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TEXAS A&M UNIVERSITY

Accelerated Design of Fusion Materials

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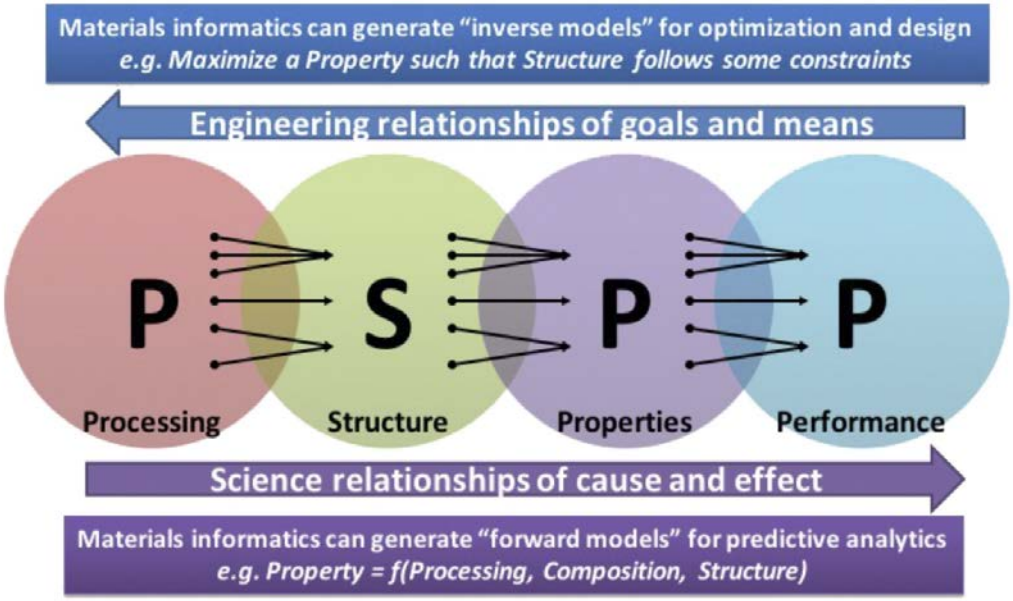
Questions:

1. **What promising AI / ML architectures can be used** for rapid discovery of new fusion materials? How might these work with material computational modeling tools? What are the pros and cons of these approaches?
2. Without considering economics, **how confident are you that we can use ML/AI to find a better performing** alloy to serve as PFC (plasma facing component) material to replace the current leading candidates (e.g., RAFM, W, V4Cr4Ti)?
3. **Which of the following properties** in Table 1.1., if any, do you believe **is *infeasible* to optimize** based on current ML/AI tools for material discovery, and why?
4. Can you name **any additional material properties** that should be optimized to make an impact for commercial FPPs? What are the relevant ranges of those properties? What tests do you need to validate these properties?
5. **Is it feasible for current ML/AL tools to automatically generate new material specifications** for existing manufacturers to fabricate commercial fusion components? If not, what is missing?
6. **What other opportunities/challenges/issues** at code and simulation level for rapid material design should we consider?

Accelerated Materials Discovery as a Goal-oriented Activity:

- Materials discovery has to be a goal-oriented activity
- Materials discovery is about navigating the materials space, with a purpose

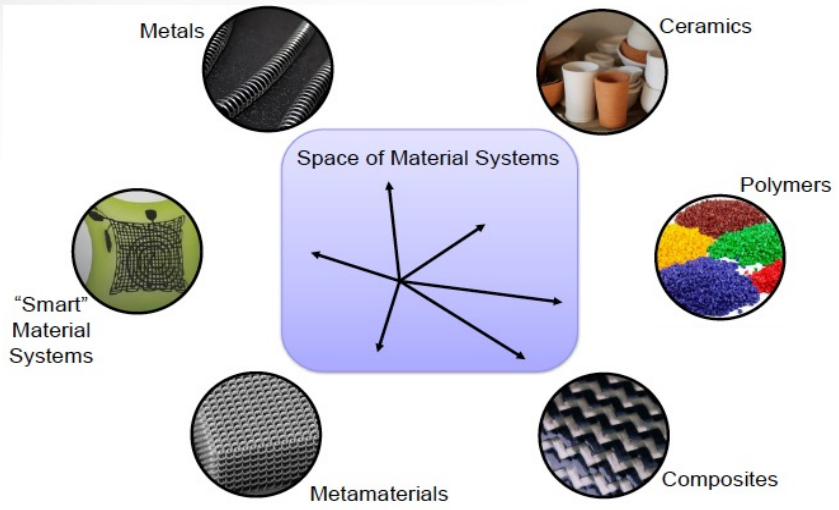


[2016 Agrawal]

Materials Design is very challenging

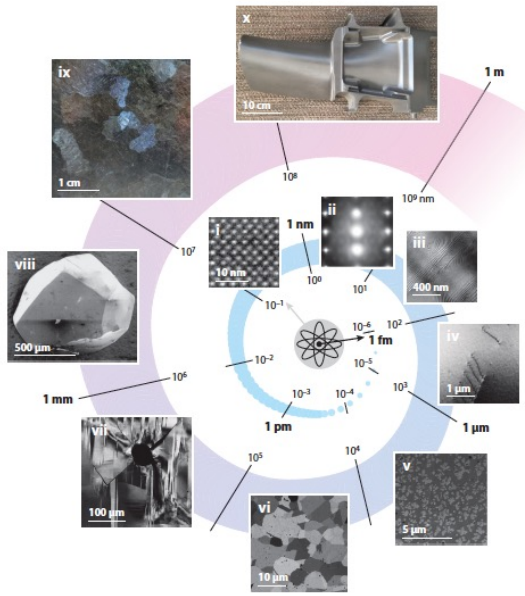
However, navigating this space is incredibly difficult/costly:

Technology Challenges are Materials-Agnostic



[2016 Paredis]

Materials Spaces are Costly to Query



Annu. Rev. Mater. Res. 2015. 45:171–93

Challenges in Materials Design

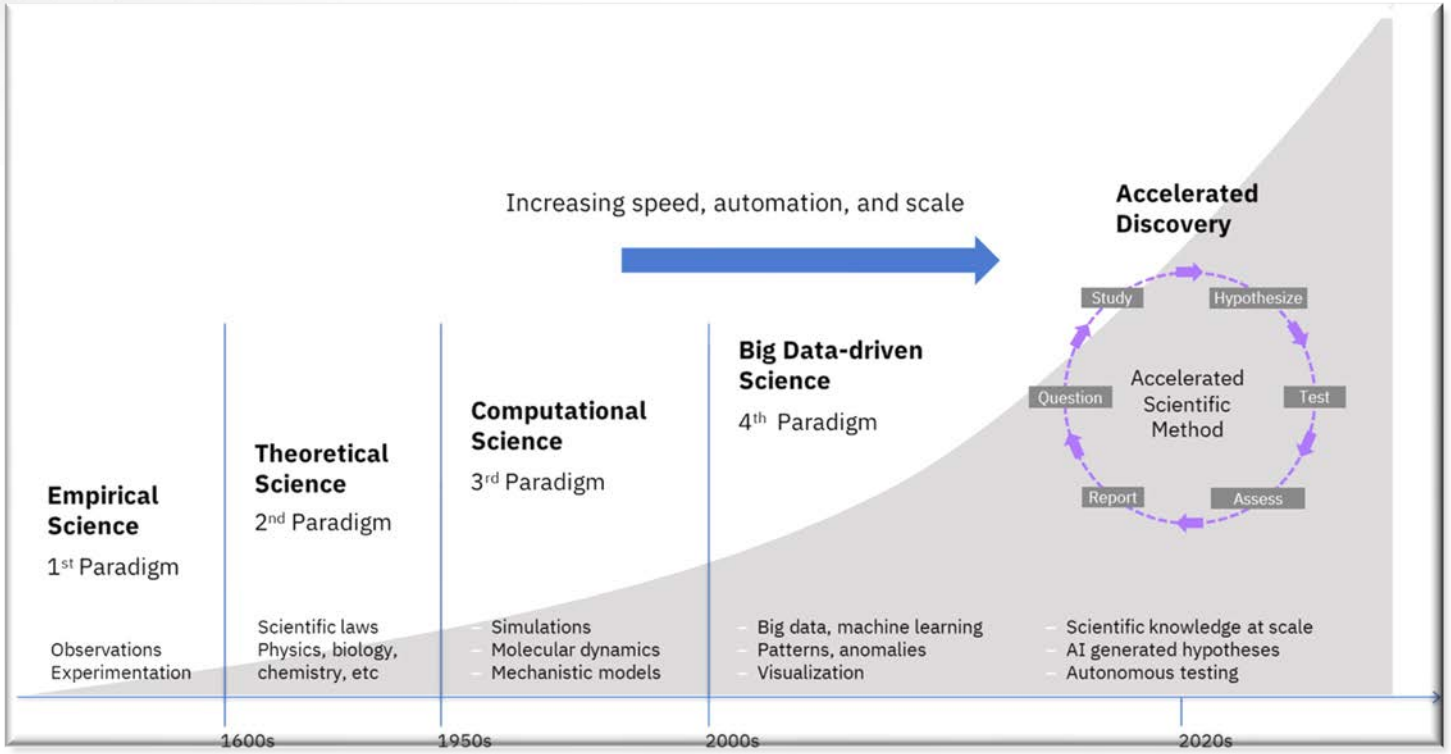
- Multiple (*Competing*) Objectives
- Multiple Constraints (problem can be constraint-dominated)
- Models and Experiments have limits:
  - Models are incomplete
  - Experiments are expensive
  - Models and experiments are uncertain
  - Some performance metrics require long exposure times
- Materials discovery problem is dynamic:
  - Externalities matter (i.e. supply chain is dynamic)
  - Preferences evolve

Notional Example:

Property	At Room Temperature (RT)	At 1300C[a]	At 20dpa (14MeV neutron equivalent) and RT	At 20dpa (14MeV neutron equivalent) and 1300C[a]
Yield Strength (MPa)	>250 MPa	>100 MPa	>250 MPa	>150 MPa
Ultimate Tensile Strength (MPa)	>350 MPa	>200 MPa	>350 MPa	>250 MPa
Failure Elongation (%)	>20%	>20%	>5%	>5%
Fracture Toughness (MPa $m^{1/2}$)	>50 MPa√m	>50 MPa√m	>10 MPa√m	>10 MPa√m
Creep Rupture Stress (MPa) @ 1000hr	NA	>80MPa	NA	>80MPa
Thermal Conductivity (W/mK)	>20 W/mK	>20 W/mK	>20 W/mK	>20 W/mK
Volumetric Swelling (%)	NA	NA	<2%	<2%
Neutron Sputtering Rate (μm/yr)	NA	NA	< 100 μm/yr	< 100 μm/yr
Fatigue Failure Cycles (N)	>50,000	>50,000	>10,000	>10,000
Total Activation Dose (on contact after 24hrs) - Rem	NA	NA	<5 Rem	<5 Rem

Opportunities in Materials Design

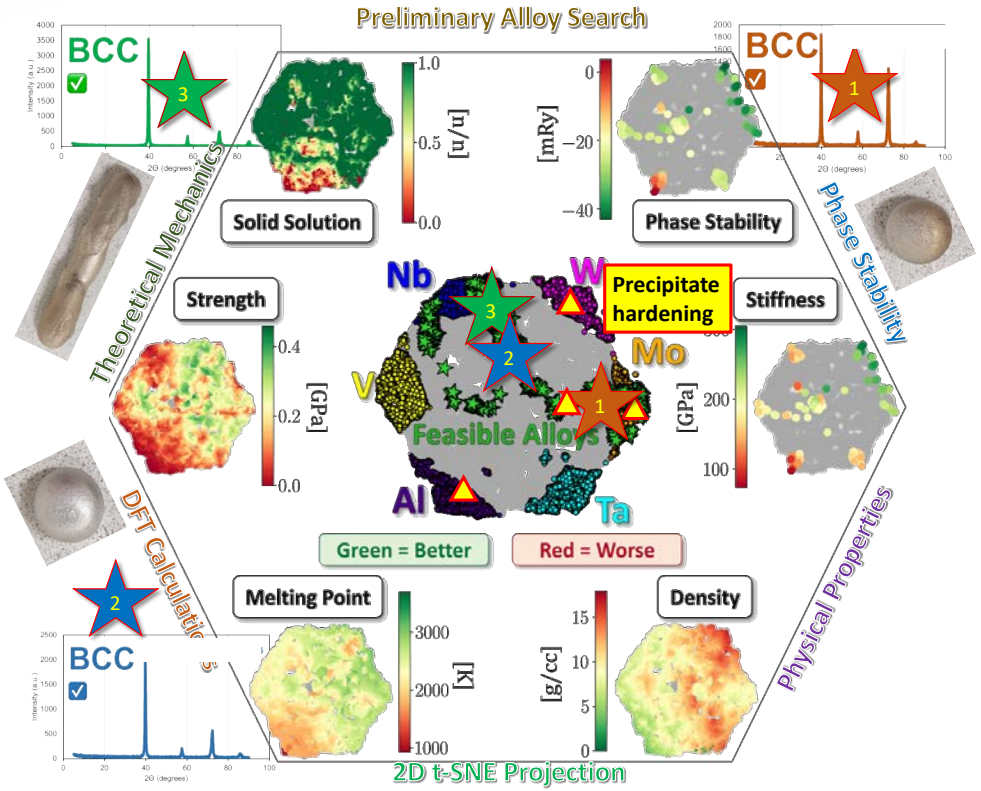
Machine Learning for decision-making, inference and acceleration of simulations hold significant promise



[Pyzer-Knapp 2022]

AI-Enabled Materials Discovery

- Frameworks must deal with constraints effectively
- Frameworks must be capable of exploring and exploiting materials design space efficiently
- They must be able to incorporate experiments **and** simulations
- They must incorporate as much physics knowledge as possible
- They must be capable of exploiting high-throughput capabilities
- They must be *dynamic* and account for evolution in the problem definition itself



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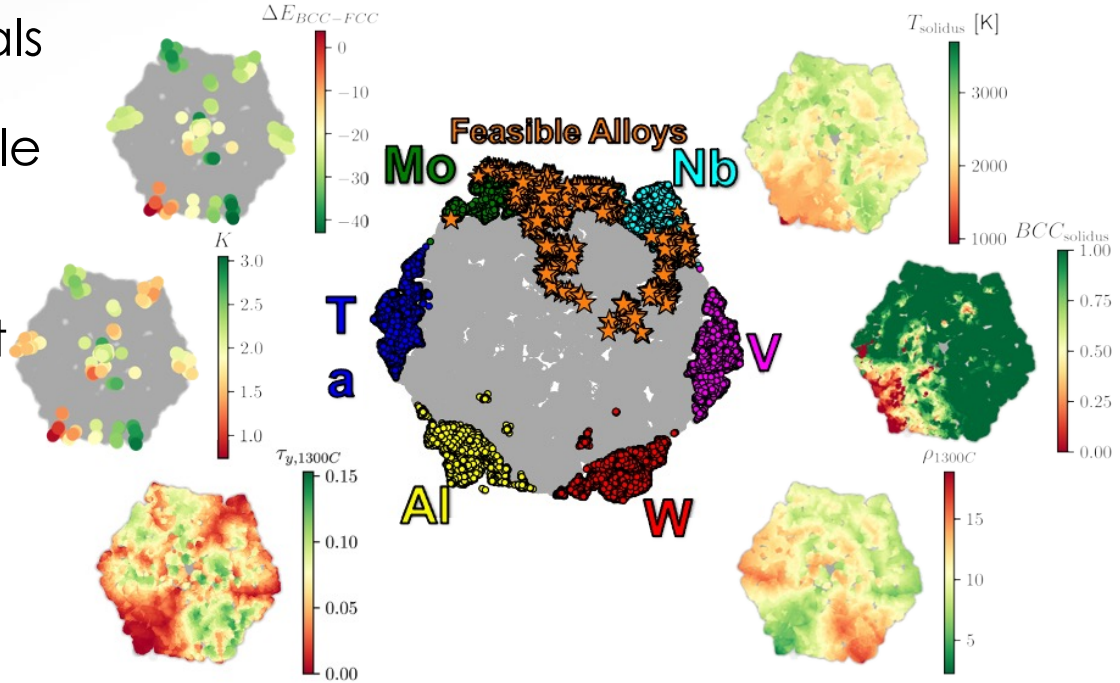
Constraint-Limited Problems

- In many challenging materials discovery problems (e.g. fusion materials), much of the available space is *infeasible*
- It is very inefficient to waste precious resources if there is not certainty in feasibility of a candidate design point
- Better approach is to satisfy constraints first, optimize later



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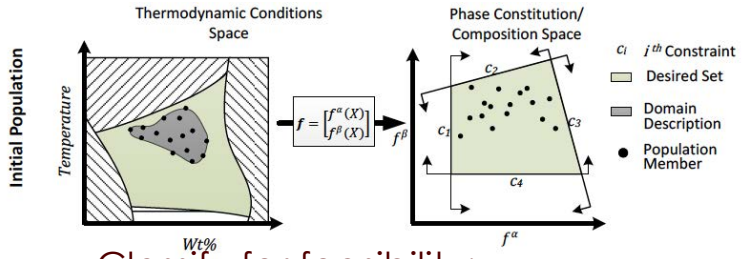
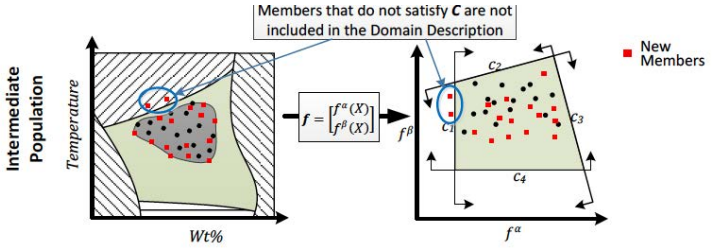
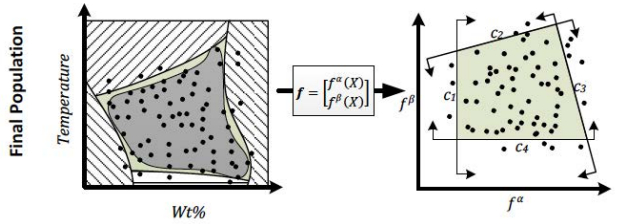
Explore Design Space:



Classify for feasibility:

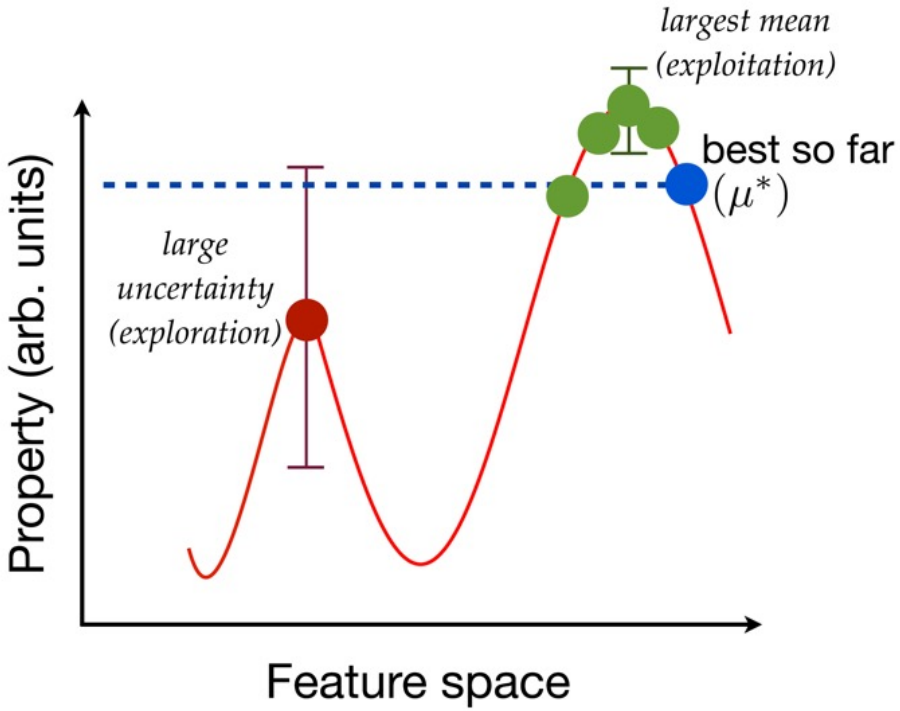


Expand the feasible region:



The Big Picture

- Exploration/exploitation of a (computational) experiment space should not be random
- Unfortunately, each experiment/computation often times is extremely costly
- With "open loop" approaches there is no prescription of what to do next once more knowledge has been gained

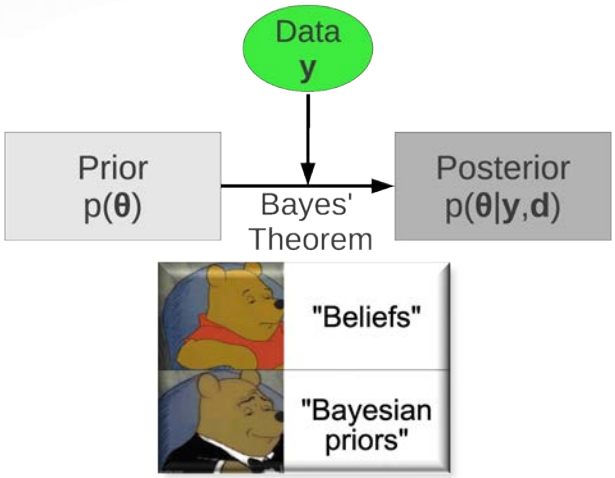


[2016 Balachandran]

Discovery as a (Black Box) Optimization

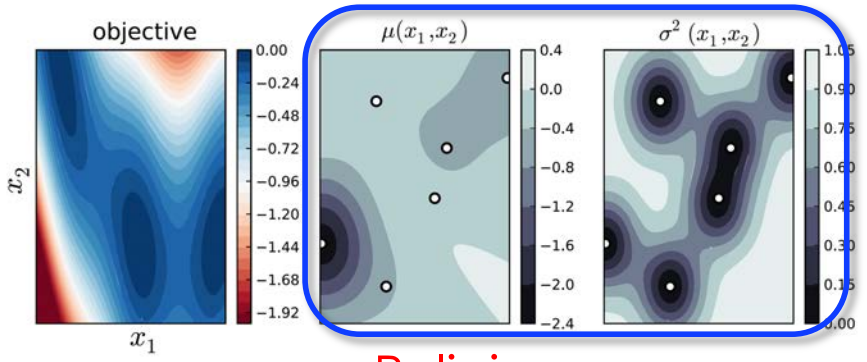
When queries to the experimental design space are expensive, we need to do better than *random exploration*

Bayesian Methods:

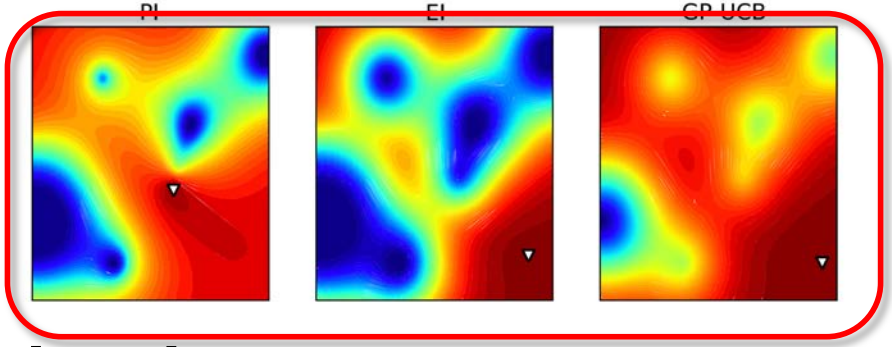


Bayesian Optimization:
Prediction of Outcomes +
Prescriptive Policies

Model



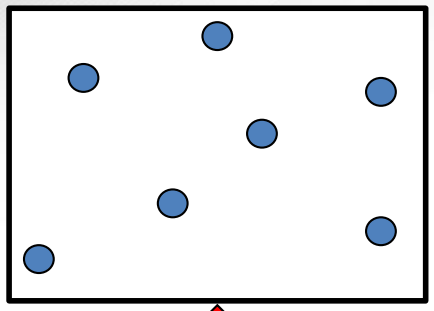
Policies



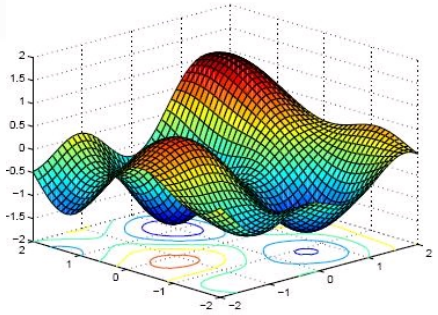
[Brochu]

Typical SOA

Initial Data



Our Current Model



Select Single (*or many*) Experiment(s)

"Autonomous systems [should] ***build and exploit own internal models*** *[and act on them]"*—N. Freitas

Run Experiment(s)

[Azimi]

Is that all there is?

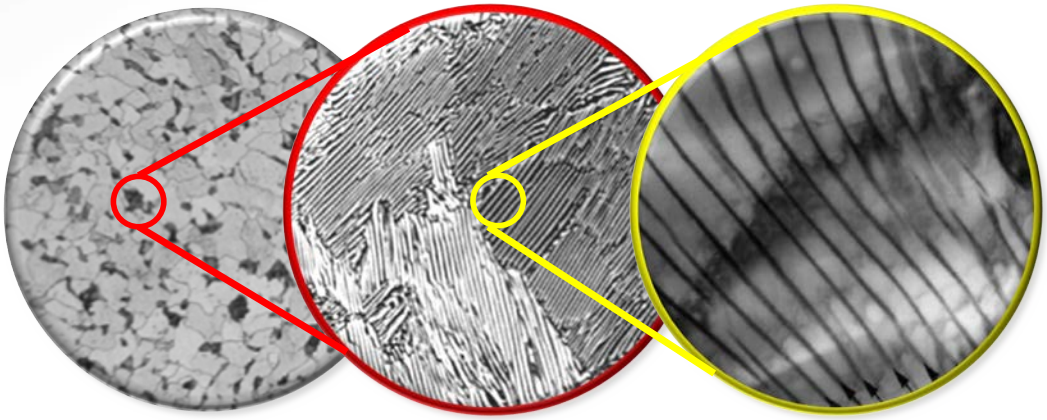
Most approaches to date to autonomous materials discovery can be mapped to a sequential ‘black-box’ optimization problem

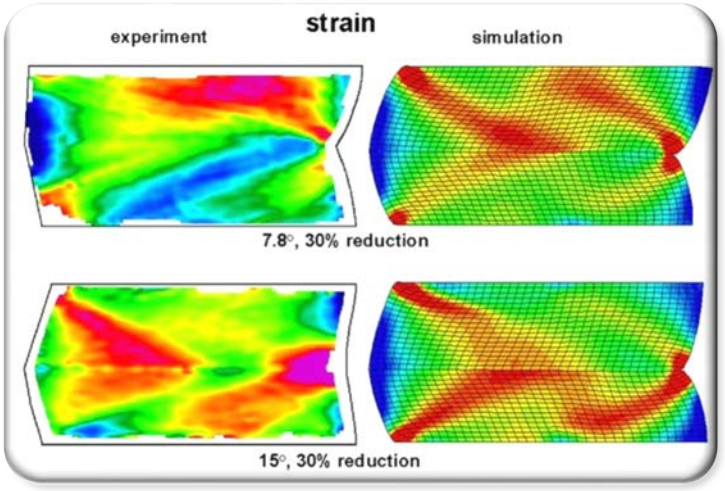
Such approaches tend to be limited, since:

- One has potentially multiple gray boxes, instead of a single black box
- It is generally necessary to account for multiple objectives and constraints simultaneously
- Sequential (one-by-one) experimentation is highly inefficient
- Incorporating physics/chemistry priors into ML/AI frameworks can accelerate process

Combining Multiple Information Sources

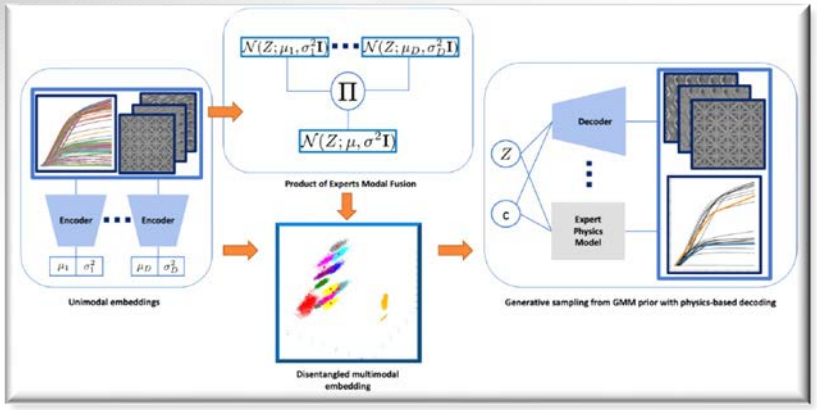
- What if we have multiple information sources at our disposal?
- In materials science, we often have **multiple sources of information** at our disposal





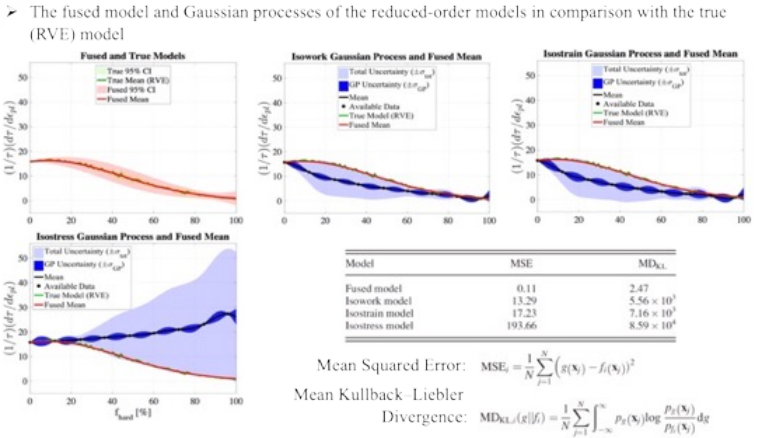
Combining Multiple Information Sources

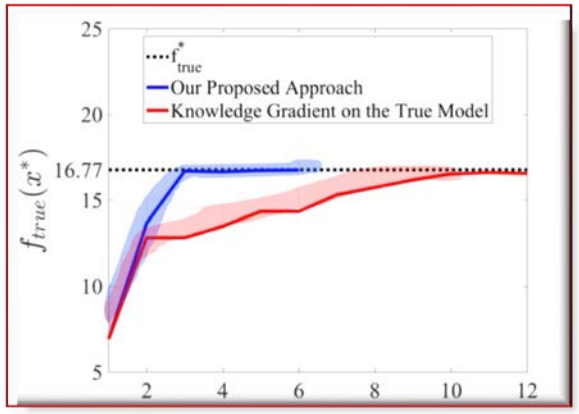
Multi-modal Learning



[Trask 2022]

Multi-Information Source BO





[Khatamsaz]

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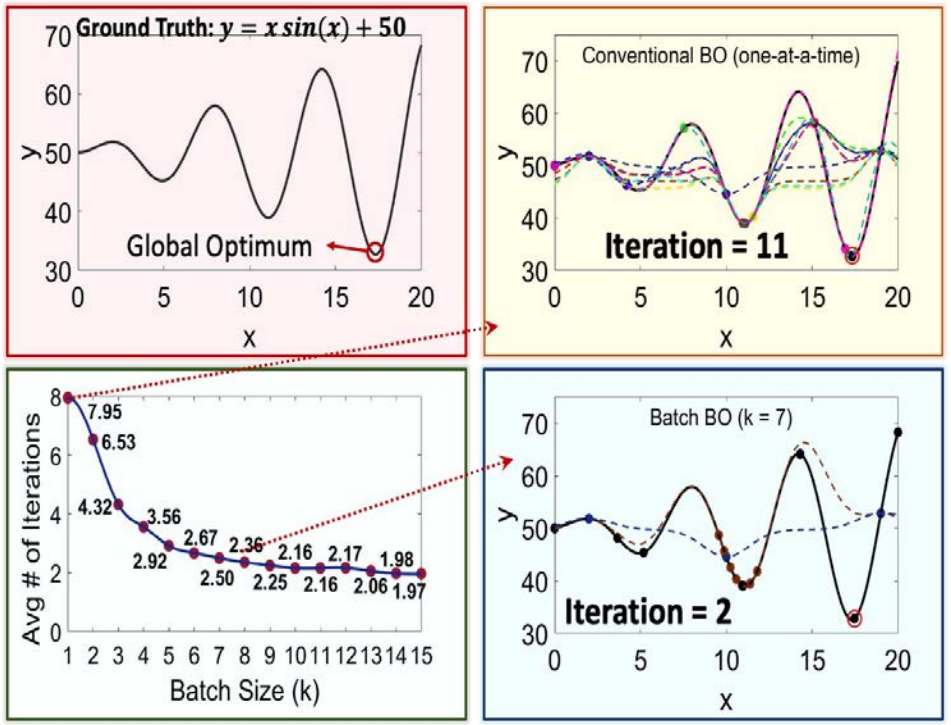
Exploiting HTP Facilities

- Conventional BO:
  - Makes strong assumption about shape and 'roughness' of underlying function (e.g. hyperparameters given sparse data)
  - Location of optimal region(s) is highly dependent on these assumptions
  - This is very risky when the amount of data is small
- Alternate Approach:
  - Assume that all shapes are possible ('roughness' of the function is multi scale)
  - Compute acquisition function for *many* possible hyperparameters at the same time



T. T. Joy, S. Rana, S. Gupta, and S. Venkatesh, "Batch Bayesian optimization using multi-scale search," *Knowledge-Based Systems*, Jun. 2019, doi: 10.1016/j.knosys.2019.06.026.

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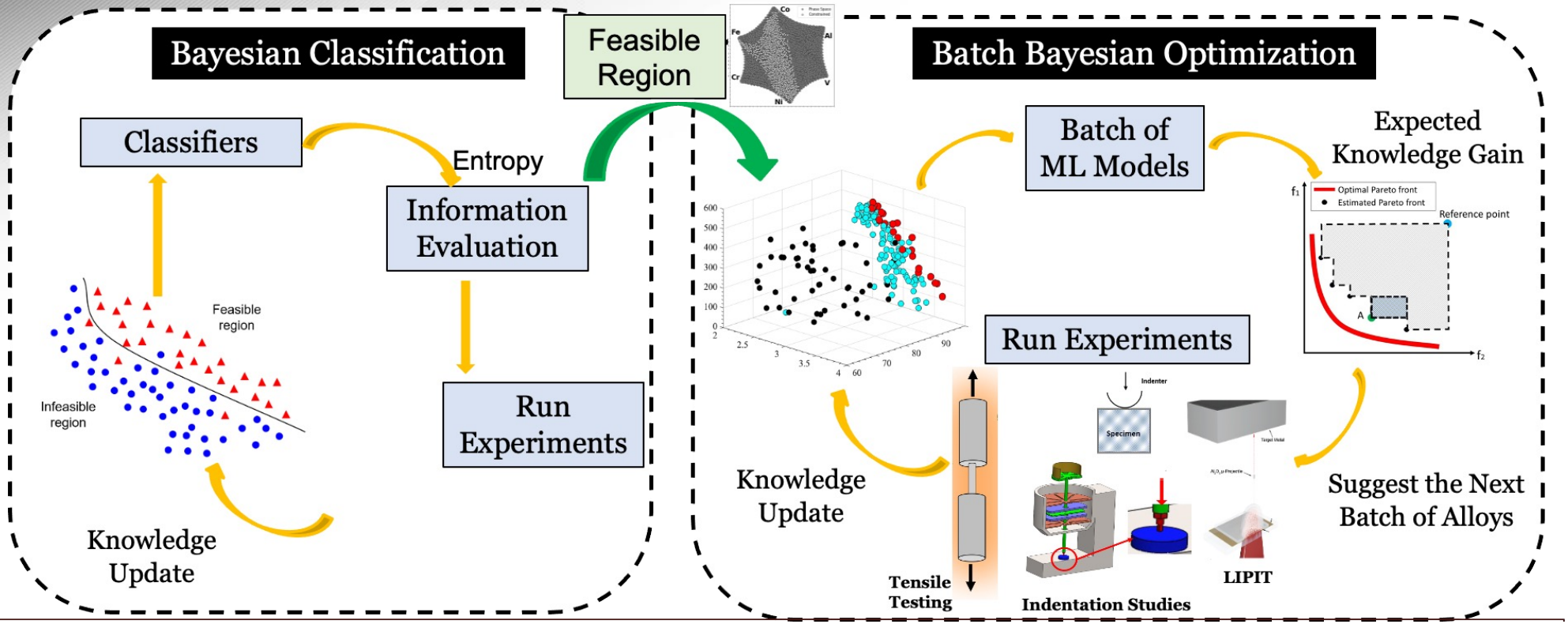
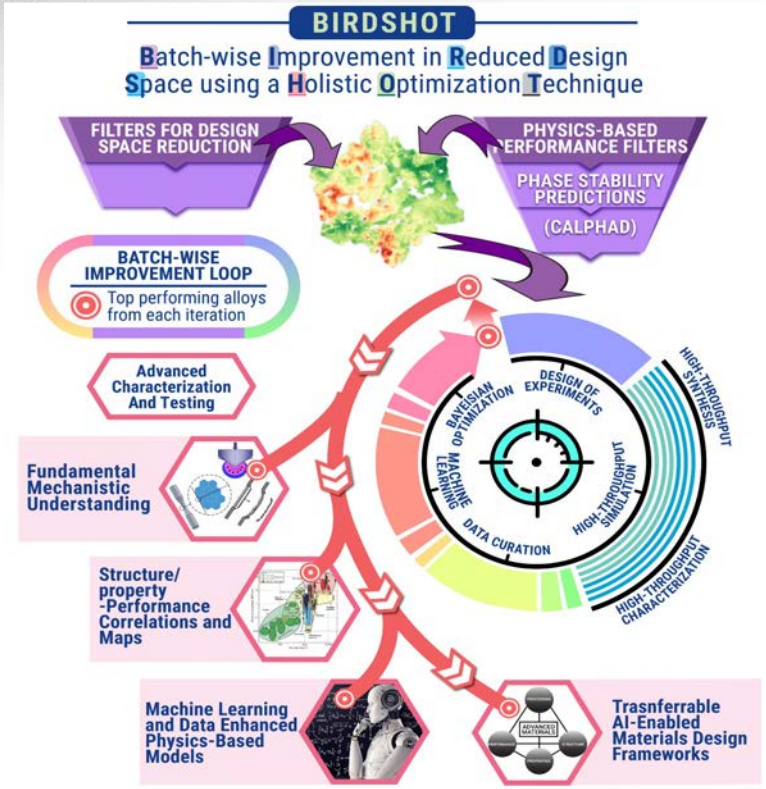
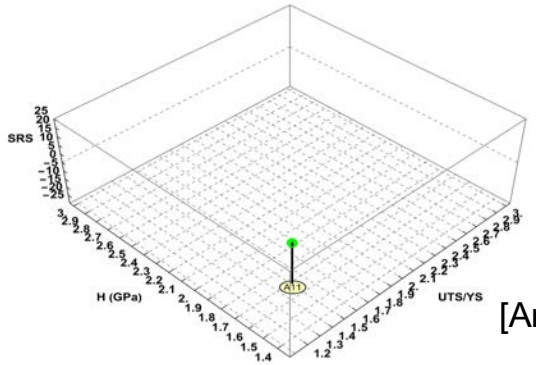
Dealing with Multiple Objectives and Constraints



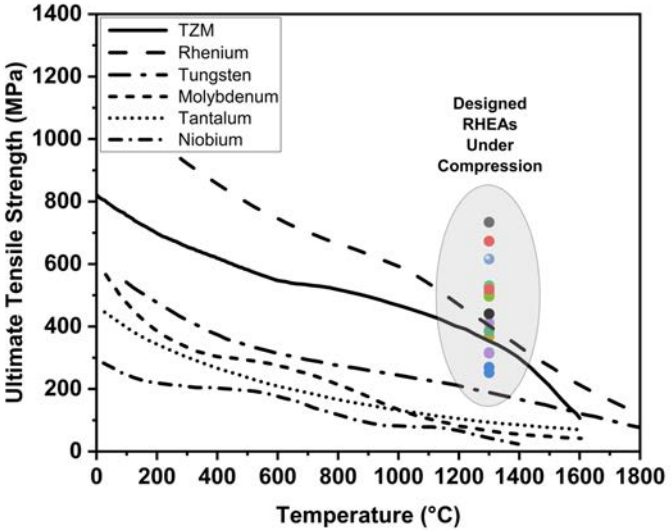
SOA in Alloy Design



[Arroyave, Allaire, Karaman 2023]



[Arroyave 2023]

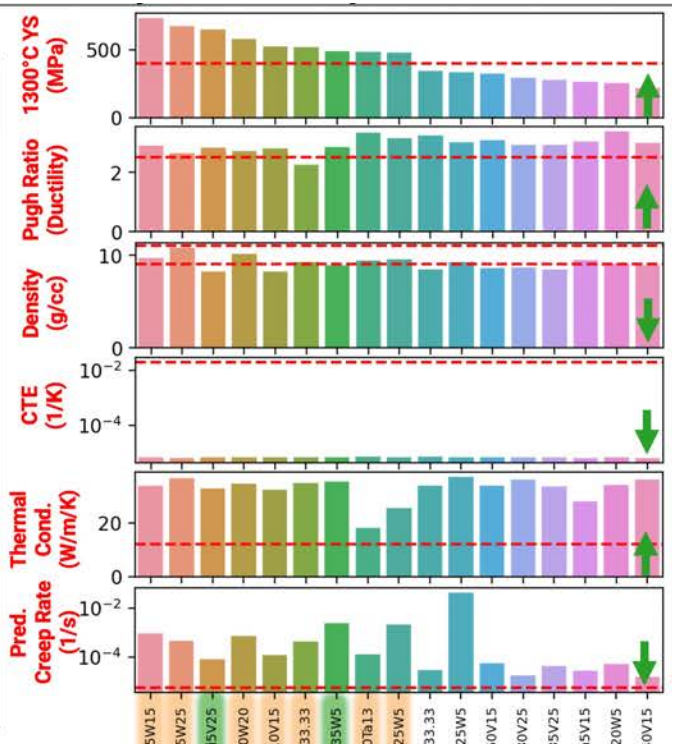


Karaman 2023]

SOA Alloy Design

Example: Application of BIRDSHOT to ULTIMATE

Property or attribute	Method of evaluation	Two-year Project Target	Go/No-Go acceptance at Q5	Information Source	Model Fidelity	Confidence in meeting Go/No-Go	Reasoning
Density	Apparent density using Archimedes method	< 9 g/cc	< 11 g/cc	MS5 Property Model	High Fidelity	High	Extremely accurate prediction
Room Temperature Tensile Ductility	Uniaxial tensile test (1)	> 1.5%	> 1%	MS6 DFT Pugh Ratio	Low Fidelity	Moderate	Nb+Ta constraint
0.2% Tensile Yield Strength at 1300 °C	Uniaxial tensile test (1)	> 400 MPa	> 200 MPa	MS7 Experiment	Medium Fidelity	Moderate	Augmented model predict solns. exist
Thermal Conductivity	Laser flash method	RT: 9-12 W/mK	> 8 W/mK	MS5 Property Model	Medium Fidelity	High	~30 W/m/K for RHEAs in general
Linear Thermal Expansion (RT-1300°C)	Dilatometry	< 2%	< 3%	MS5 Property Model	Medium Fidelity	High	~10^{-4} % for RHEAs in general
200 MPa, 100h creep strain at 1300 °C	Uniaxial tensile creep test (1)	< 2%	n/a	n/a	Low Fidelity	Moderate	Contrell-Jaswon Model for Min. Creep



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Where do we move from here?

Add Physics/Chemistry to BO

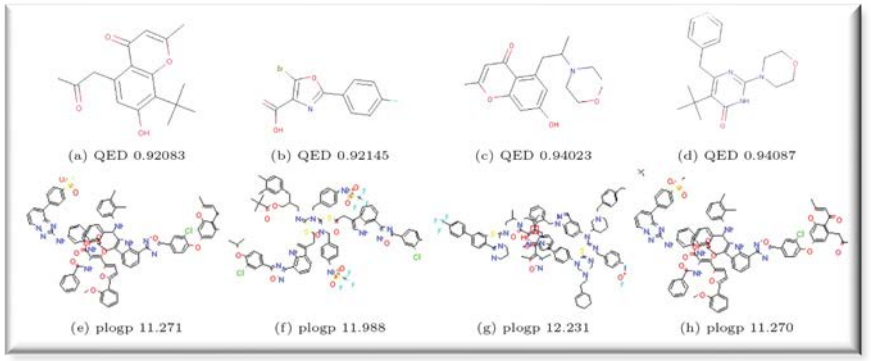
Standard BO uses off-the-shelf kernel functions that assume a Euclidean space

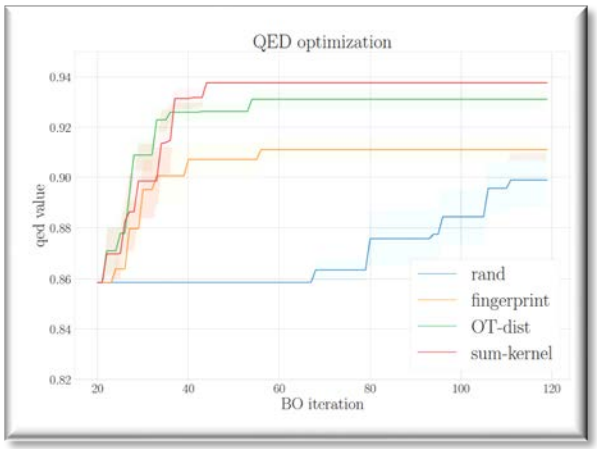
This may not be the best representation of the problem

It may also lead to unsafe design choices

A solution could be to inject physics/chemistry priors into the kernel function itself

In ChemBO, for example, the kernel was constructed over the molecular graph space

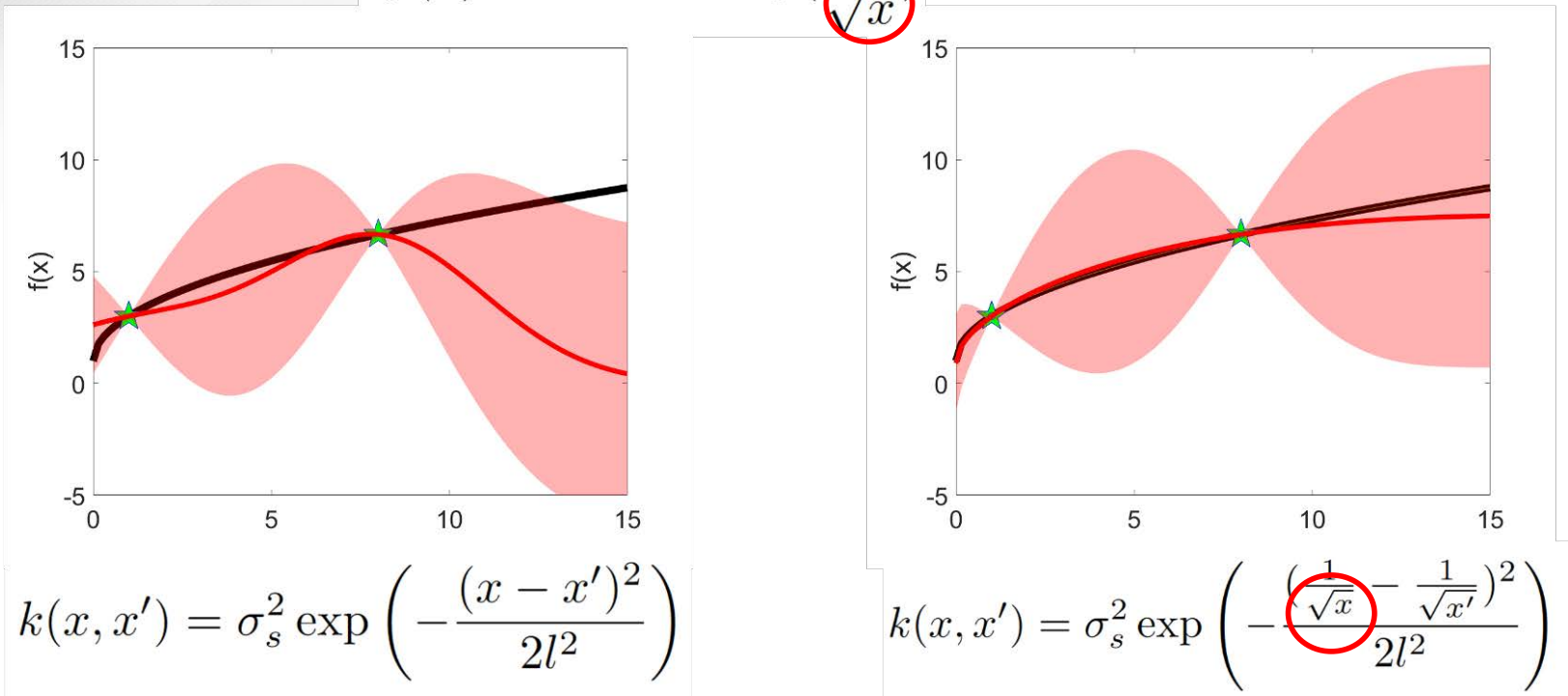




[Korovina 2020]

Add Physics/Chemistry to BO

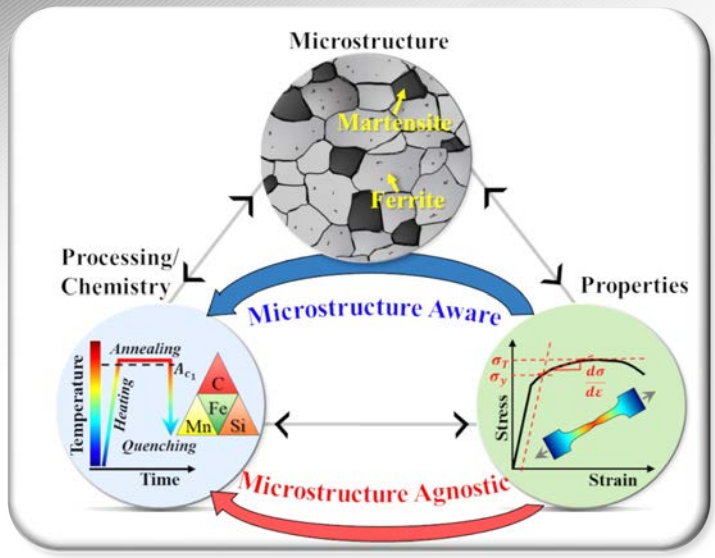
$$f(x) = 1 + 2 \times \exp(\frac{1}{\sqrt{x}})$$



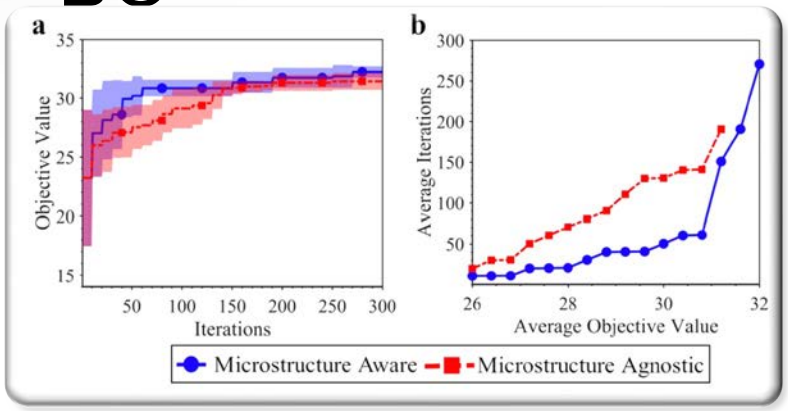
$$k(x, x') = \sigma_s^2 \exp\left(-\frac{(x - x')^2}{2l^2}\right)$$

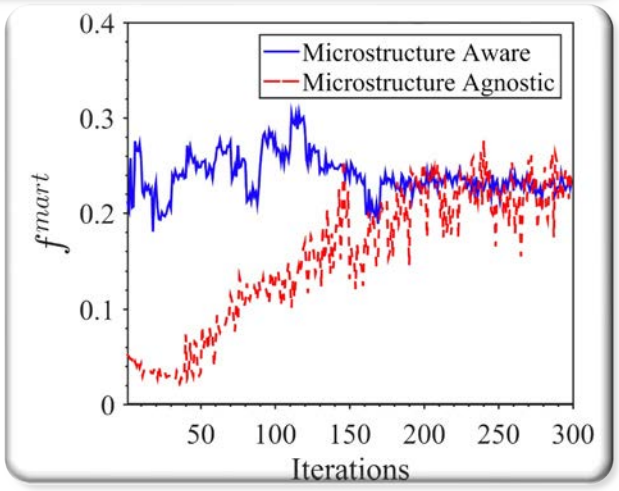
$$k(x, x') = \sigma_s^2 \exp\left(-\frac{(\frac{1}{\sqrt{x}} - \frac{1}{\sqrt{x'}})^2}{2l^2}\right)$$

Add PSP Relationships to BO



- Example: we have compared microstructure-agnostic BO vs microstructure-aware BO
- Our results have shown that explicitly exploiting PSP relationships leads to faster solutions than when only exploiting PP

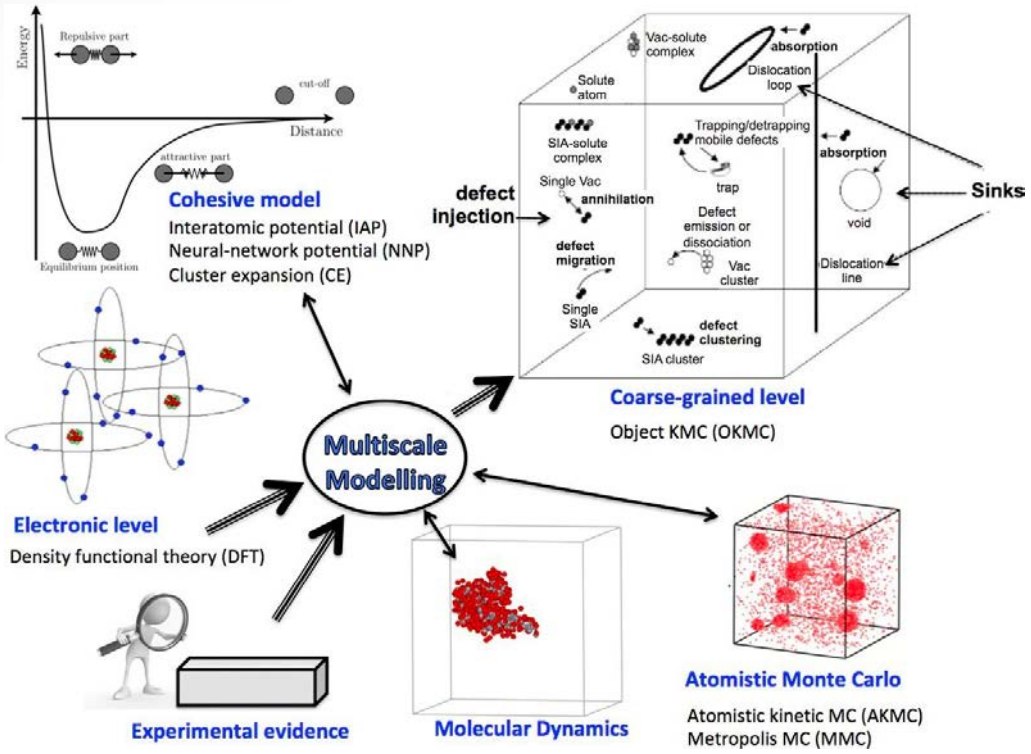




[Khatamsaz 2022]

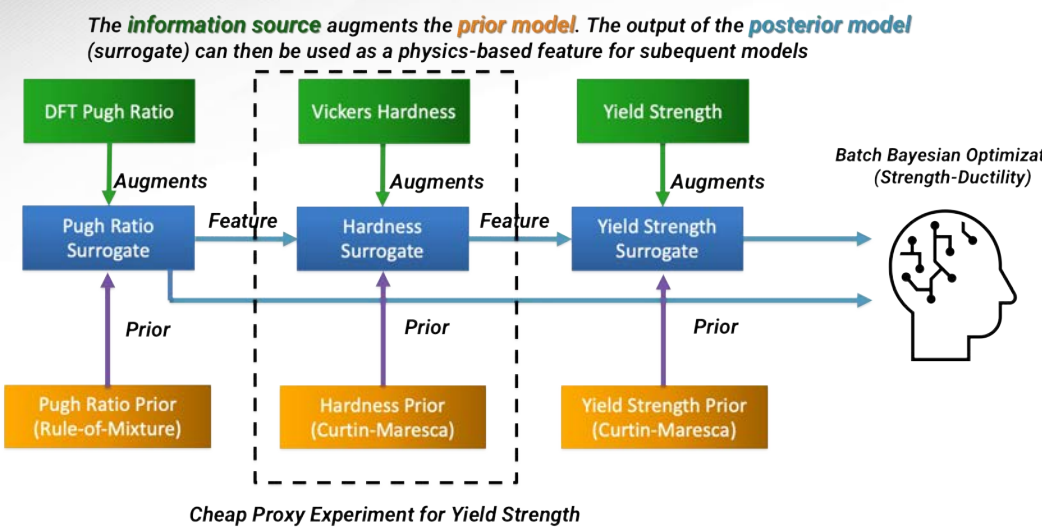
Accelerate Physics-based Models

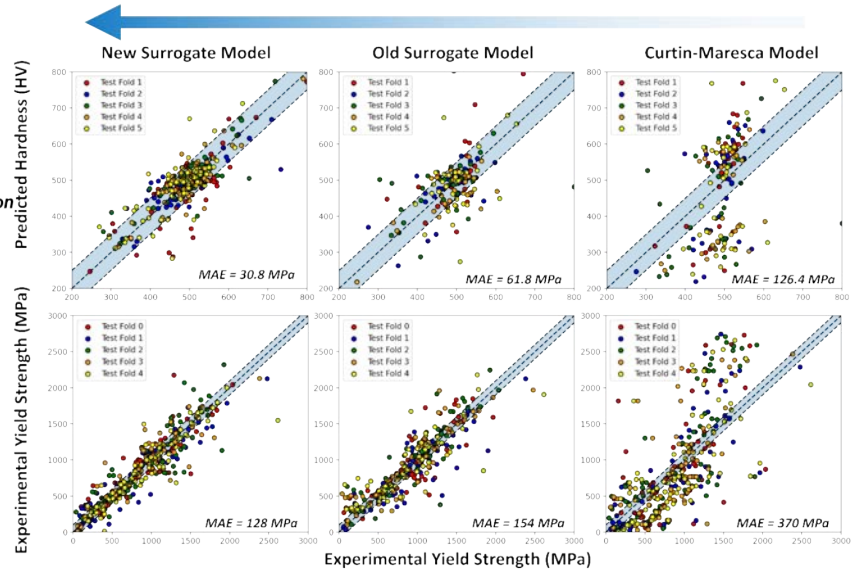
- Physics-based models are expensive
- They can be accelerated using ML
- There are many examples relevant to fusion/fission:
  - ML Potentials
  - ML Accelerated MD
  - ML Accelerated KMC



[Castin 2018 CMS]

Augment Data-only models with Priors





[Vela 2023]

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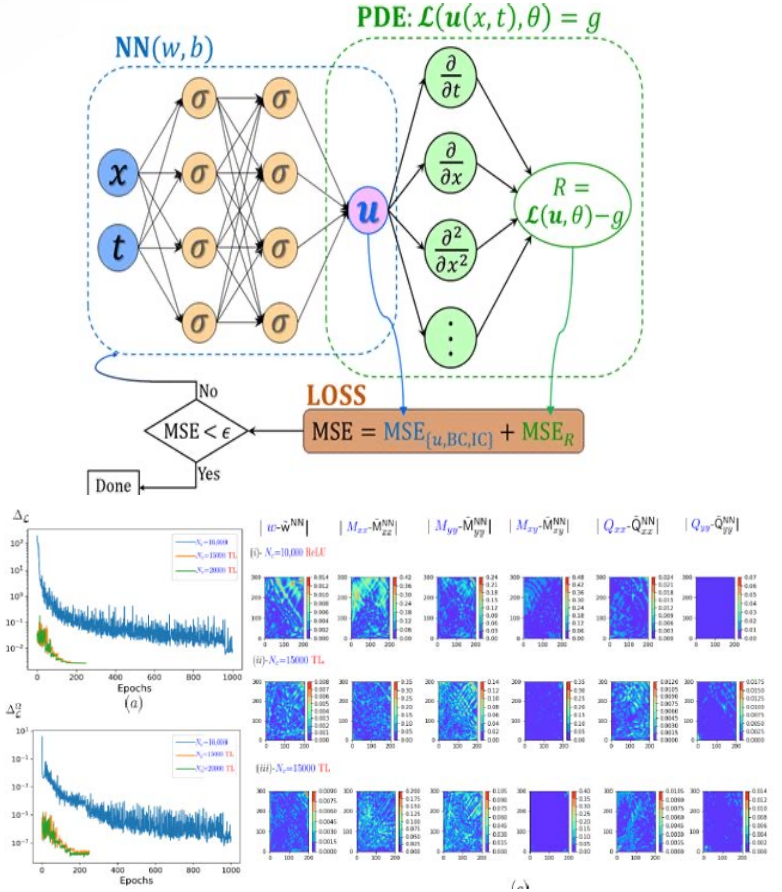
  - ML Potentials
  - ML Accelerated MD
  - ML Accelerated KMC
  - Physics Informed NNs



[Roy 2022]

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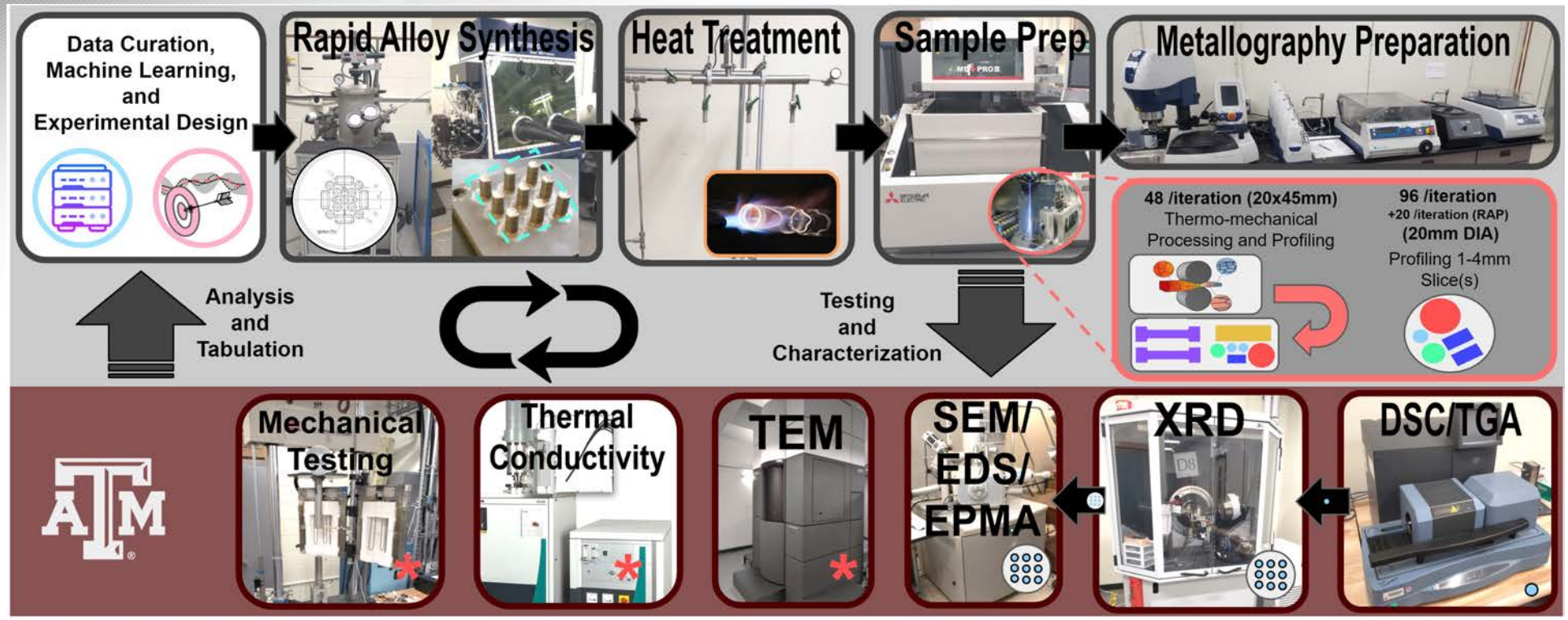
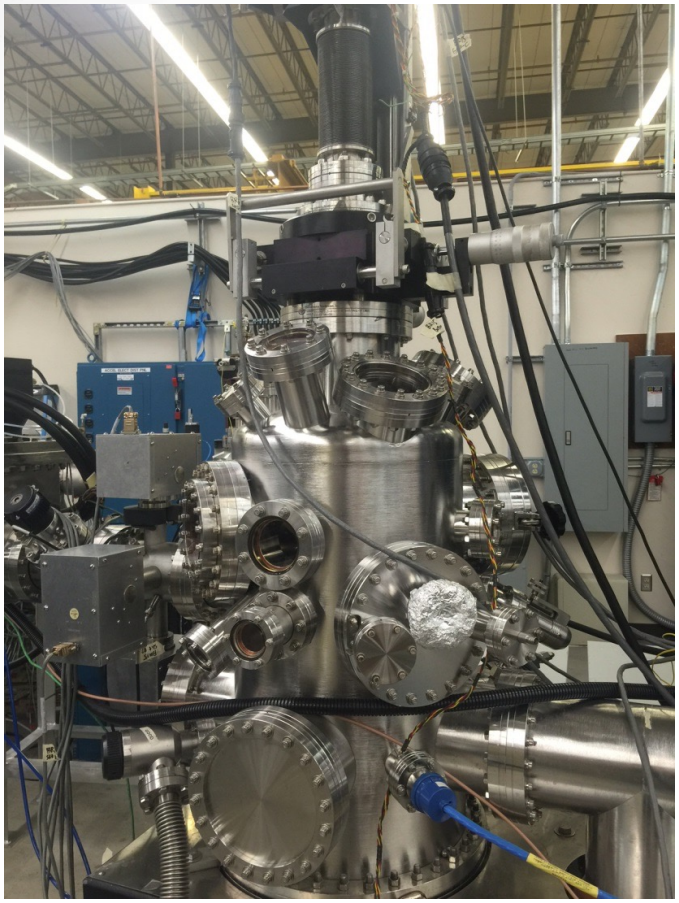
Develop Integrated Synthesis/Characterization/Testing Platforms



[Karaman 2023]

Develop Accelerated HTP Irradiation Tests

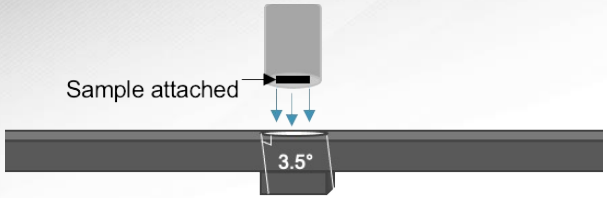


Multiple (kinds of) radiations
Multiple temperatures
Multiple energies

[Shao 2022]

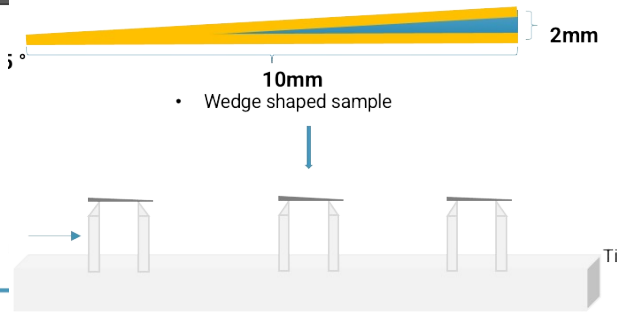
Design Samples for HTP Characterization

Example: HTP Oxidation

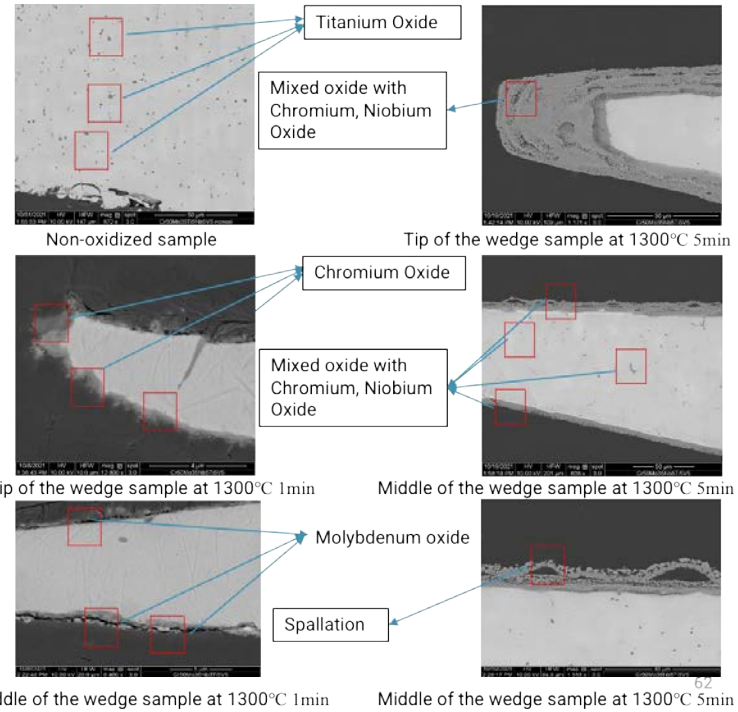


- Polishing with customized sample holder (3.5°)
- Polishing both top and bottom

- Place the sample inside box furnace
- Varying parameters



- Wedge shaped sample
- Place the sample on top of alumina rods
- Minimize contact area between sample and rods



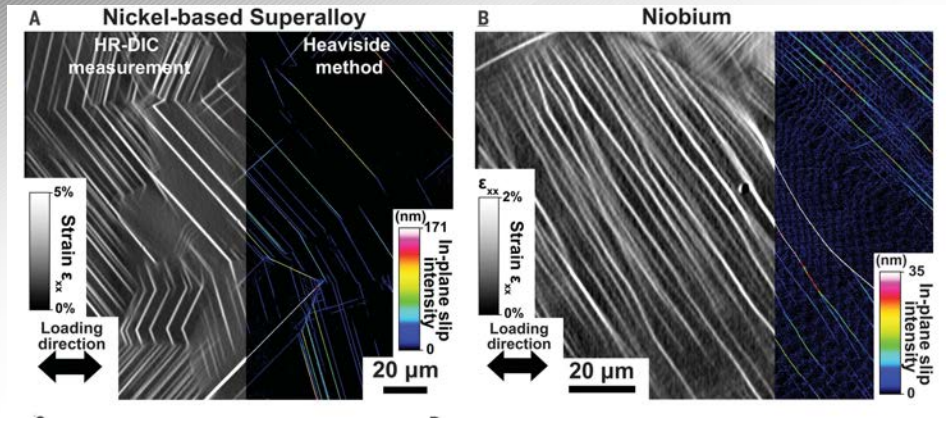
Non-oxidized sample | Tip of the wedge sample at 1300°C 5min

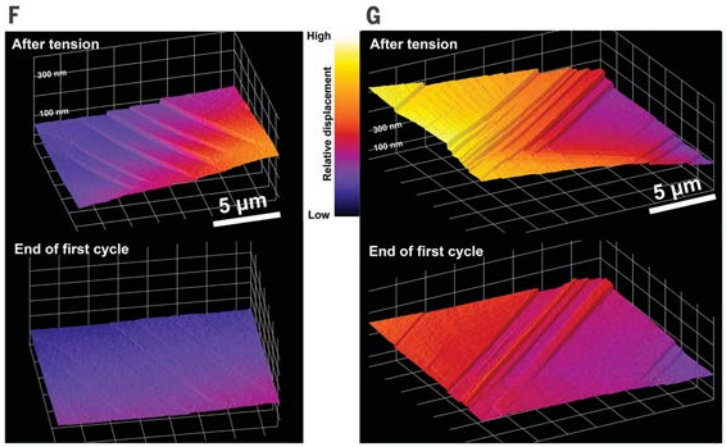
Tip of the wedge sample at 1300°C 1min | Middle of the wedge sample at 1300°C 5min

Middle of the wedge sample at 1300°C 1min | Middle of the wedge sample at 1300°C 5min

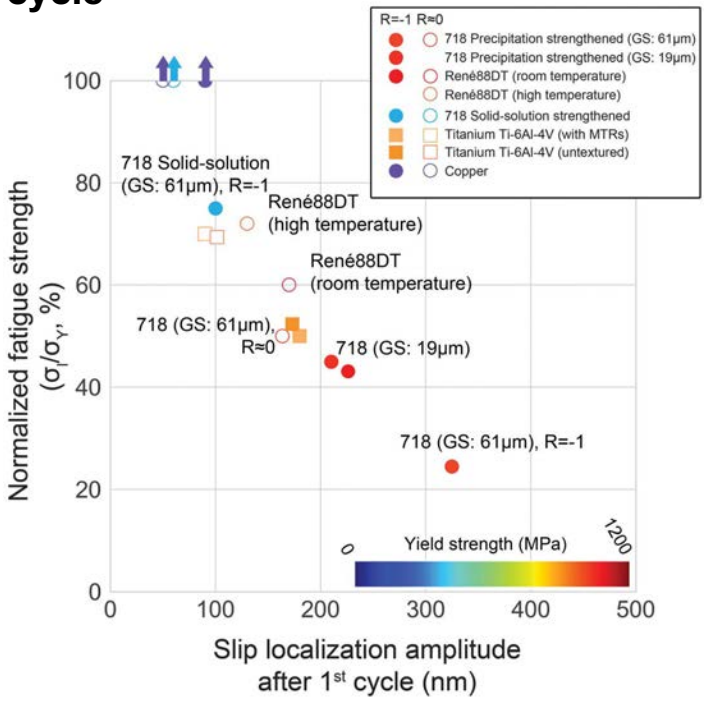
[Radovic 2022]

Develop Fast Methods to Assess Long-evolving Properties





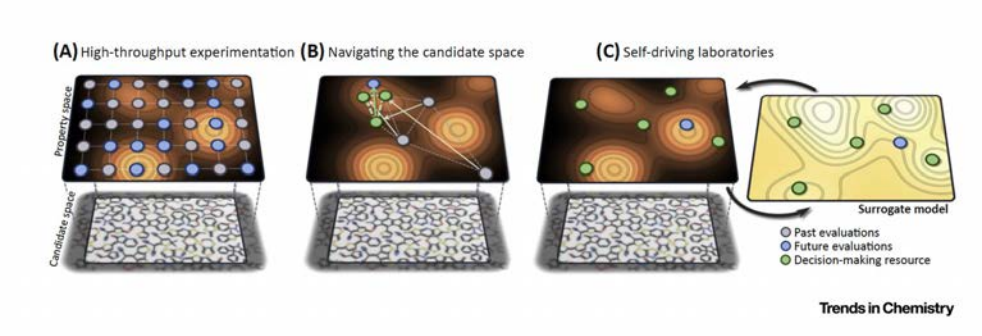
High Cycle Fatigue resistance assessment after **one cycle**



[Stinville 2022]

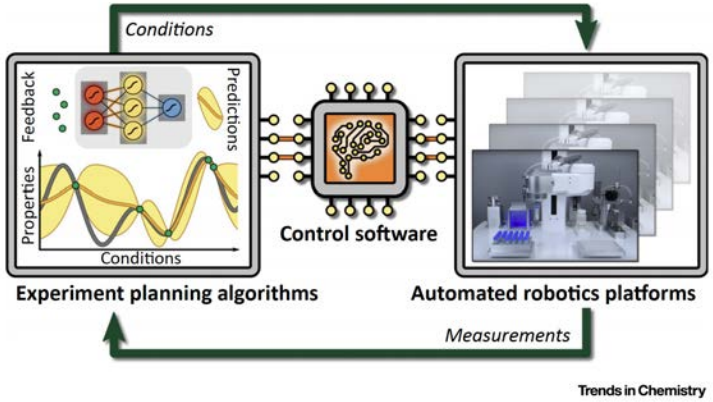
Blue-Sky: Develop Integrated Cyber-Physical Platforms

Self-driven Laboratories:



[Haase, 2019]

In practice:
Decision-Making Algorithm* + Robotics



*Given their data-efficiency, most algorithmic decision support is based on Bayesian Optimization (BO) approaches

My own (naïve) thoughts

1. What promising AI / ML architectures can be used for rapid discovery of new fusion materials? How might these work with material computational modeling tools? What are the pros and cons of these approaches?
   - BO-based approaches, Physics—Informed ML Inference and Acceleration
2. Without considering economics, how confident are you that we can use ML/AI to find a better performing alloy to serve as PFC (plasma facing component) material to replace the current leading candidates (e.g., RAFM, W, V4Cr4Ti)?
   - I am (mildly) confident that there may be better options than current candidates
3. Which of the following properties in Table 1.1., if any, do you believe is *infeasible* to optimize based on current ML/AI tools for material discovery, and why?
   - % elongation at fracture, swelling, creep, fatigue will be **extremely challenging to design for**
4. Can you name any additional material properties that should be optimized to make an impact for commercial FPPs? What are the relevant ranges of those properties? What tests do you need to validate these properties? –No idea
5. Is it feasible for current ML/AL tools to automatically generate new material specifications for existing manufacturers to fabricate commercial fusion components? If not, what is missing?
   - To make this possible, we **must** consider co-design (materials and process)
6. What other opportunities/challenges/issues at code and simulation level for rapid material design should we consider?
   - **Orders of magnitude acceleration (diffusive times at atomic scales)**

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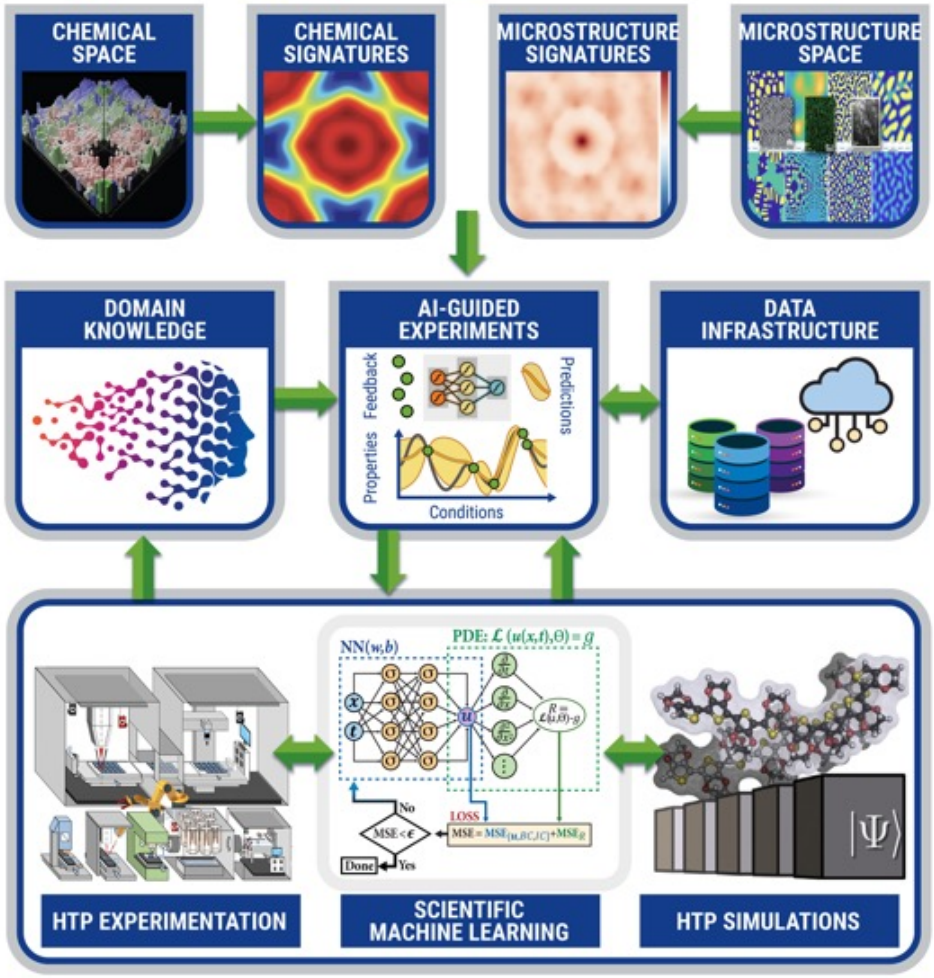
Final Remarks

- Alloy discovery occurs in the **sparse data regime** (this is NOT a big data problem)
- From our experience, iterative alloy discovery loops with multiple objectives and constraints with de-localized resources have a discovery rate ~20 alloys/month
- Deployment of BO itself can be quite expensive, requiring supercomputing power (~1000 cores for 3 days per iteration)
- Integrated synthesis-processing-characterization-testing platforms may accelerate discovery rate (~20 alloys/week?)
- Rate of discovery is limited by slowest task in discovery loop
- Further advantages arise when using physics-informed ML
- Ideally, we want **cyber-physical** platforms, with experimental platforms coupled with dedicated supercomputing resources



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Thanks!