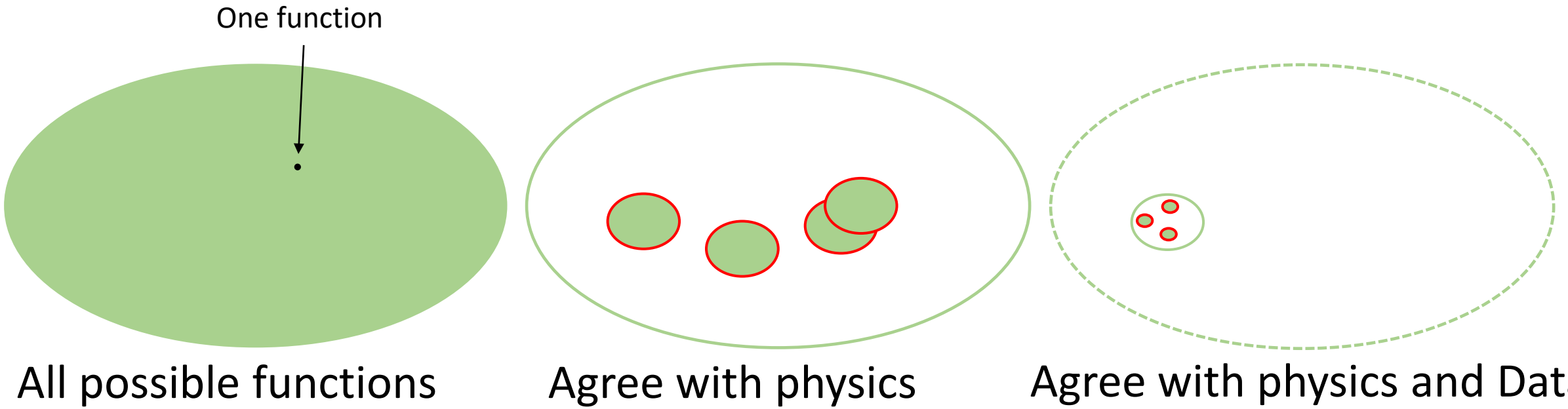
Uncertainty in Function

Physics-Informed

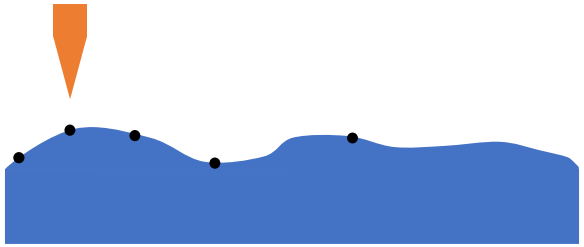




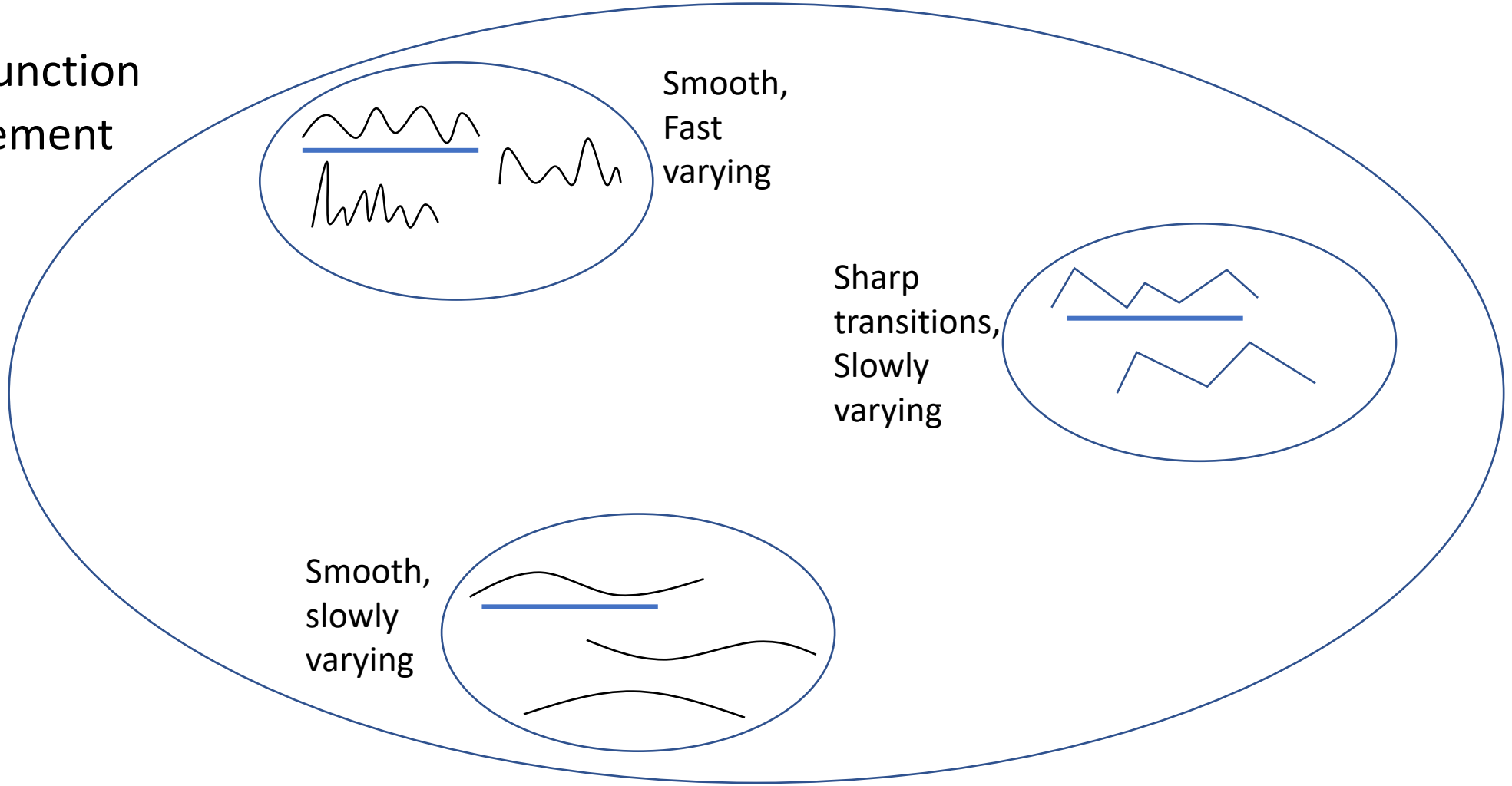
- Not all solutions are realistic
  - Physics of Measurement: e.g., Negative values
  - Physics of Target Function: e.g., Smoothness



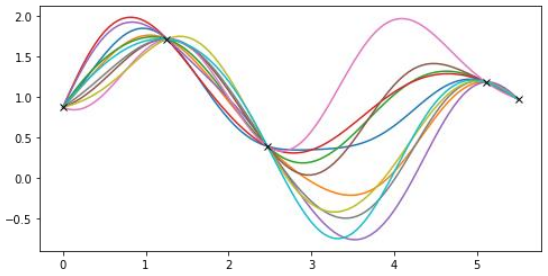
Example

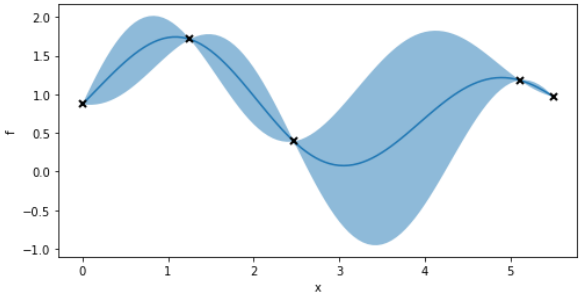


- Physics of:
  - Target Function
  - Measurement



Function vs **Hypotheses**





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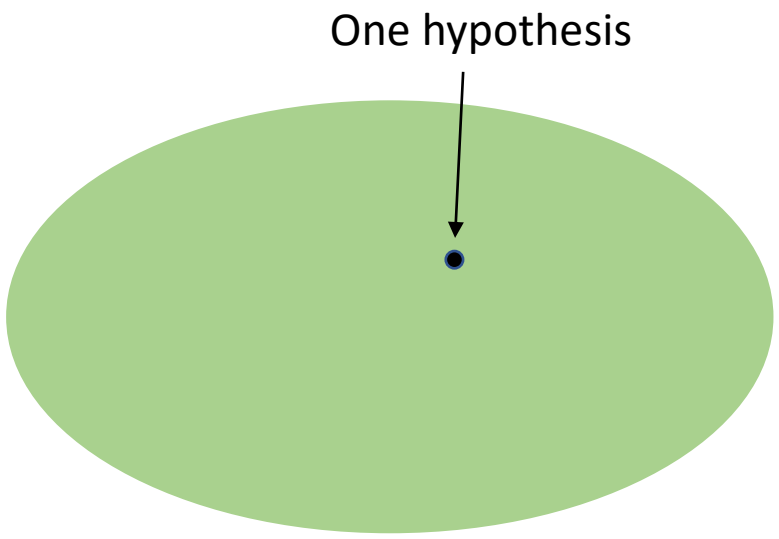
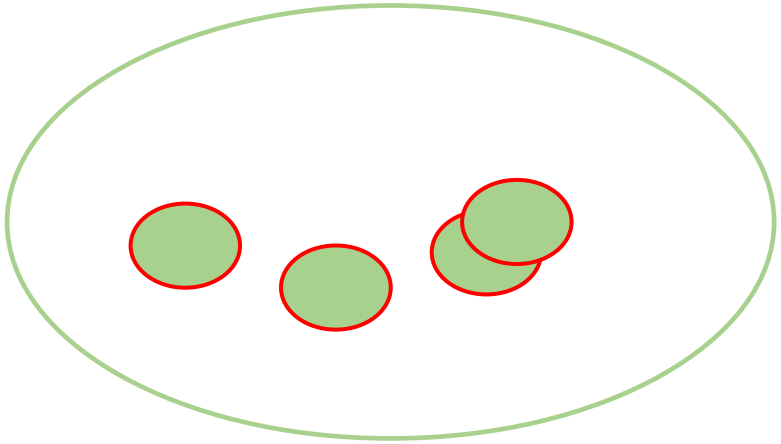
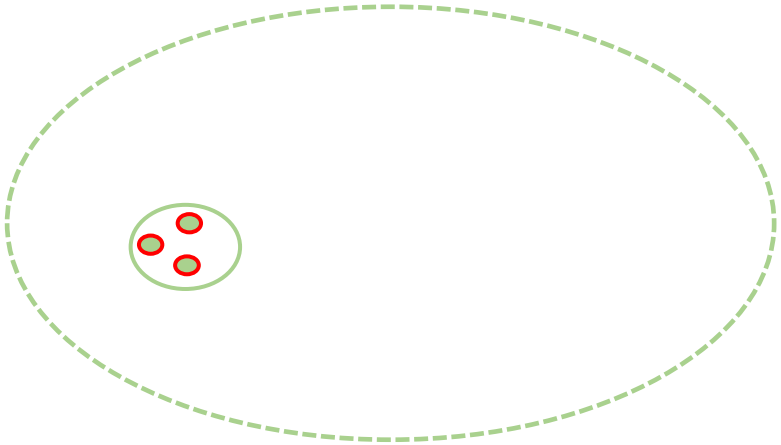


All possible hypotheses

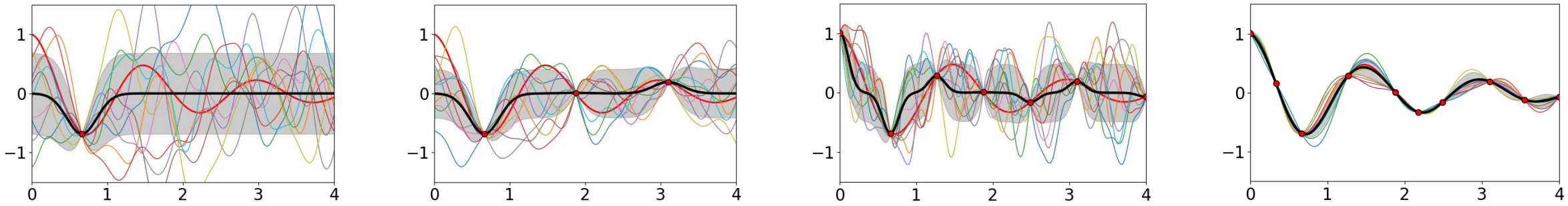


Agree with physics



Agree with physics and Data

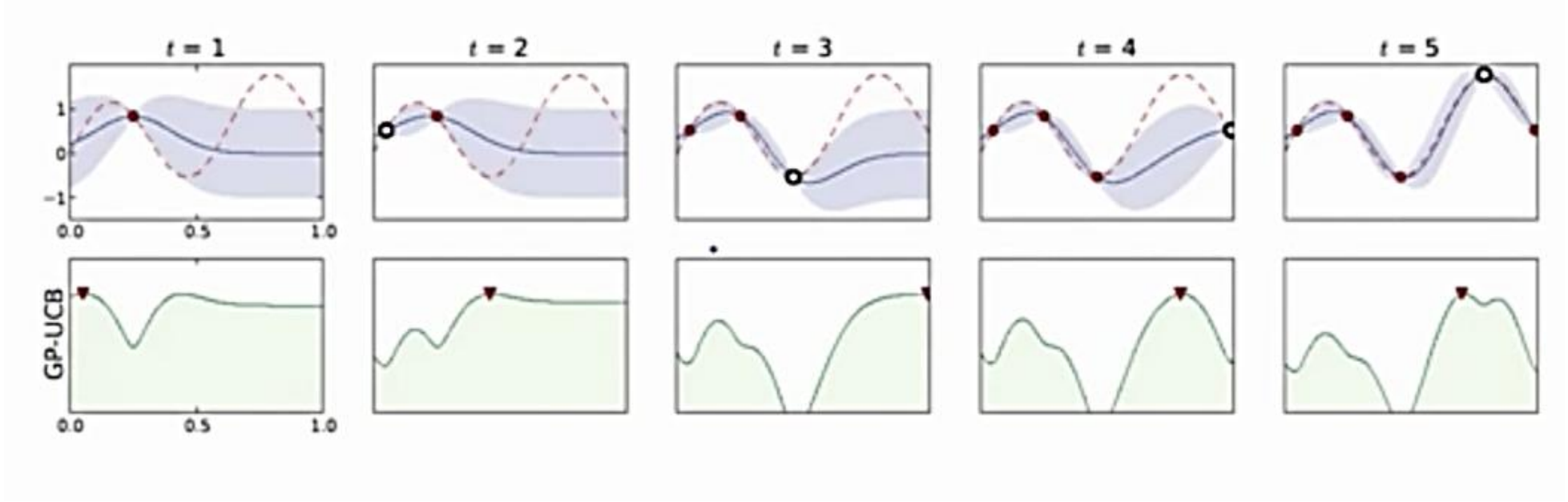
Active Learning



- Goal:
  - ~~Measure faster~~
  - Measure smarter! -> “Measure” the function/hypothesis
- Methods:
  - Point of greatest uncertainty
  - Look-ahead, e.g., risk minimization
  - etc.

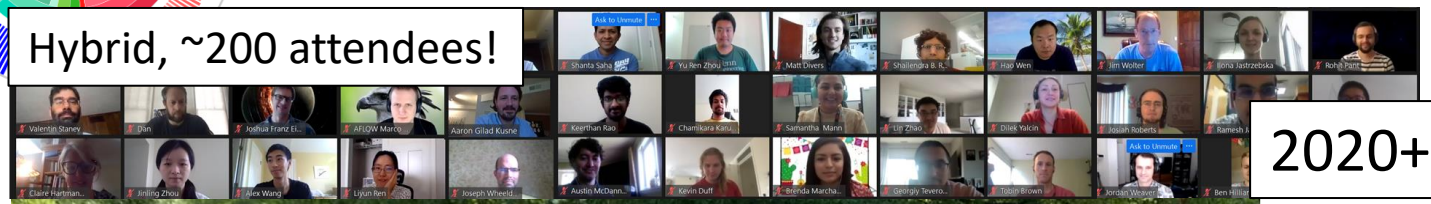
Bayesian Optimization

- Set an objective -> Find extrema.
- exploit Uncertainty to improve optimization

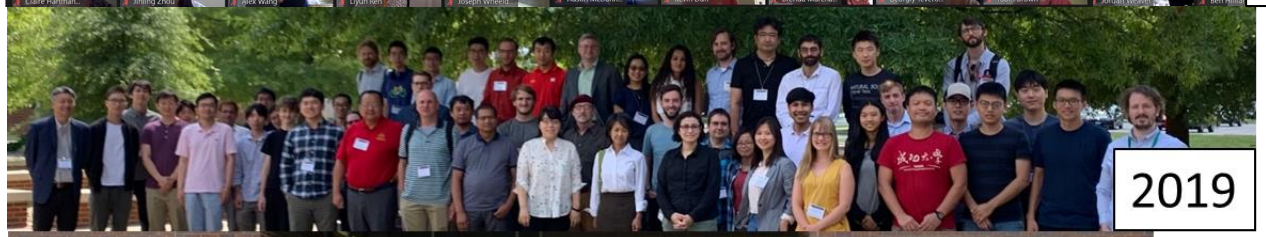


https://towardsdatascience.com/shallow-understanding-on-bayesian-optimization-324b6c1f7083

Annual Machine Learning for Materials Research Boot Camp and Workshop



Hybrid, ~200 attendees!



2019

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Introduce researchers from industry, national labs, and academia to ML theory and tools for rapid data analysis.

- 4 days of lectures and **hands-on** exercises (e.g. noise reduction, unsupervised and supervised techniques, computer vision, etc.) includes ML for robot science!

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https://www.nanocenter.umd.edu/events/mlmr/

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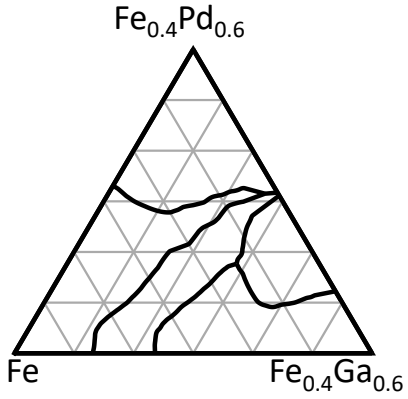
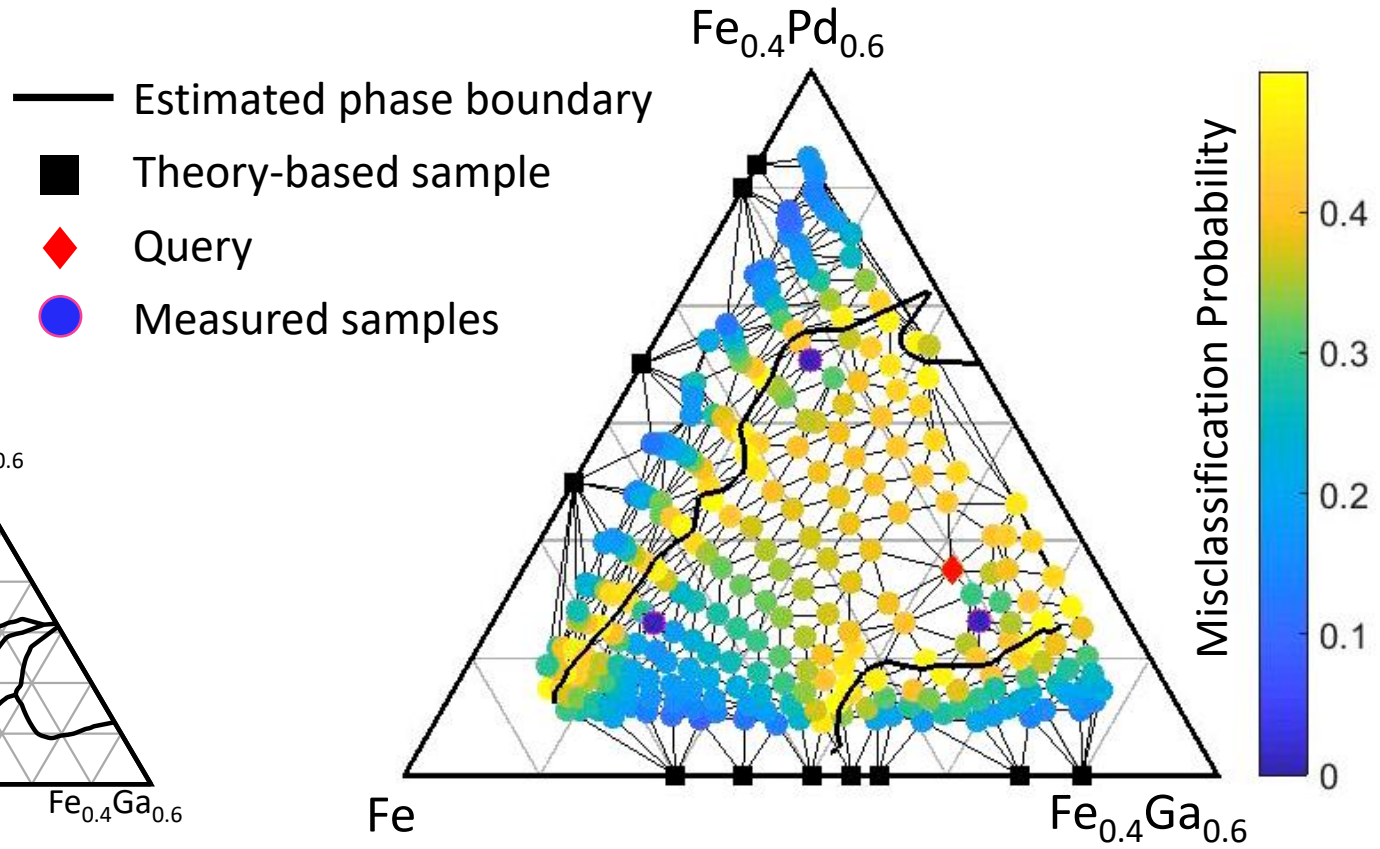
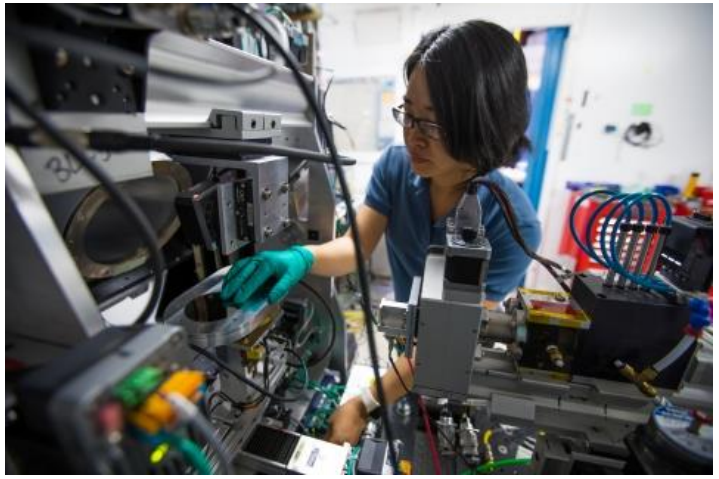
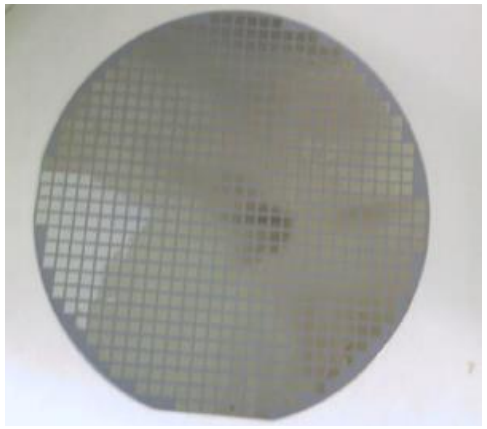
Examples @ NIST

Autonomous Phase Mapping



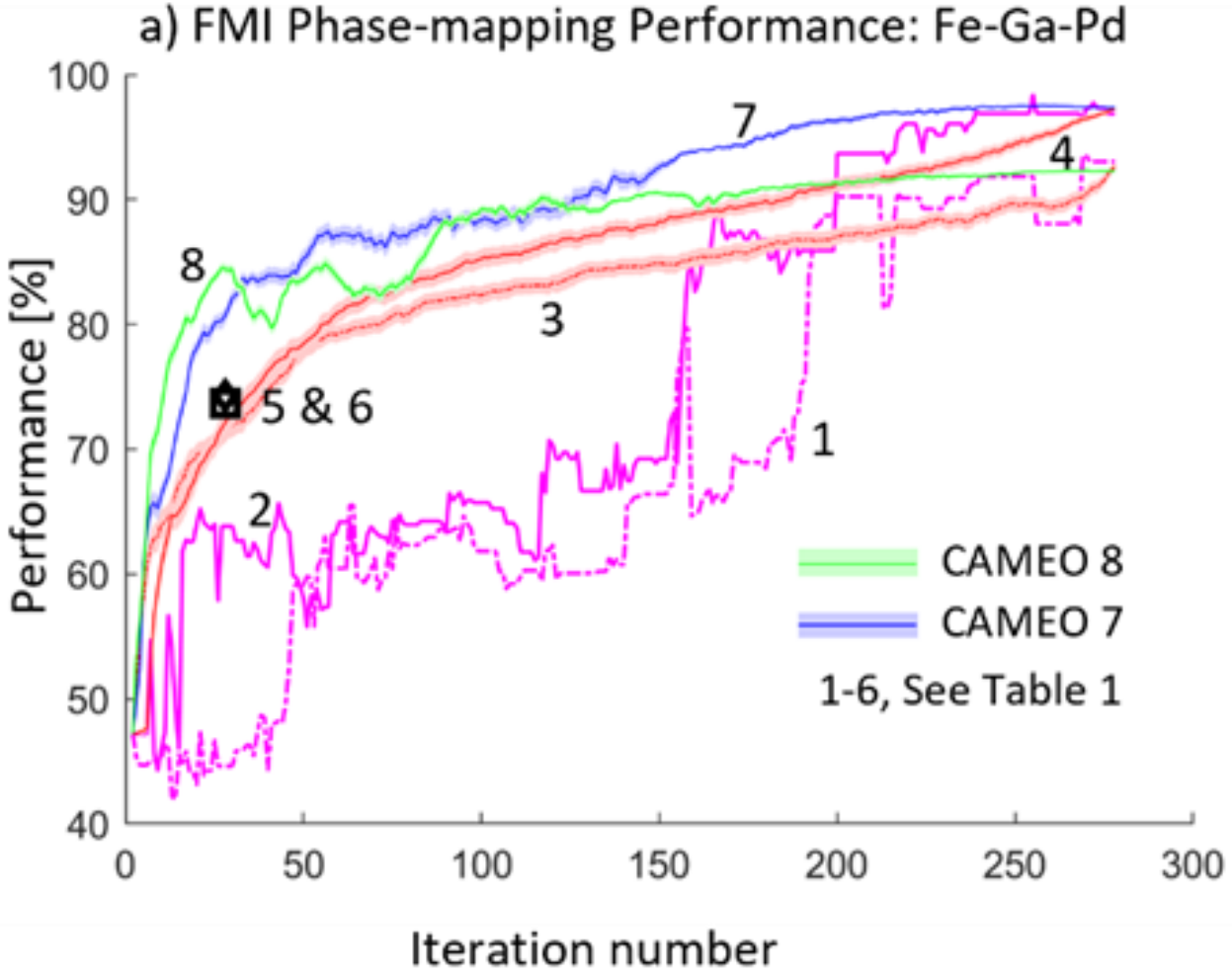






AI is controlling X-ray diffraction systems at SLAC & in the lab!

CAMEO: Physics in the Machine

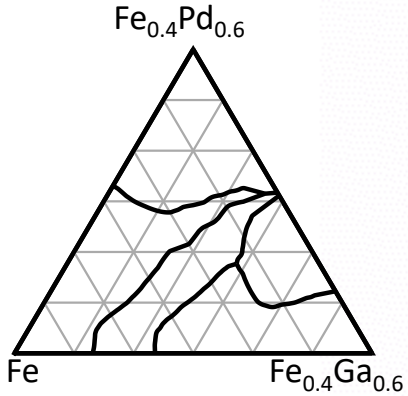


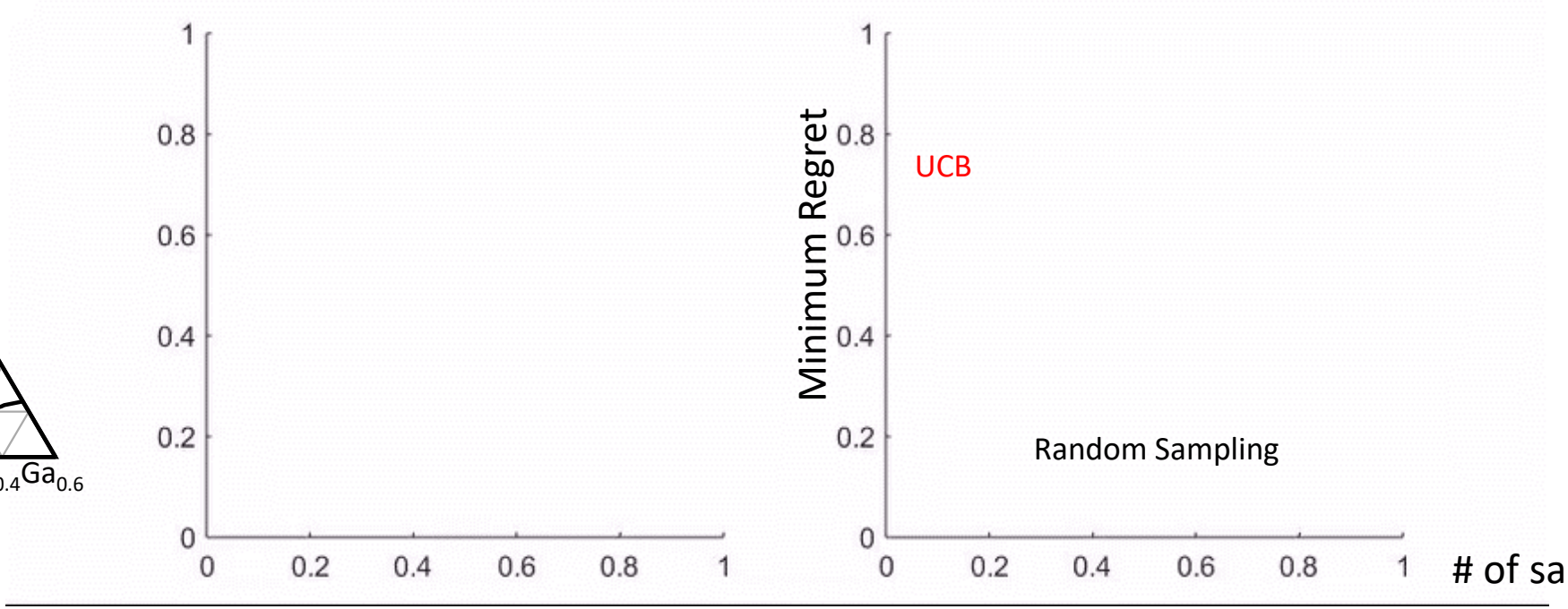
Index	Phase-mapping	Prior	Sampling	Performance for #27 [%]
8, CAMEO	CAMEO	Y	Risk Minimization	85
7, CAMEO	CAMEO	N	Risk Minimization	80
6	CAMEO	N	10 %	74
5	HCA + 1NN	N	10 %	74
4	CAMEO	N	Random	72
3	HCA + 1NN	N	Random	71
2	CAMEO	N	Sequence	64
1	HCA + 1NN	N	Sequence	45

Kusne, et. al., **Physics In the Machine**, Front. Phys. 10:815863 (2022)

Functional Property Optimization - Phase Map Informed

- At every measurement Collect XRD and Magnetization

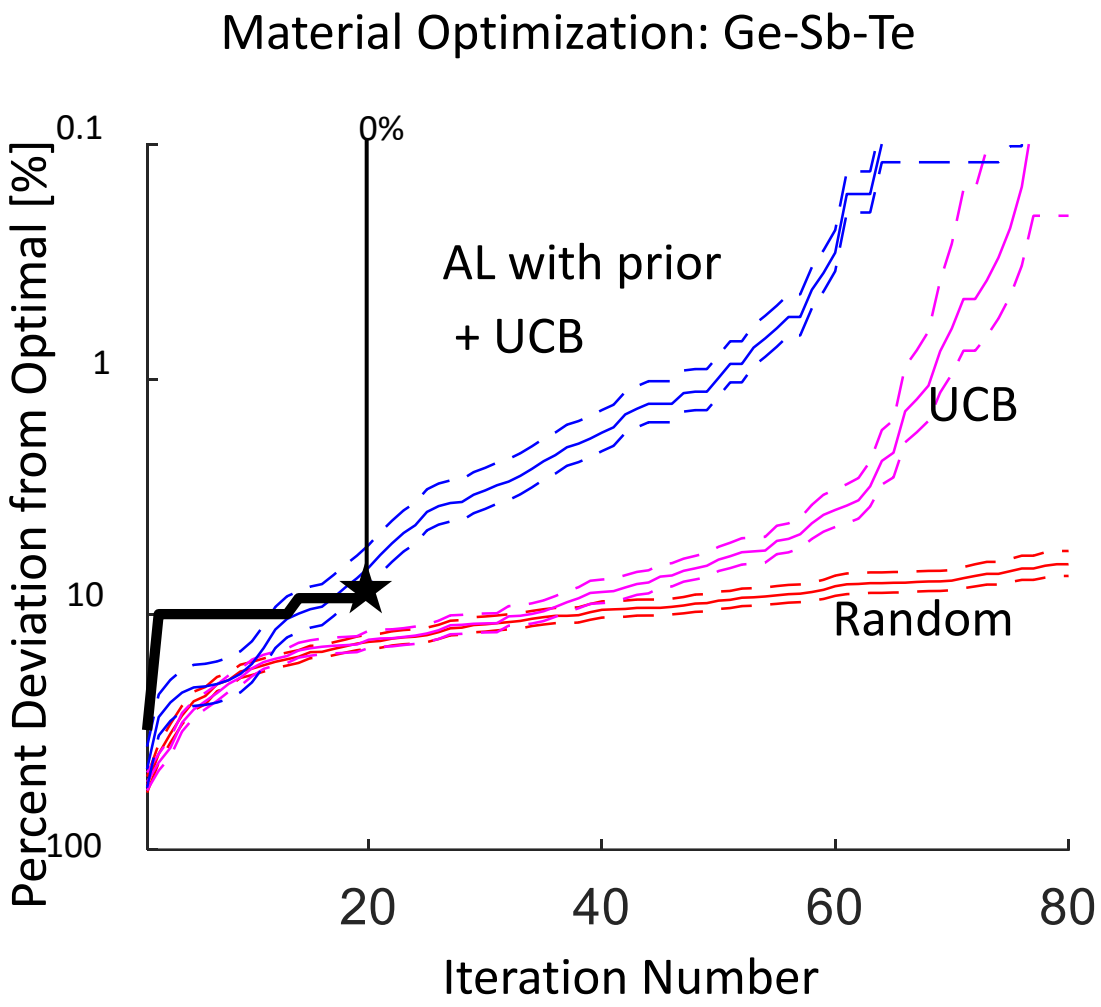




Kusne, et al. Nature Communications 11.1 (2020)

CAMEO: Find best phase change material

- 10x faster Exploration & Discovery
- New material discovered.
  - Novel nanocomposite phase change memory material
  - Superior to previous best material.



Kusne, et al. Nature Communications 11.1 (2020)

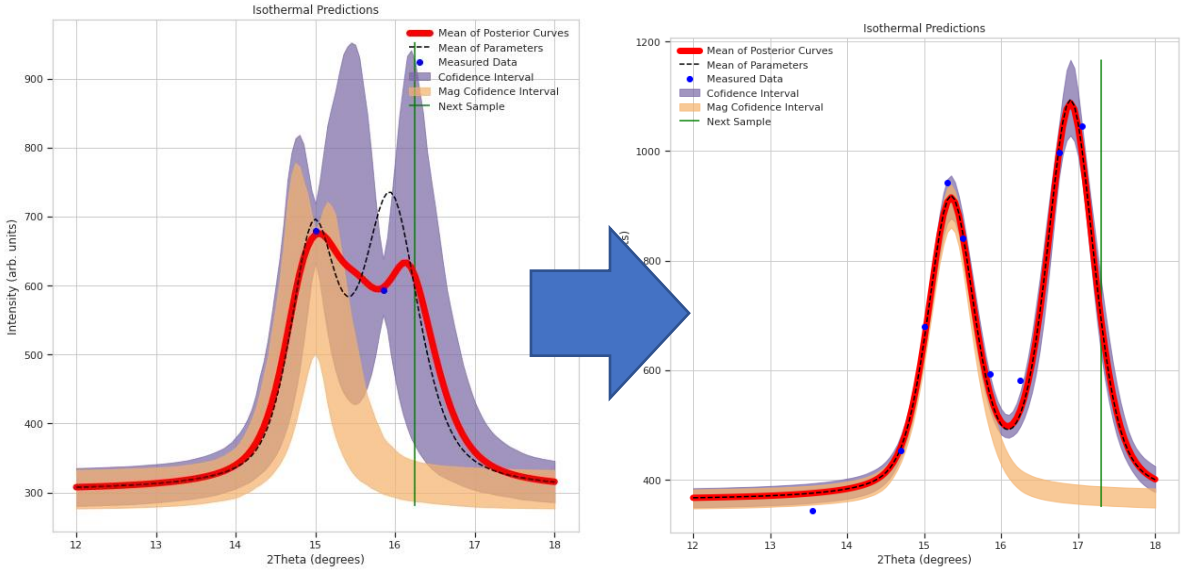
ANDiE: Autonomous Neutron Diffraction Explorer

- Discovers magnetic structure and dynamics parameters
- Built in magnetic structure and neutron scattering physics
- 5x acceleration over current methods.
- Run at: NIST, ORNL

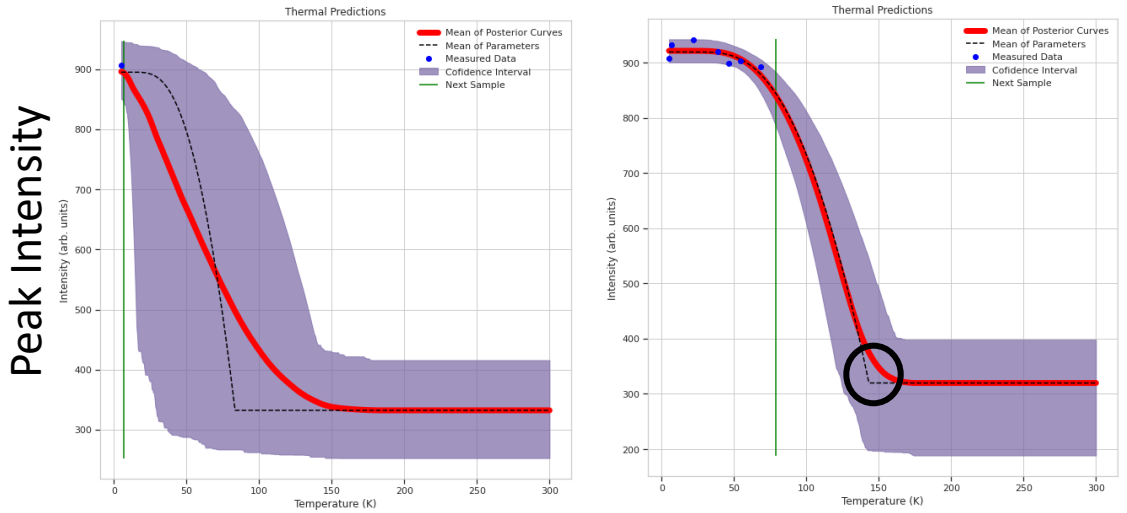
Austin McDannald

> McDannald. Applied Physics Reviews 9.2 (2022): 021408.

Peak Parameters



Neel Temperature



Real time experiment-theory autonomous interaction for phase diagram determination: step by step

Ichiro Takeuchi & JC Zhao
UMD

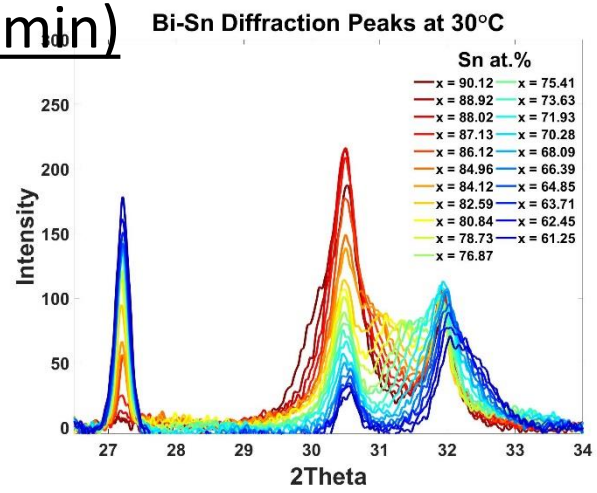
Start at room temperature;
Determine the solvus point
(GP for boundary determination)

Once solidus is reached (no more Bi peak), jump to the liquidus line and continue up with Sn peak

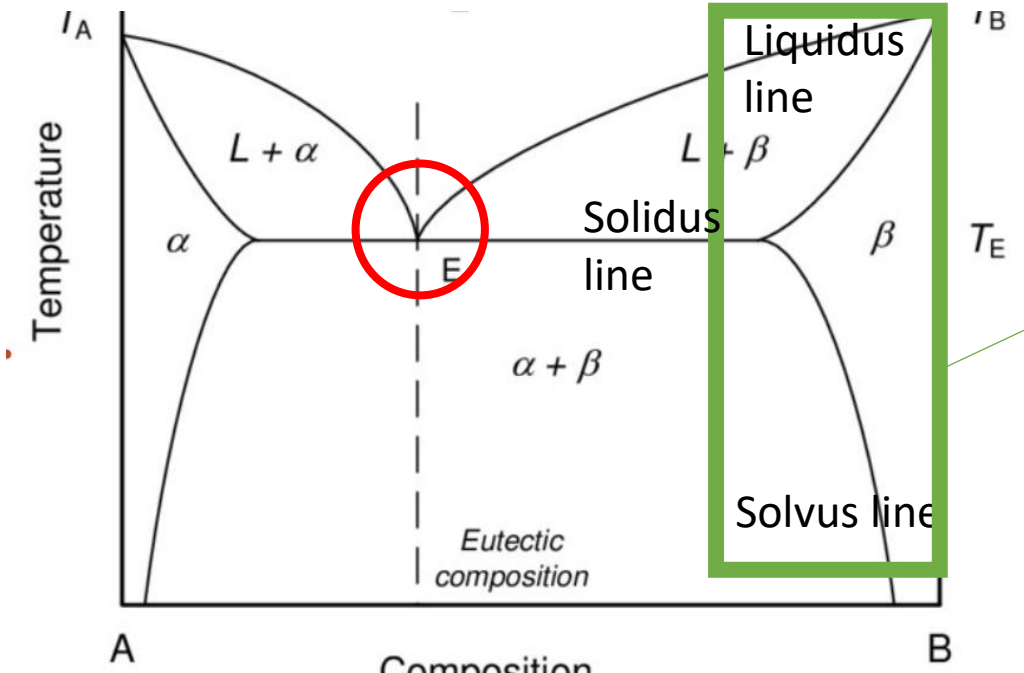
Input to Thermo-calc to determine the lines with uncertainty (< 1 sec)

Jump to the next temperature guided by Thermo-cal, so as to follow the solvus line

closed-loop cycle!
(< 30 min)



Determine the boundary at each temp



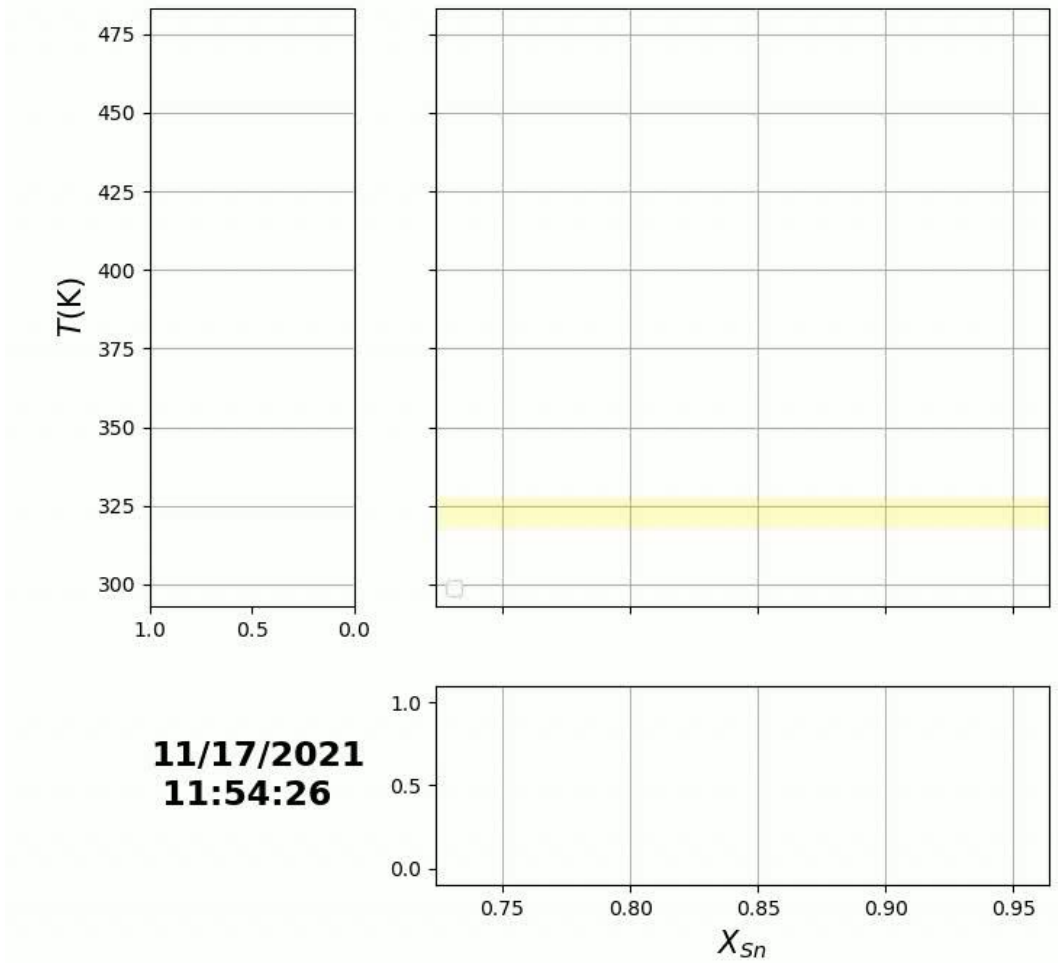
The only assumption is phase diagram looks like this in this region!

Real time experiment-theory autonomous interaction for phase diagram determination: video capture

Thermo-calc calculated uncertainty at higher temp

Thermo-calc takes less than 1 sec

Experiment takes ~ 30 min per temperature



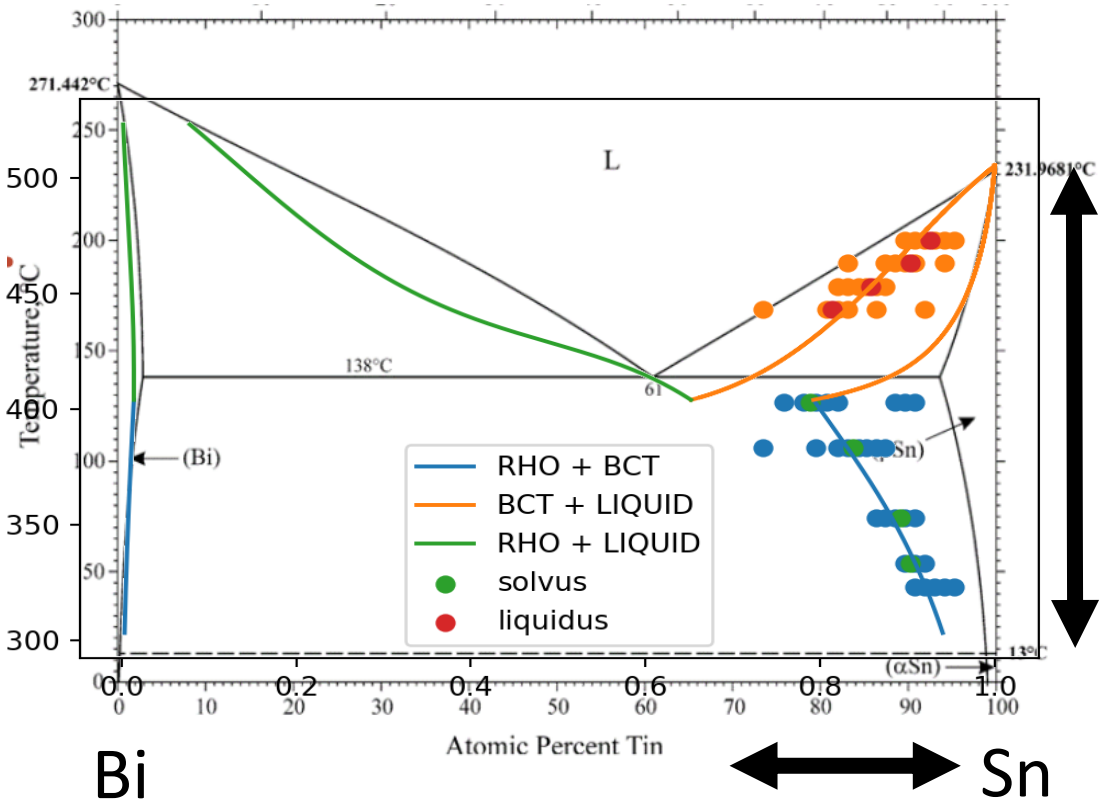
Typically takes 50 XRD measurements:
~ up to 5-6 hours for the whole run

Instead, if we did entire grid, would take over 50 hours

GP at each temperature to find the boundary (solvus or liquidus)

Hoatong Liang

Real time experiment-theory autonomous interaction for phase diagram determination: the result of bulk vs thin film comparison



Sn-Bi composition spread (~300 nm)

From a limited measurement range (composition and temperature), entire phase diagram is obtained

Extrapolation by combining physics with ML

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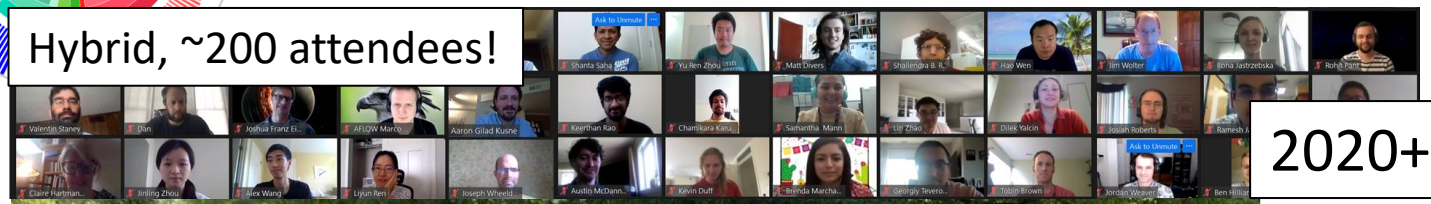

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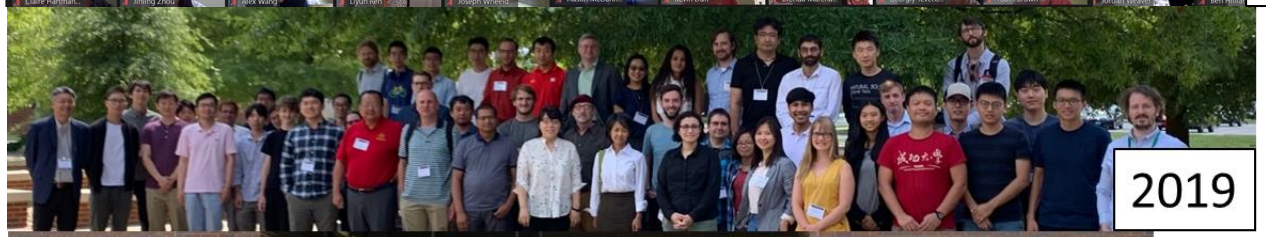

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