Design of Engineering Material Systems from an Engineering Design Perspective

Chris Paredis
Georgia Institute of Technology
George W. Woodruff School of Mechanical Engineering
H. Milton Stewart School of Industrial and Systems Engineering
Director, Model-Based Systems Engineering Center
chris.paredis@me.gatech.edu

Overview

- What is Design?
  - My perspective and mental model of design
  - Design as a search and learning process
- Design Research
  - Current research topics in design
  - Research methodology
- Design Research in a DEMS context
  - Bottom-up vs. Top-down

What is Design?

Design is a Process with a Purpose… Maximizing Value

- “Everyone designs who devises courses of action aimed at changing existing situations into preferred ones”

  — Herbert Simon, The Sciences of the Artificial

- How do we, engineers, change existing situations?

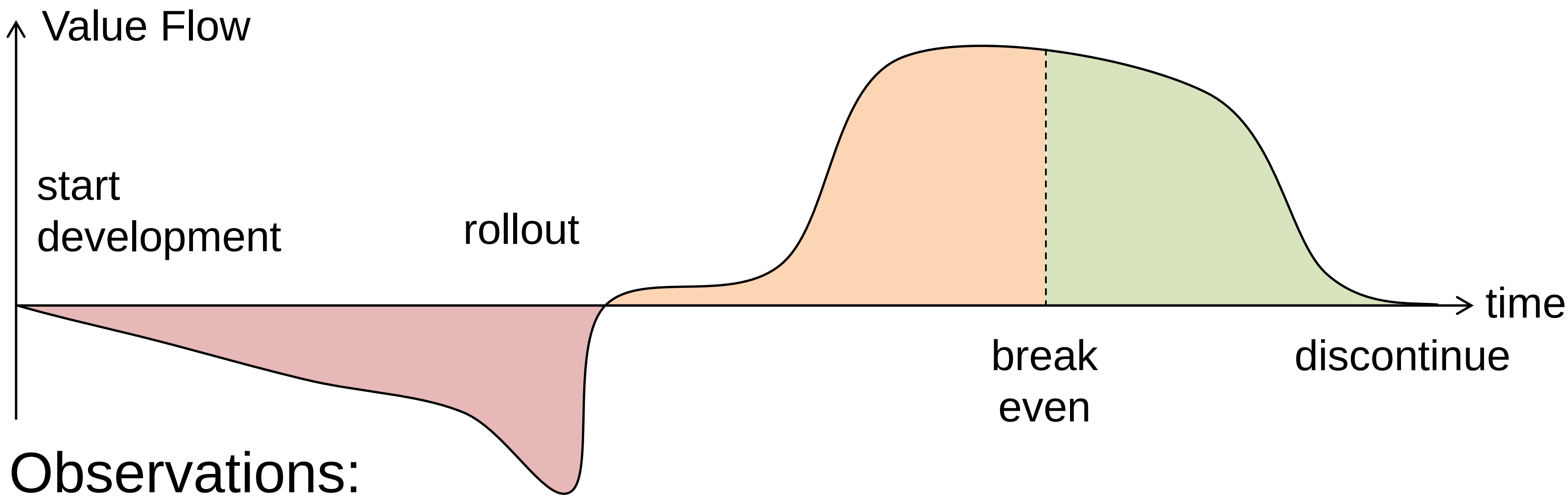
→ By creating or improving artifacts — such as materials…

- Design is a planning process
  - Primarily a process of information transformation
  - We develop a systematic plan—a model—for how to add value
  - In the final phase, we produce the artifact by executing the plan

In Design, we create a model for how to add value

What do we Mean by Preferred Outcomes?

Value over the Product Lifecycle



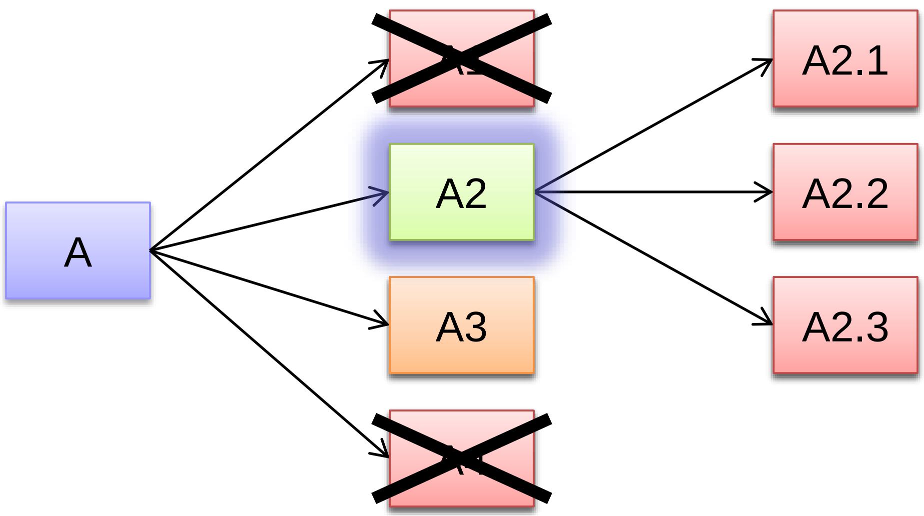
- Observations:
  - Value flows occur in the future → must account for time preferences
  - Value flows are uncertain → must account for risk preferences
  - The cost of development influences the overall outcome → must trade off cost/time of development vs quality of artifact → heuristics

$$\mathcal{A}\colon \max_{a \in A} \mathrm{E}\left[u\left(NPV\left(a, t(\mathcal{A}), C(\mathcal{A})\right)\right)\right]$$

Search: A Directed Process for Adding Value

Strategy for Adding Value Effectively

- Ideation → Analysis and Evaluation → Selection or Pruning



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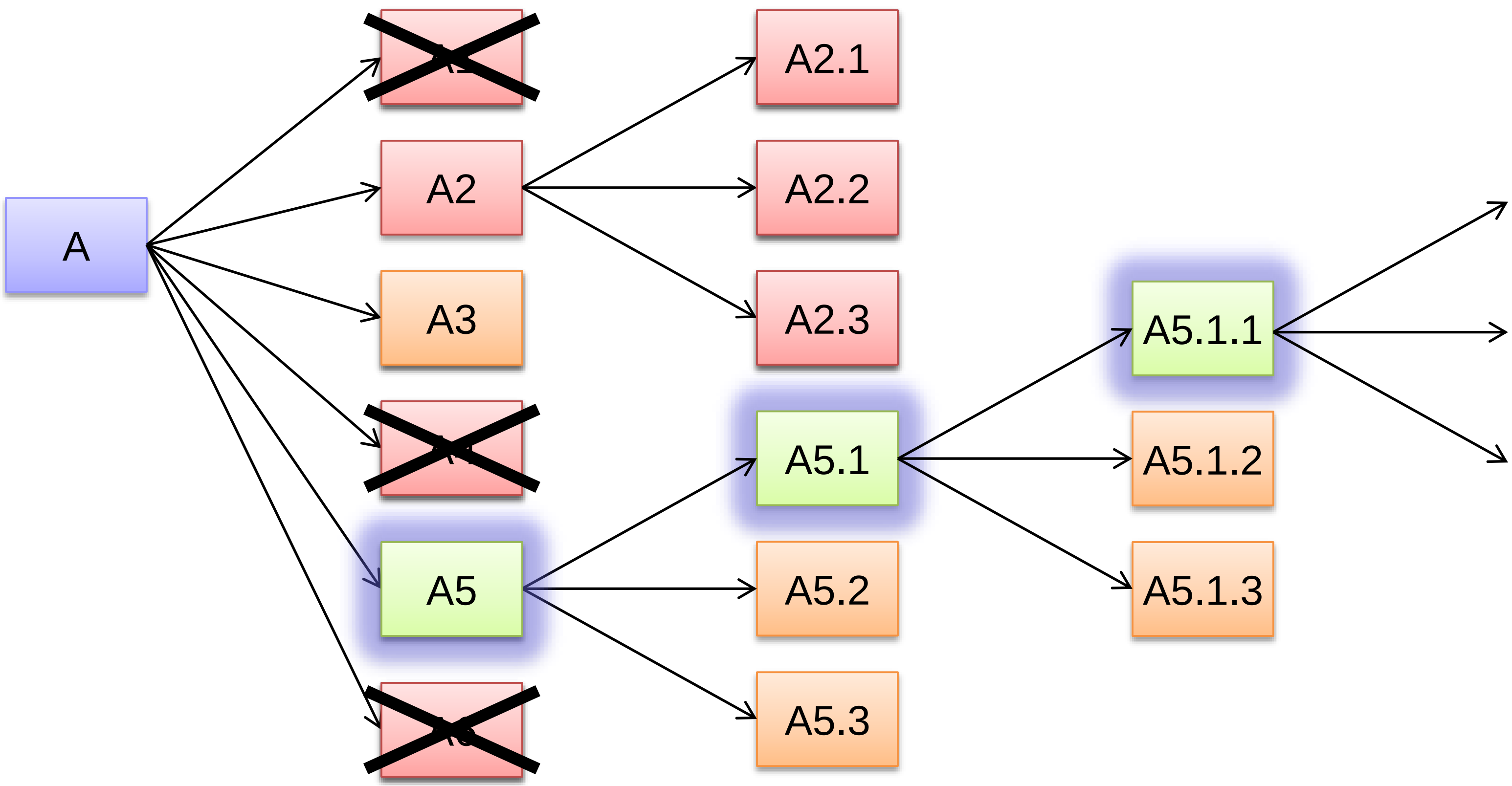

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Design as Search

Reframing as a Process Search

$$\mathcal{A}: \max_{a \in A} \mathrm{E}[u(NPV(a, t(\mathcal{A}), C(\mathcal{A})))]$$

- Maximization from a process perspective:

$$\mathcal{P}: \max_{p \in P} \mathrm{E}\left[u\left(NPV\left(a(p), t(p), C(p)\right)\right)\right]$$

  - In Design, we make choices about the process, and only indirectly about the artifact
  - Process choices are irreversible; artifact “choices” can be reconsidered
  - Because the cost of optimizing the process is often larger than the expected benefit, we rely on **heuristics**

Design as Learning

- Explore a new, previously unknown set of alternatives
  → In the course of the search process, we learn!

- The new knowledge has value beyond the current search process… it can be captured/stored and applied towards future problems

- We need to find a good balance between:
  – Exploitation of existing knowledge
  – Exploration to gain new knowledge

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Design Research

- Computational — Decision support tools
  - Representation
  - Uncertainty analysis and decision making under uncertainty
  - Design optimization, reasoning & inference
  - Knowledge capture and reuse — modeling, ontology engineering
- Design as a human activity
  - Ideation, creativity, abstraction, systems thinking,…
  - Sensemaking, framing
  - Multiple decision makers, systems of systems
  - Design in an organizational context — decomposition & delegation, concurrency, organizational design

Design Research Methodology

- Goal:
  - Understand — develop explanatory models
  - Improve — develop better methods and tools
- Collecting evidence in support of research claims
  - Deductive arguments based on theoretical foundations
  - Computational experiments
  - Controlled human subject studies
  - Field work — observation of design teams in context

Design research ≠ Solving a design problem

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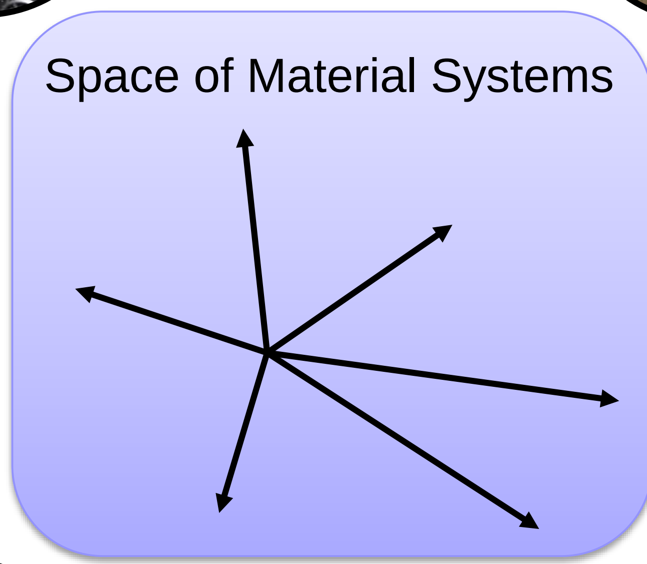
An Ever-Expanding Space of Alternatives

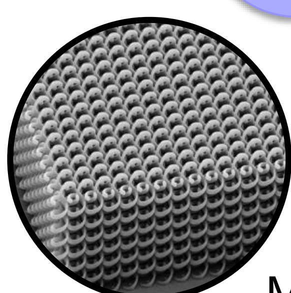
Metals

Ceramics

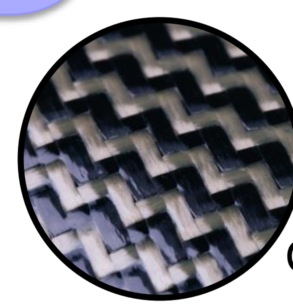


“Smart” Material Systems

Polymers

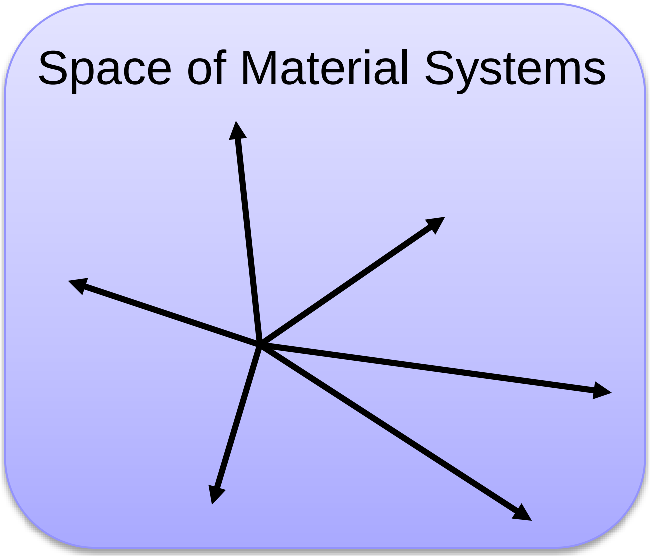


Metamaterials

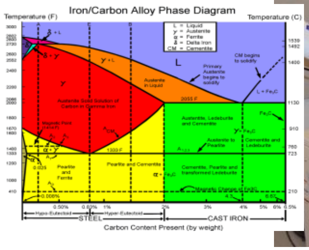


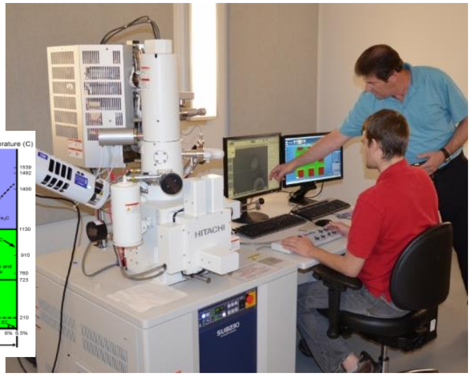
Composites

Bottom-Up Exploration



Bottom-Up Exploration

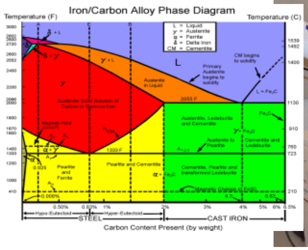


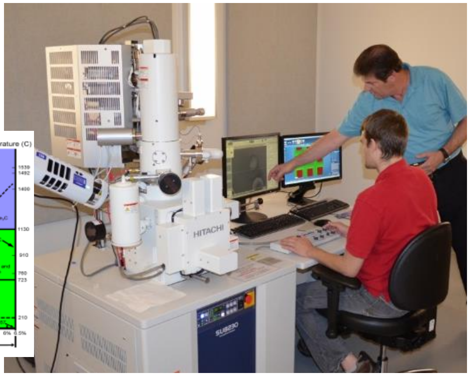


Bottom-Up Exploration

- More efficient experimentation
  - Faster generation of samples
  - Faster characterization
  - … even if it requires sacrificing some accuracy
- More focused experimentation
  - Focus on areas of the materials space that are likely to be of interest, to be "valuable"
  - Bio-inspiration

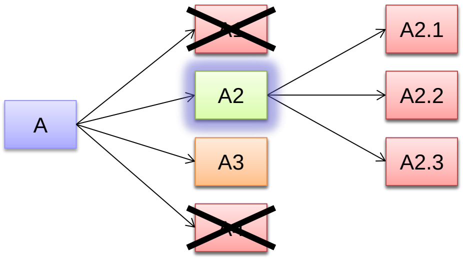
Bottom-Up Exploration

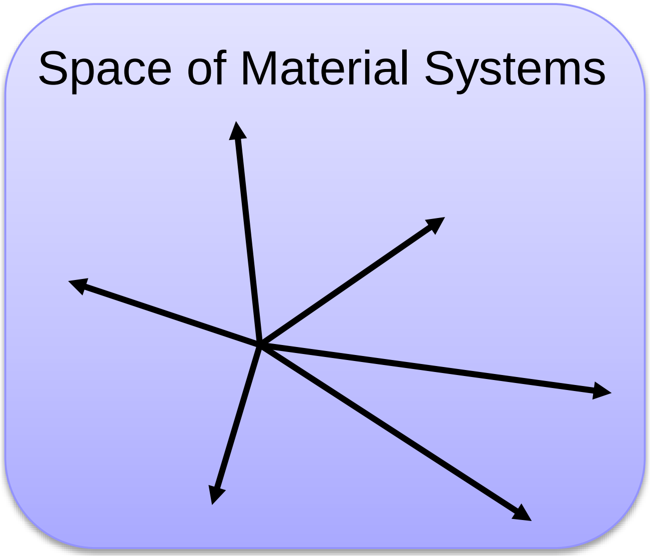




Top-Down Exploration

Top-Down Exploration





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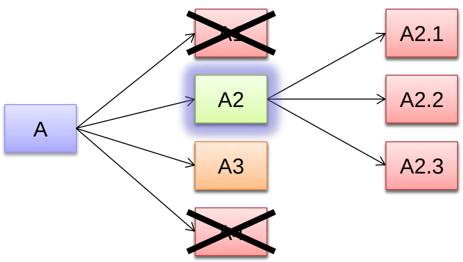
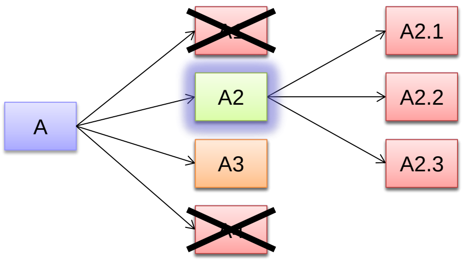


- Better exploration algorithms
  - Decomposition and Parallelization
  - Effective pruning
  - Suitable representation of alternatives
  - Use of most valuable analysis/prediction
    - » Requires info about accuracy and cost of predictions
- Better predictive models
  - Good tradeoff between accuracy and cost
  - Inexpensive…but limited accuracy
  - More accurate…but more expensive

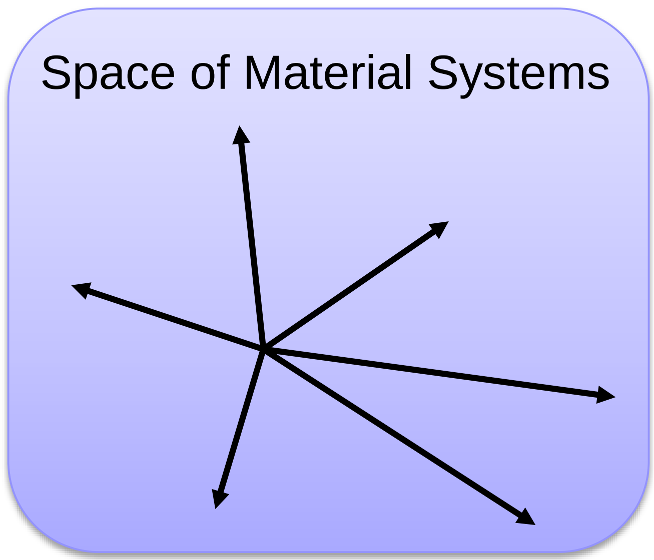
Bottom-Up vs Top-Down Exploration

Top-Down Exploration



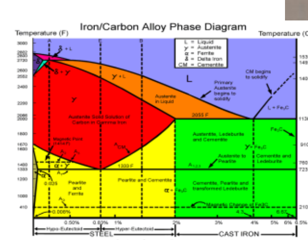
Efficient Search
- Divide and Conquer
- Model-based prediction

Informs



Focused, systematic, efficient experimentation

Bottom-Up Exploration



Informs

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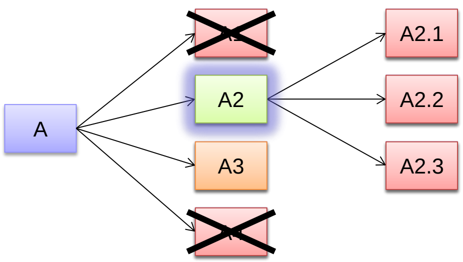
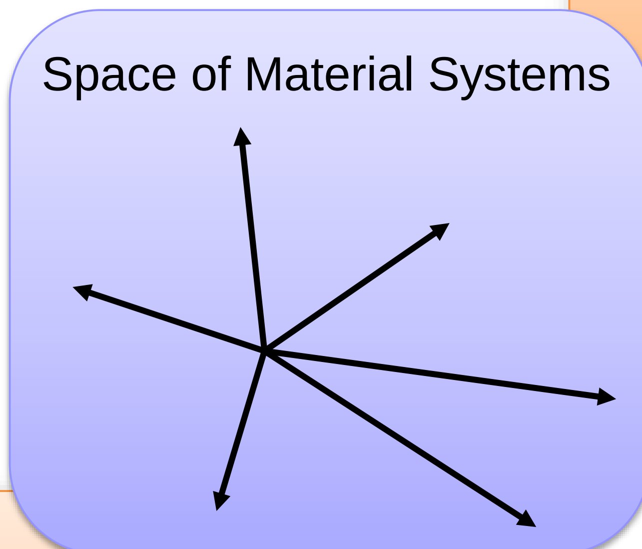


Efficient Search
- Divide and Conquer
- Model-based prediction

- How best to capture experimental observations in models?
  - Which abstractions?
  - Which formalisms?



- How best to guide the experiments towards promising alternatives?
  - Which tradeoffs?
  - Which accuracy?

Focused, systematic, efficient experimentation

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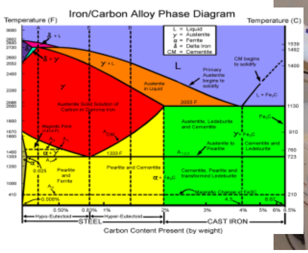

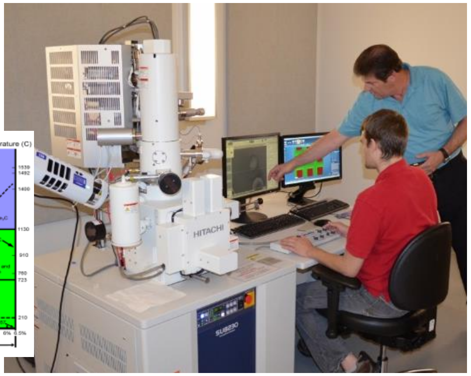

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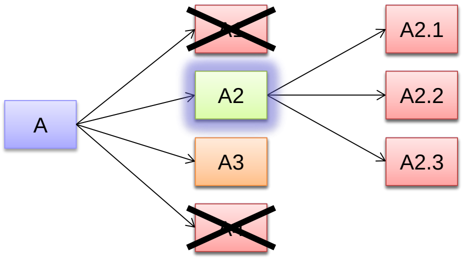

Efficient Search
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- In advance vs in-the-loop?
- How to update?
- Human role?

Focused, systematic, efficient experimentation

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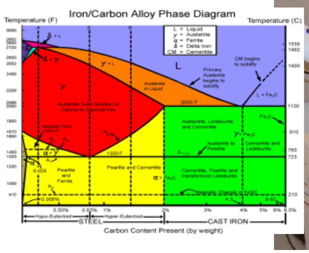

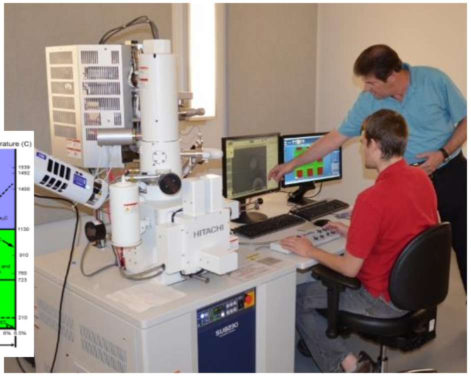

Design Faux-Pas

- I care about multiple materials properties → I should use a multi-objective optimization formulation
  - Theoretically/mathematically, Pareto frontiers are incompatible with decision-making under uncertainty
  - Pareto frontiers reduce the preferences space by one dimension → but how to choose a single alternative?
- "Inverse design" — what the heck does that mean?
- We will use atomistic/DFT analyses to predict properties and then do so a million times in a genetic algorithm

Summary

- Design → Efficiently, purposefully, and systematically search for alternatives leading to preferred outcomes
- How can we explore an almost infinite space of material systems more efficiently?
  - Determine how best to capture materials knowledge for design purposes
  - Use design to guide the discovery of new, valuable materials
- Research Methodology
  - Collect evidence in support of claim that the search for material with desired properties is more efficient/effective