AI FOR R&D AND MANUFACTURING

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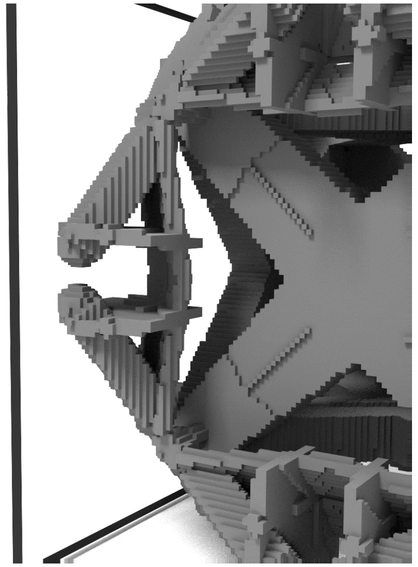
MIT

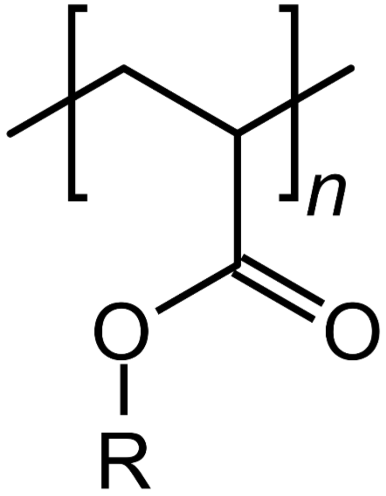
Why AI for R&D and Manufacturing?

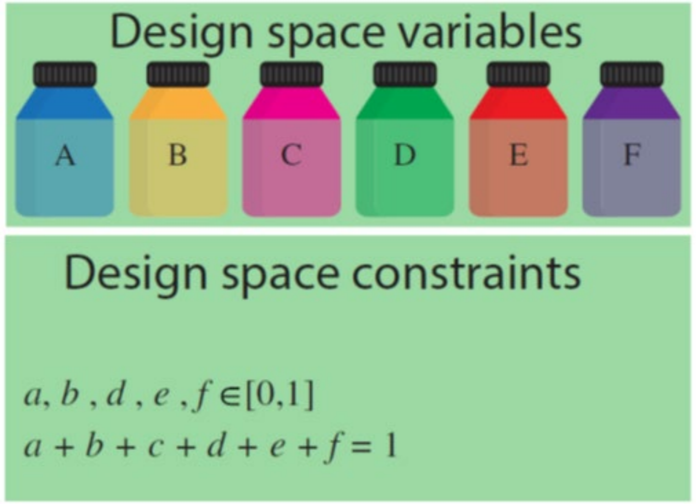
- Automatically evaluate many more designs than a human can do manually
  - Accelerate product design process
  - Reduce R&D costs
  - Generate higher performing products
- Provide a layer of intelligence for manufacturing processes
  - Automatically tune manufacturing process
  - Improve yield and accuracy
  - Predict and schedule maintenance

Design Space

- A family of designs representing a given category
- Examples of a design space
  - a parametric design in CAD
  - all possible polyacrylate polymers
  - concentration of components in a formulation

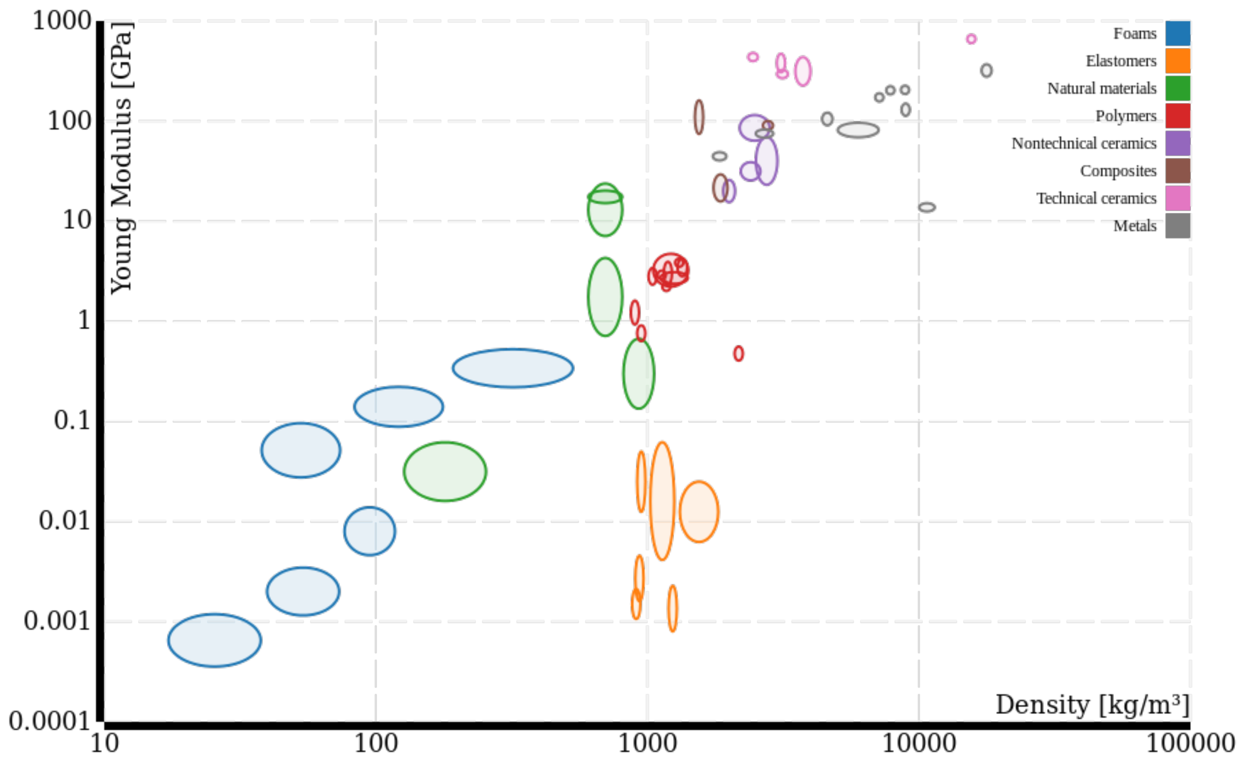






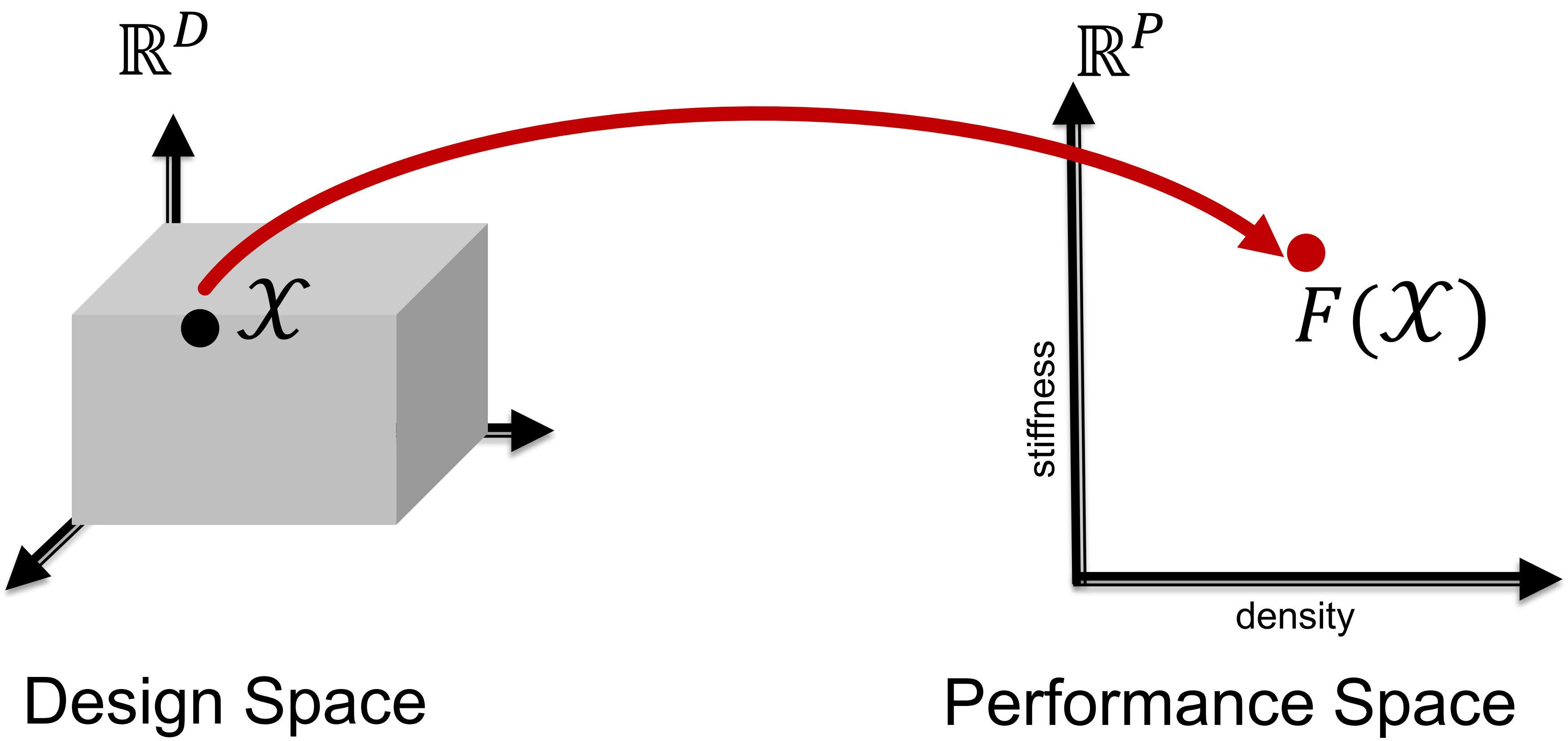
Performance Space

- Range of material properties
- Ashby/material property charts



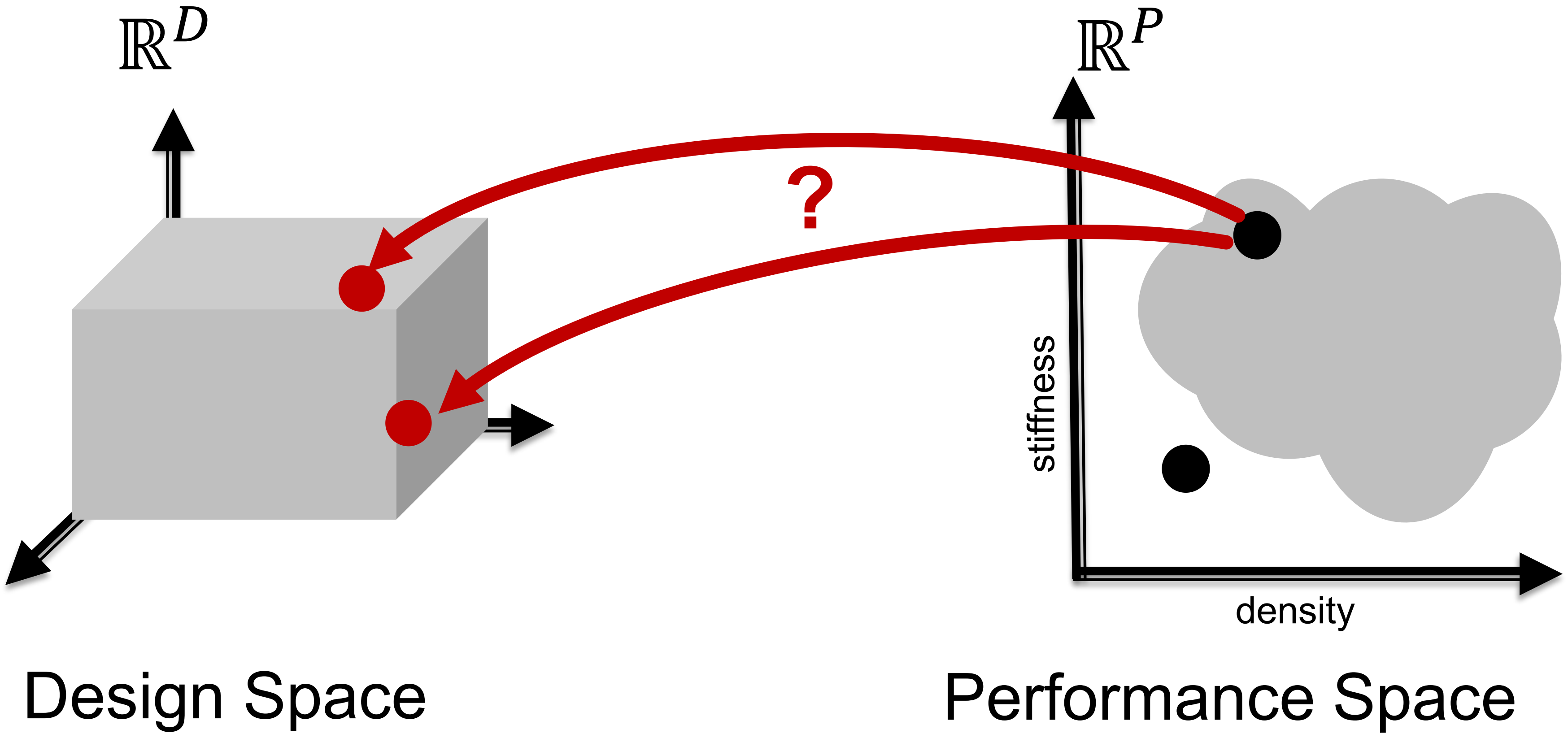
From Design to Performance

- Numerical simulations (or real experiments) map a point in design space to a point in performance space

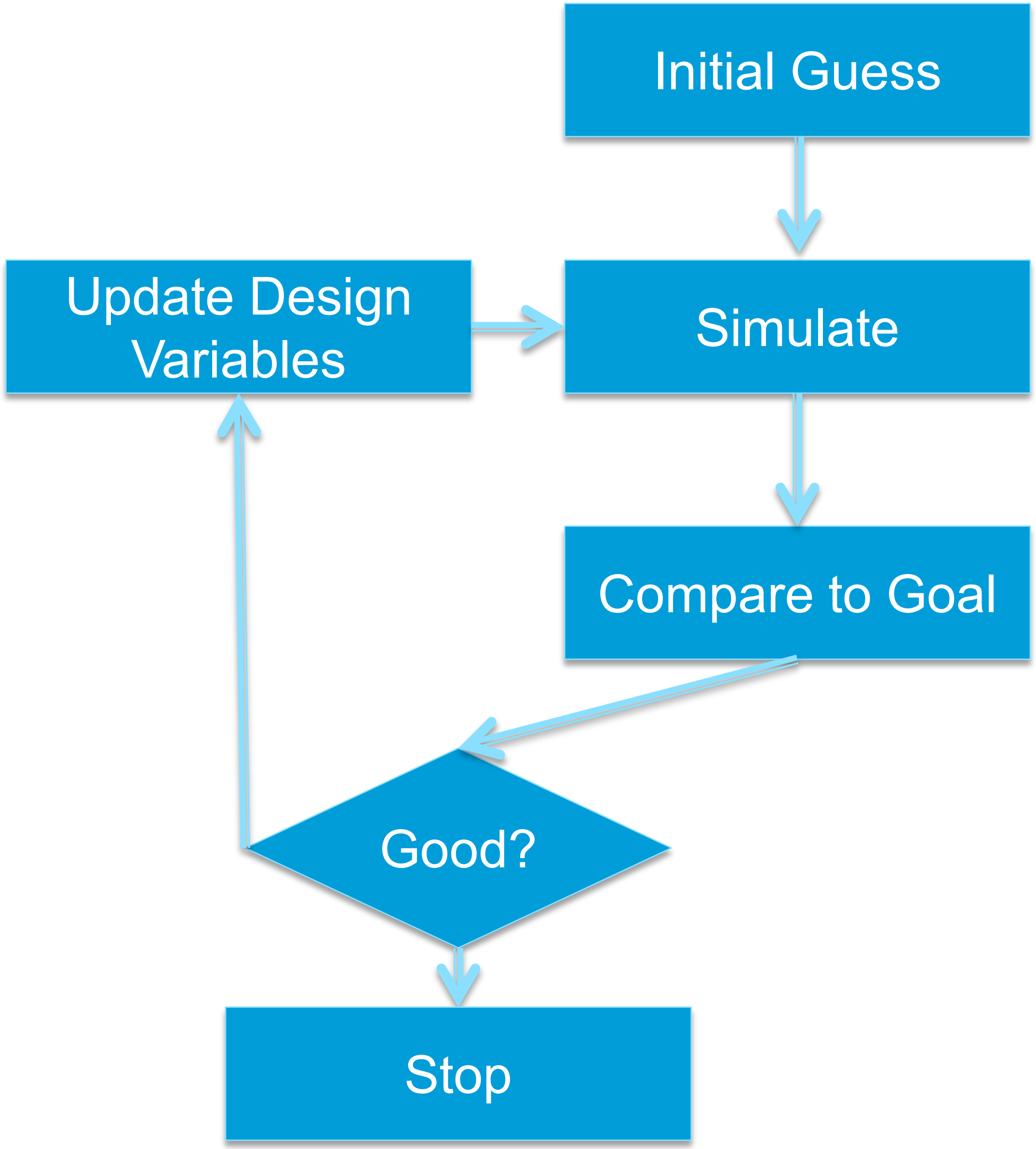


Inverse Design

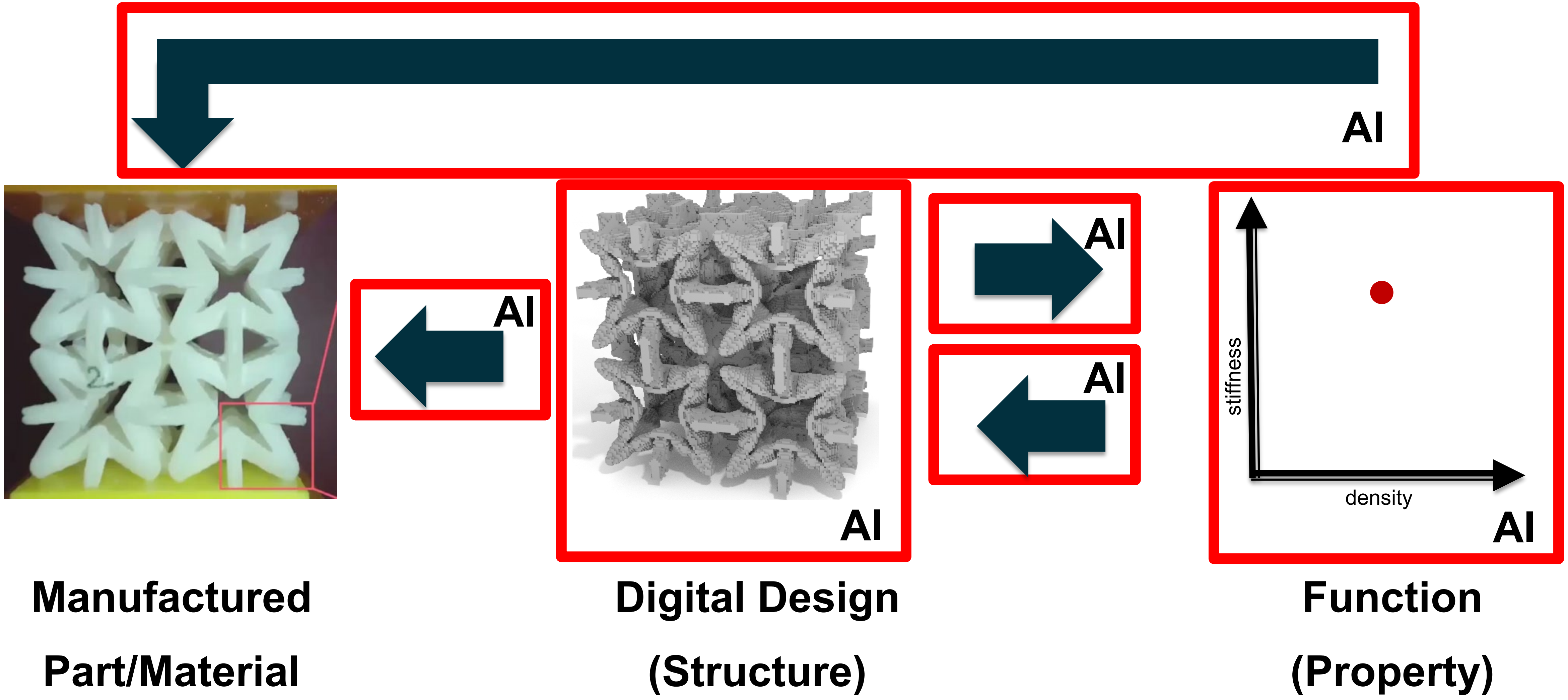
- Inverse problem is much more difficult



Inverse Design Involves Search

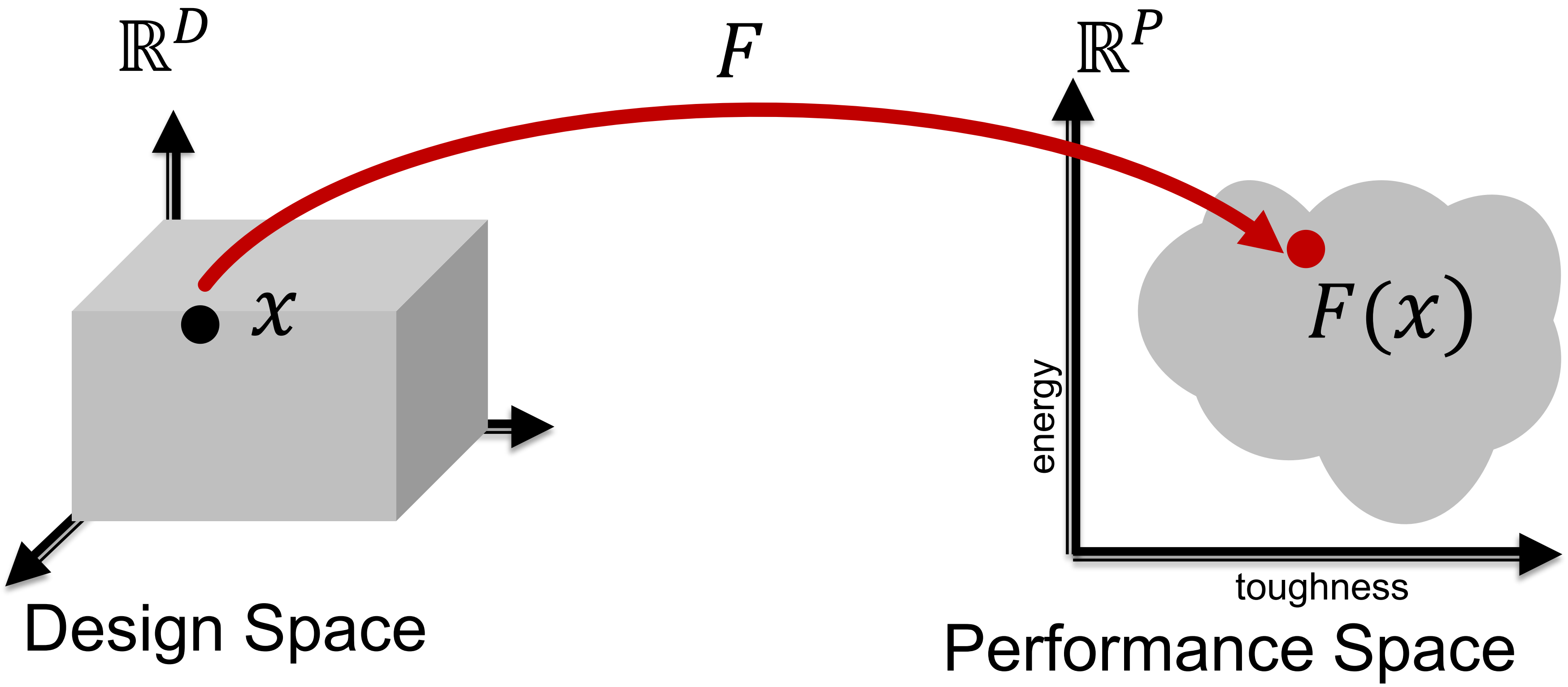


AI-based Computational Design

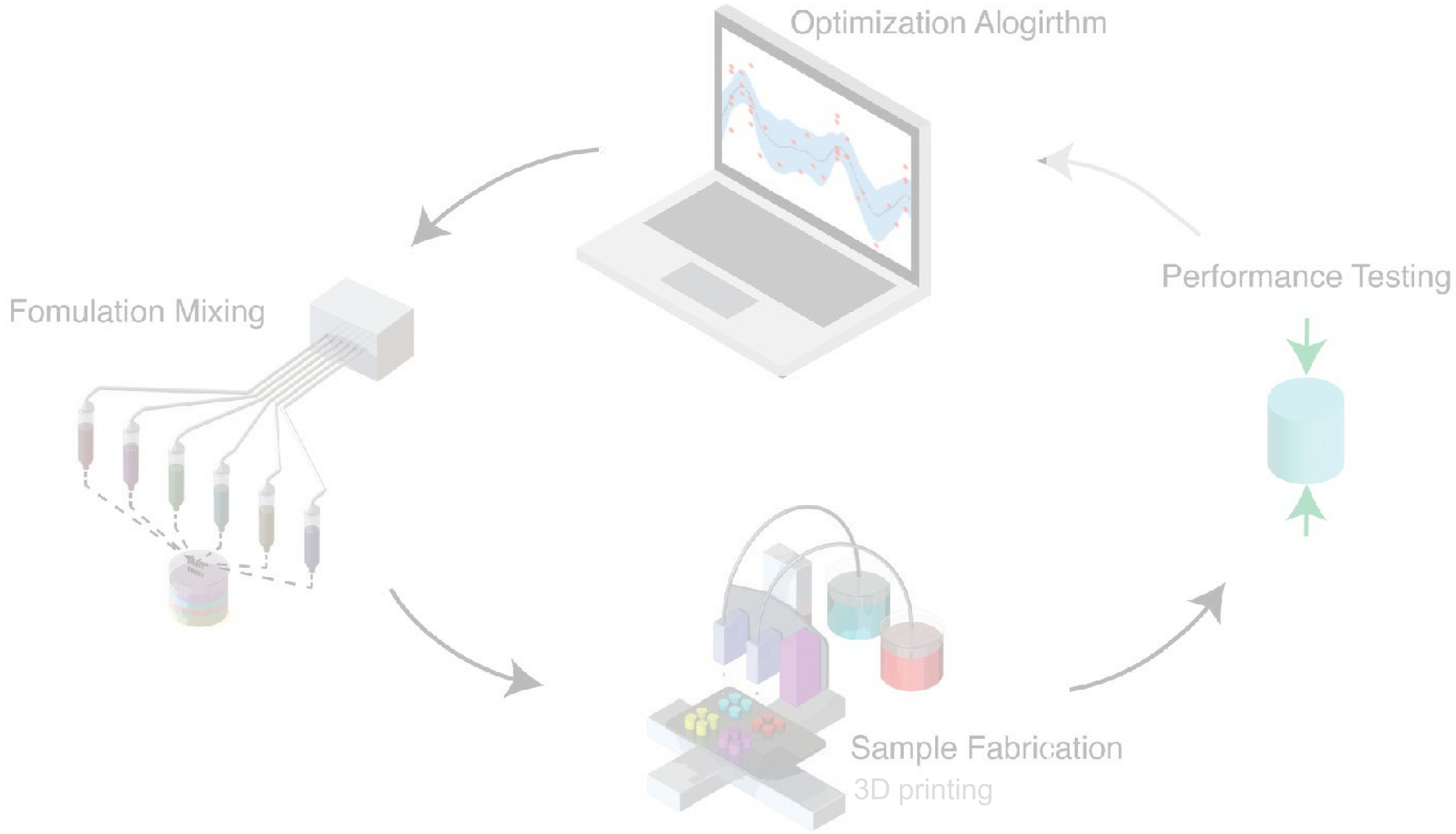


Combined AI Forward and Inverse

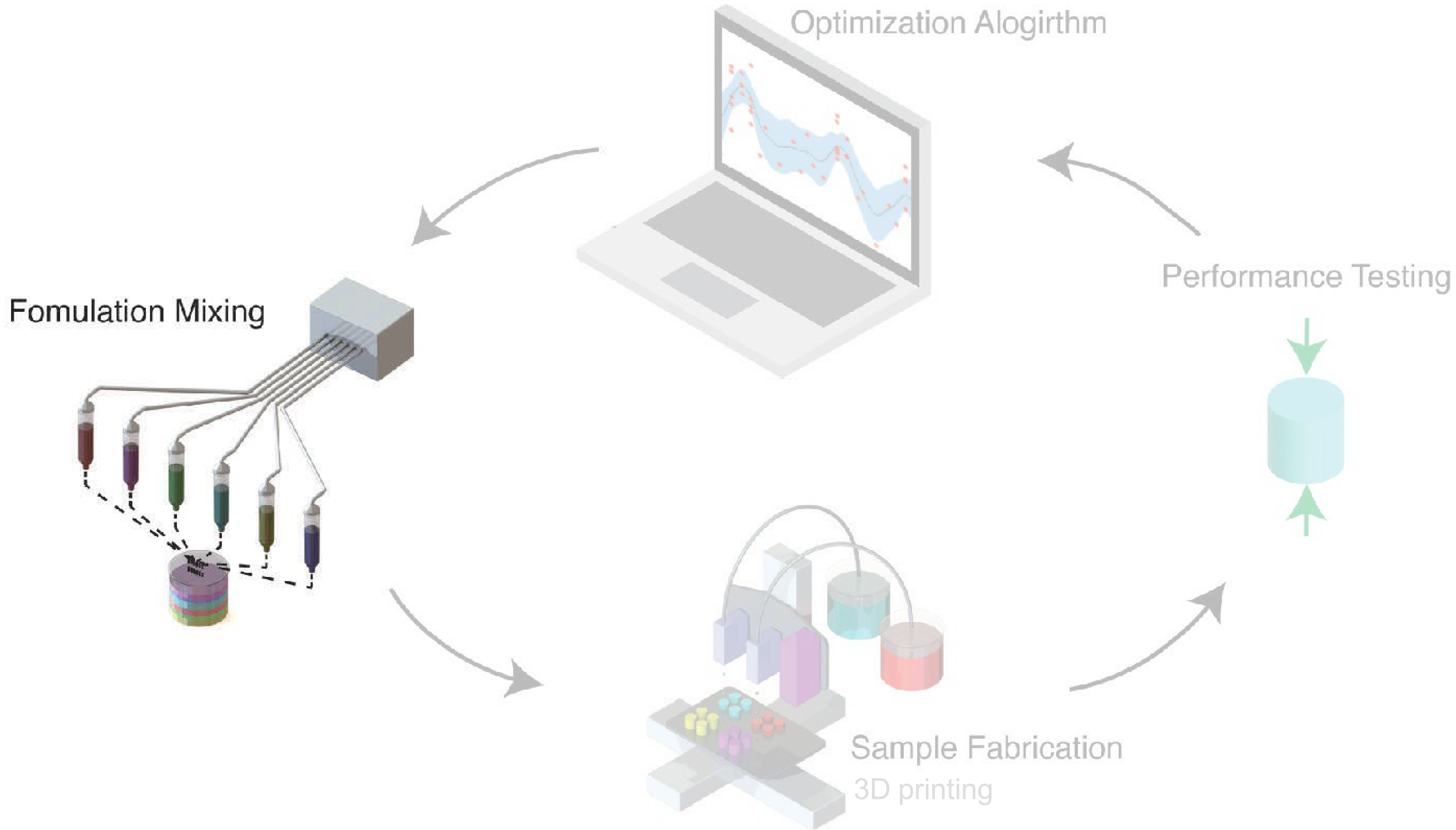
- Numerical simulation does not exist (or it is very slow to compute)
- We can make samples (e.g., materials) and measure their properties
- Samples are made sequentially or in batches
- How to select which samples to evaluate?



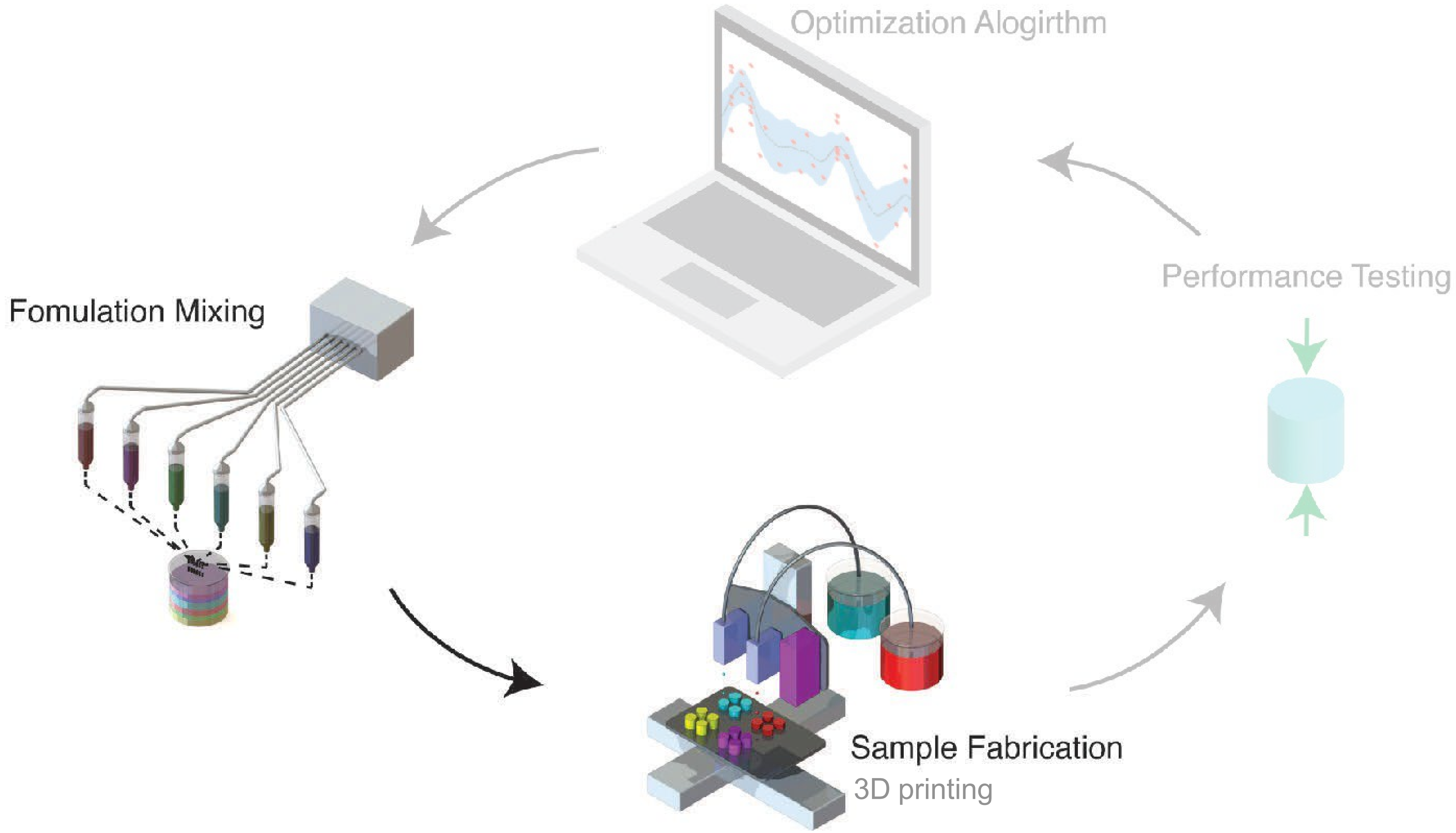
Discovery of Optimal Formulations



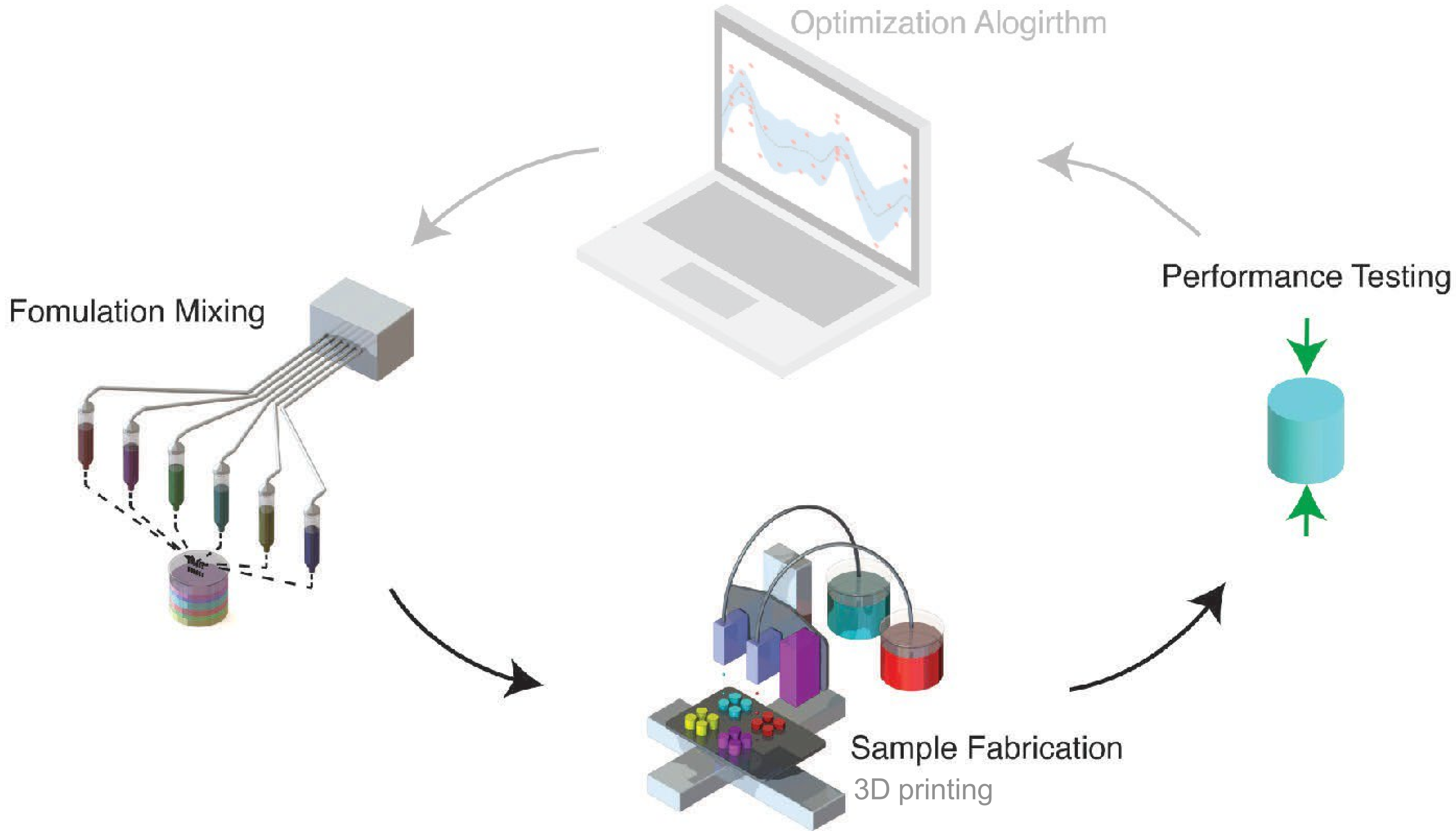
Discovery of Optimal Formulations



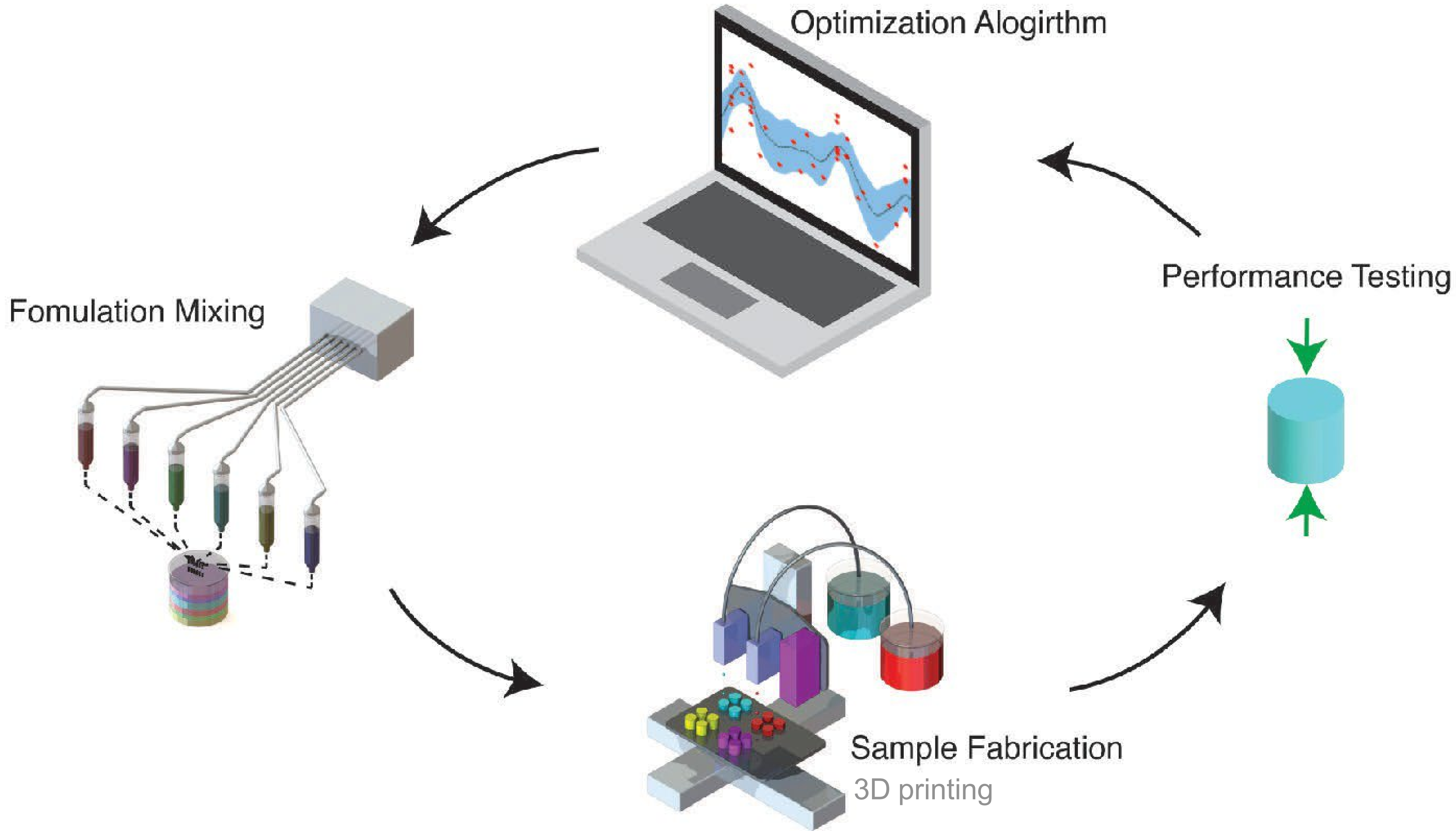
Discovery of Optimal Formulations



Discovery of Optimal Formulations



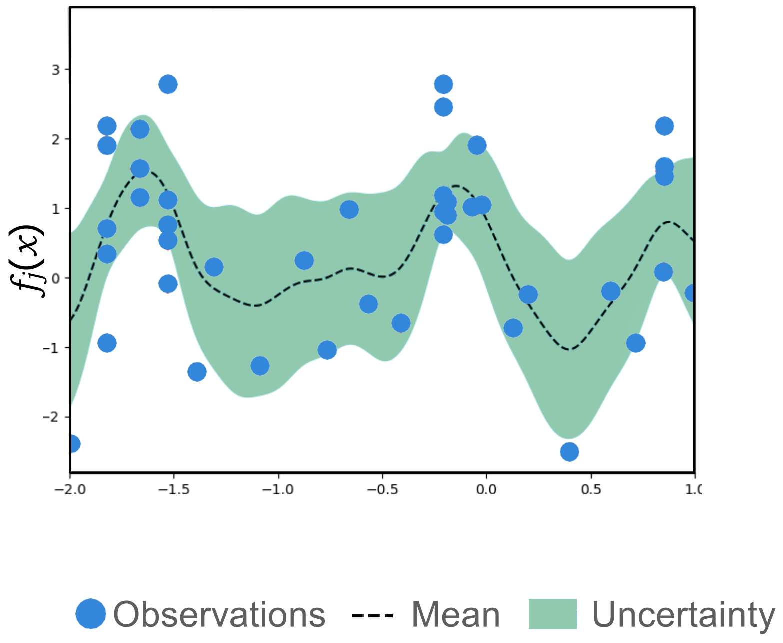
Discovery of Optimal Formulations



Multi-objective Bayesian Optimization

Surrogate model

Fit GPs for each objective f_j

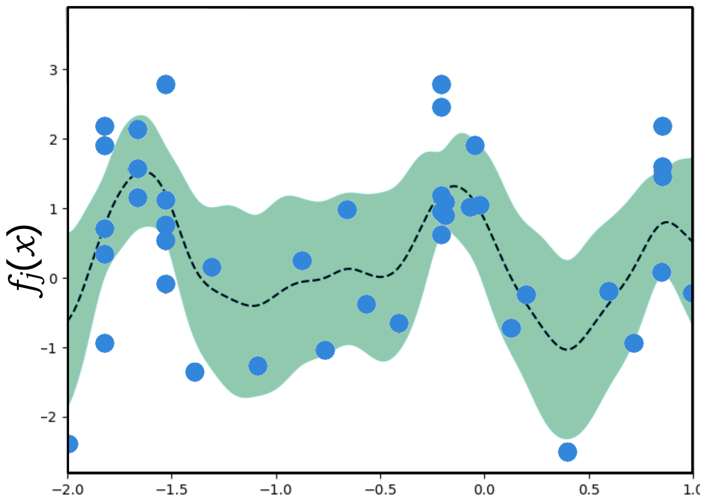


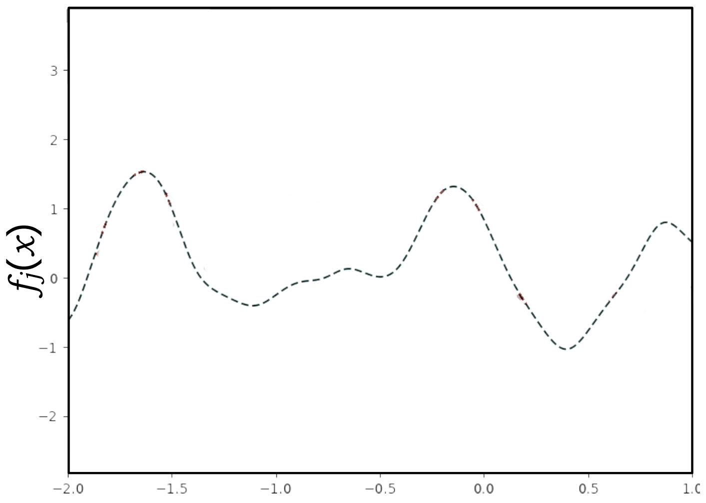
Multi-objective Bayesian Optimization

Surrogate model → Acquisition function

Fit GPs for each objective f_j

Approximate functions f_j from mean of GPs





Observations --- Mean Uncertainty

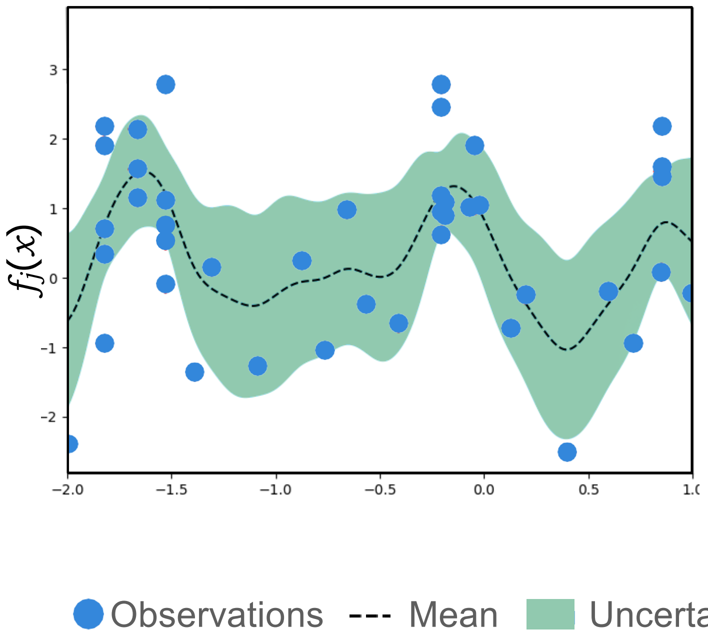
Multi-objective Bayesian Optimization

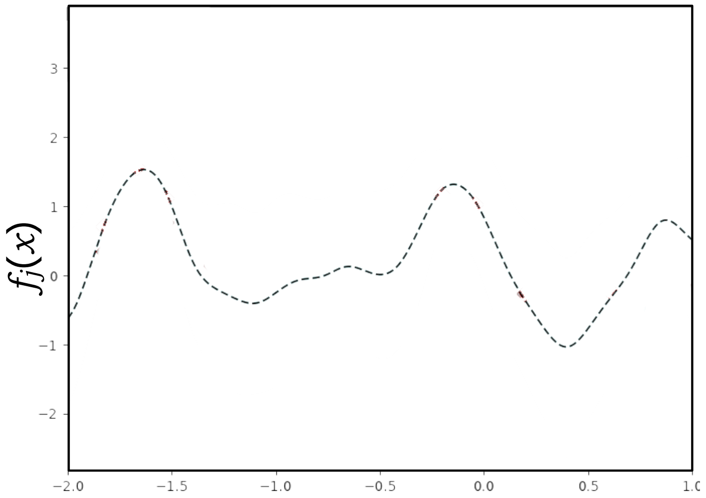
Surrogate model → Acquisition function → Multi-objective solver

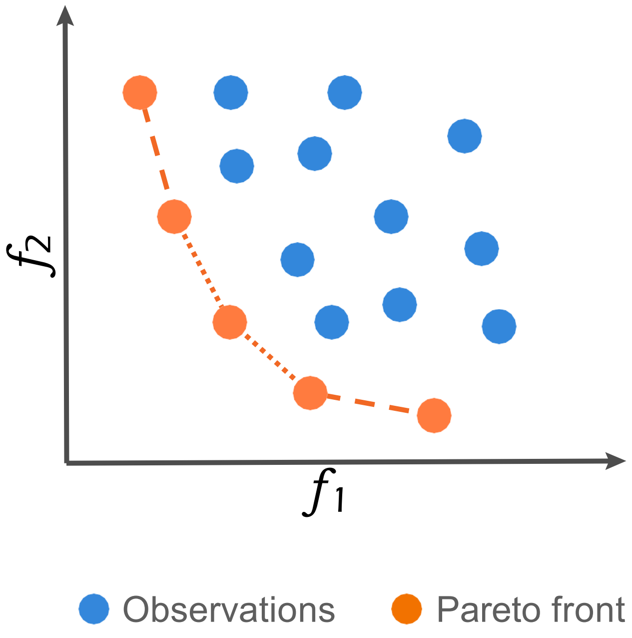
Fit GPs for each objective f_j

Approximate functions f_j from mean of GPs

Approximate Pareto set and front over all f_j







Multi-objective Bayesian Optimization

Surrogate model → Acquisition function → Multi-objective solver → Selection

Surrogate model

Fit GPs for each objective f_j

Acquisition function

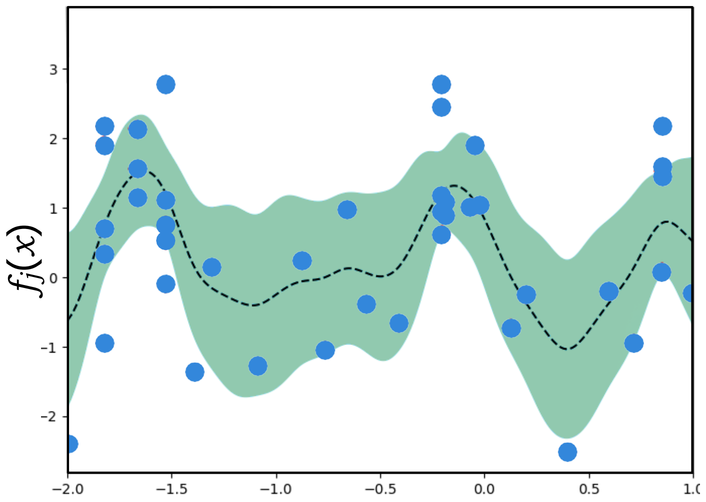
Approximate functions f_j from mean of GPs

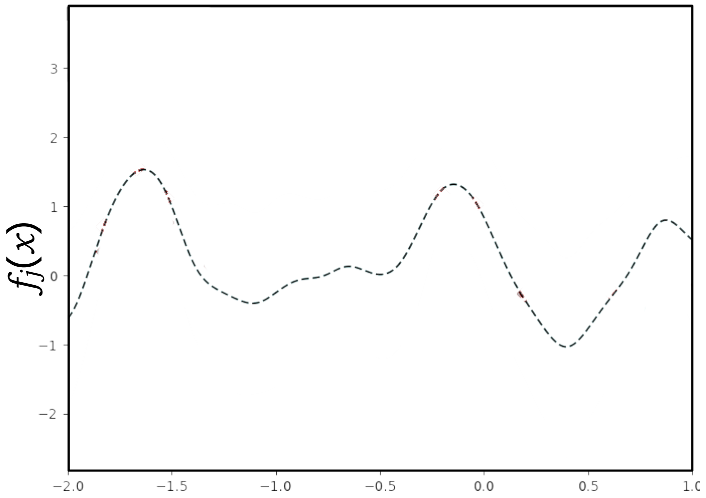
Multi-objective solver

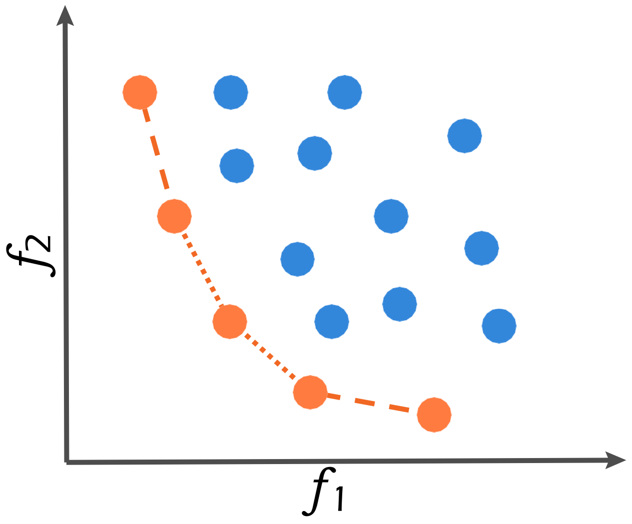
Approximate Pareto set and front over all f_j

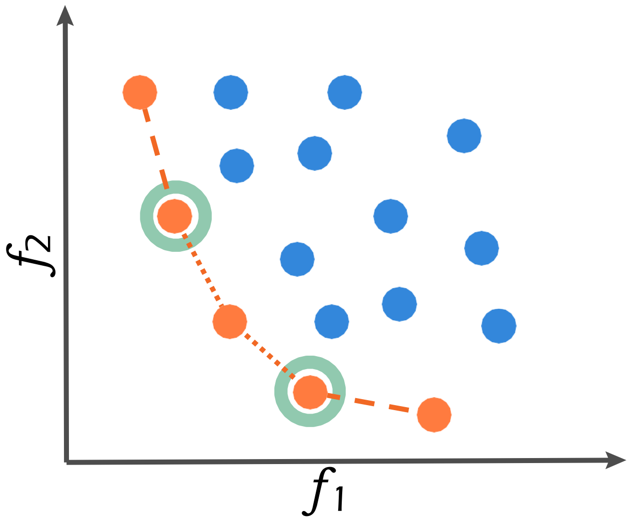
Selection

Propose a batch of points to evaluate next









Observations --- Mean Uncertainty

Observations Pareto front

Selected points

Multi-objective Bayesian Optimization

Evaluate proposed points

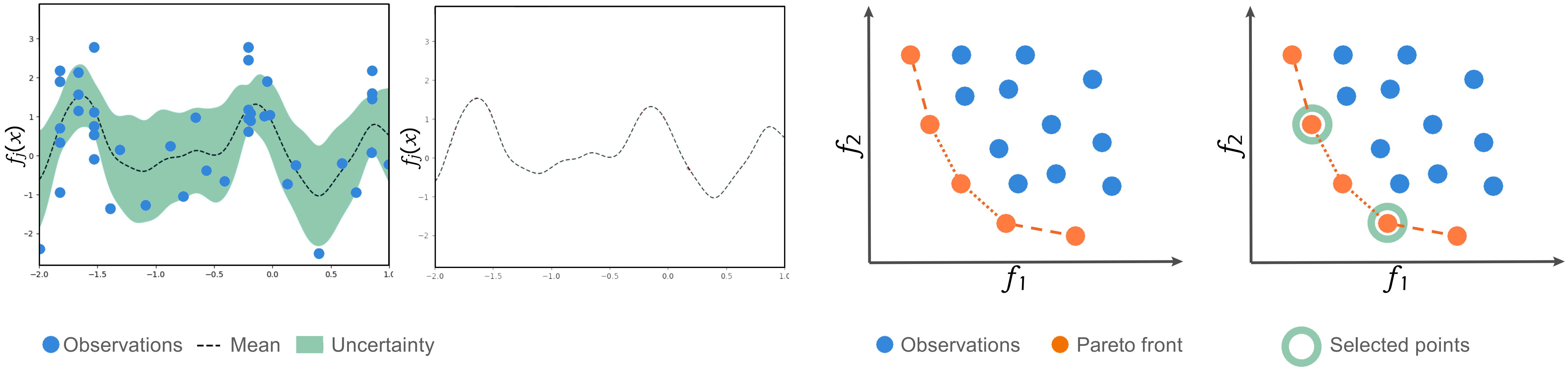
Surrogate model → Acquisition function → Multi-objective solver → Selection

Fit GPs for each objective f_j

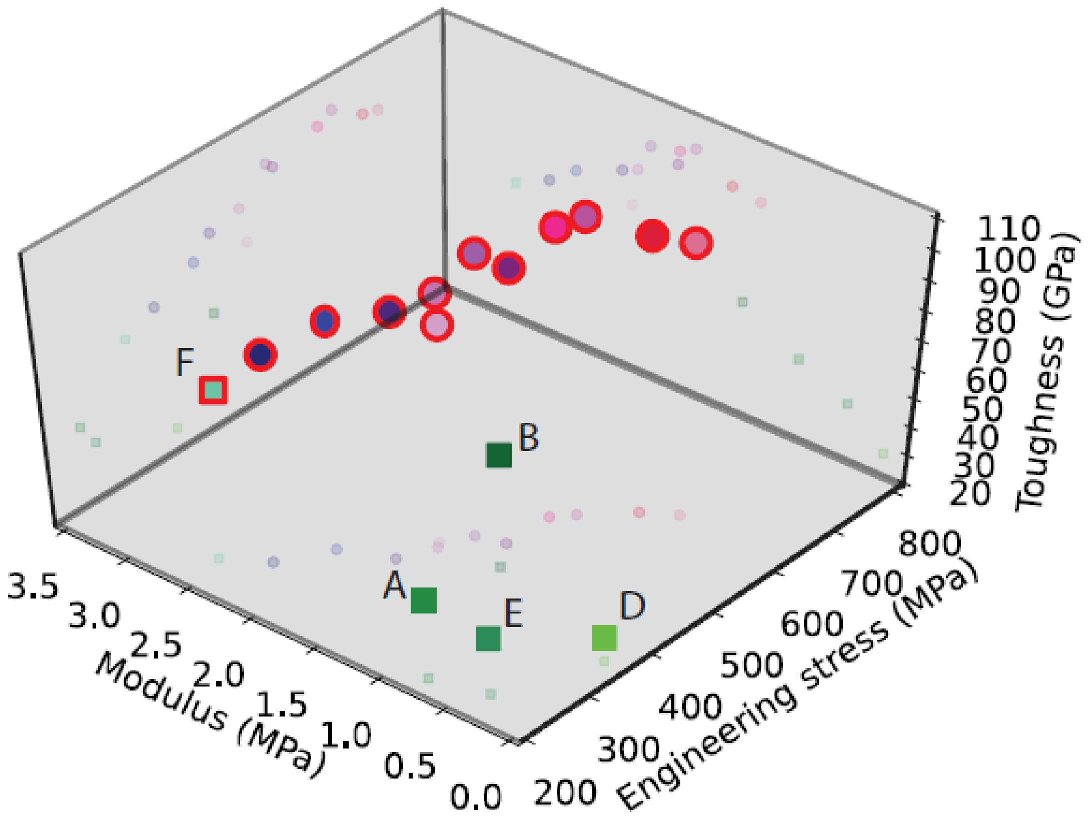
Approximate functions f_j from mean of GPs

Approximate Pareto set and front over all f_j

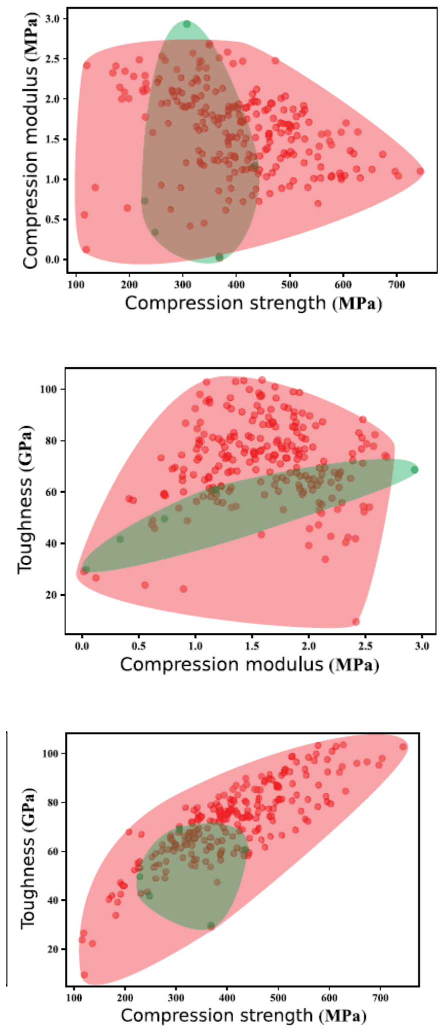
Propose a batch of points to evaluate next



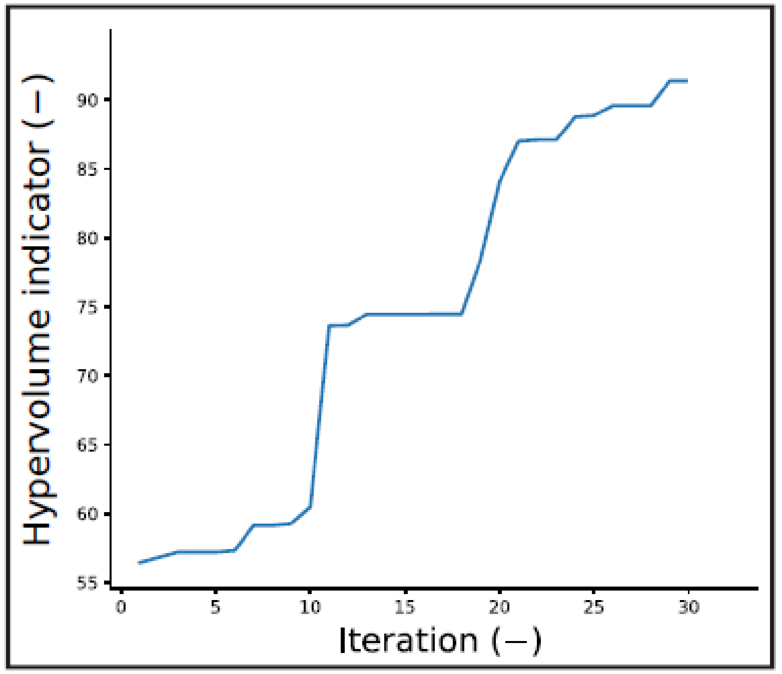
Results



Toughness (GPa)
Modulus (MPa)
Engineering stress (MPa)
A
B
D
E
F

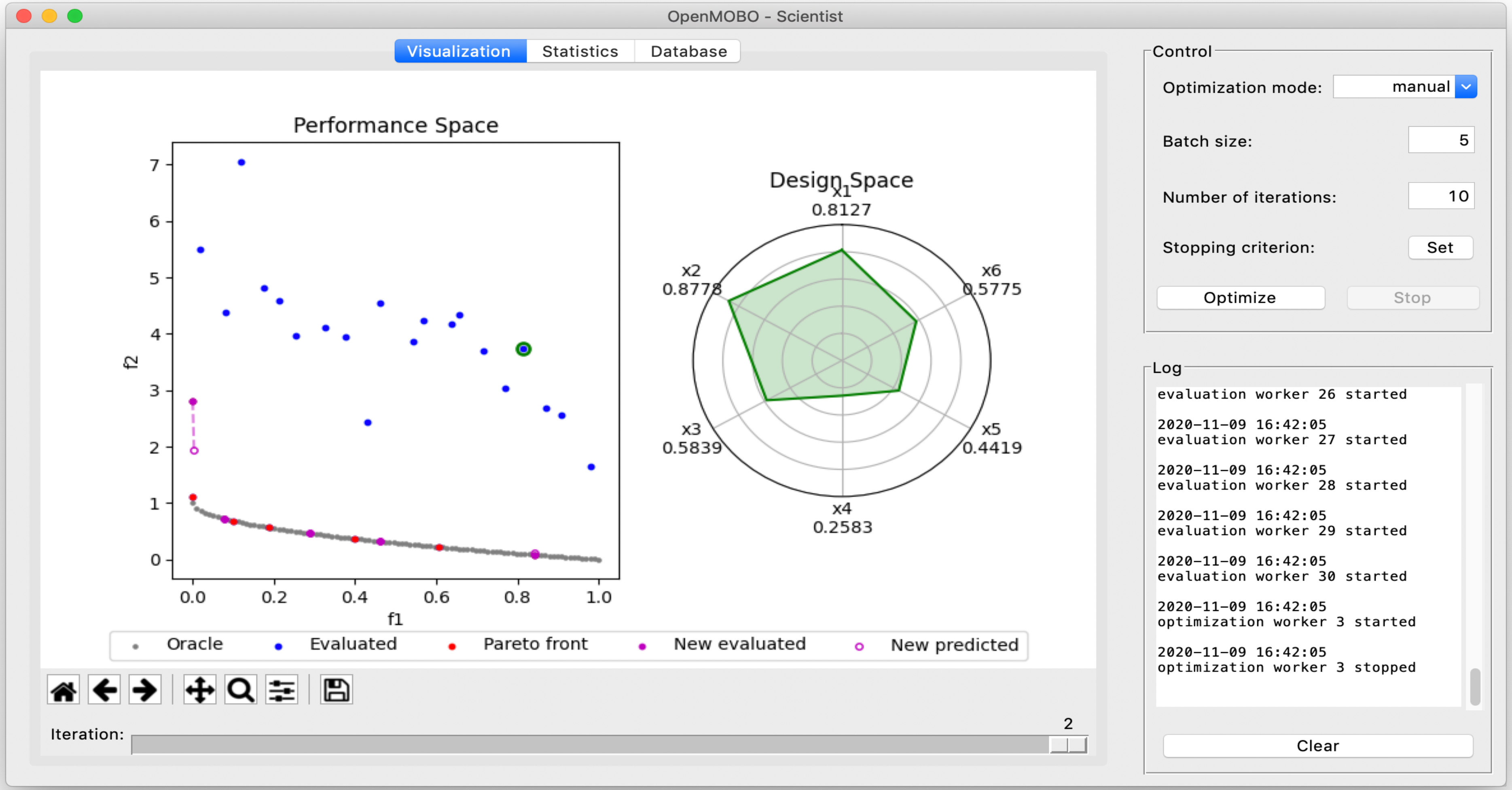


Compression modulus (MPa)
Compression strength (MPa)
Toughness (GPa)
Compression modulus (MPa)
Toughness (GPa)
Compression strength (MPa)



Hypervolume indicator (−)
Iteration (−)

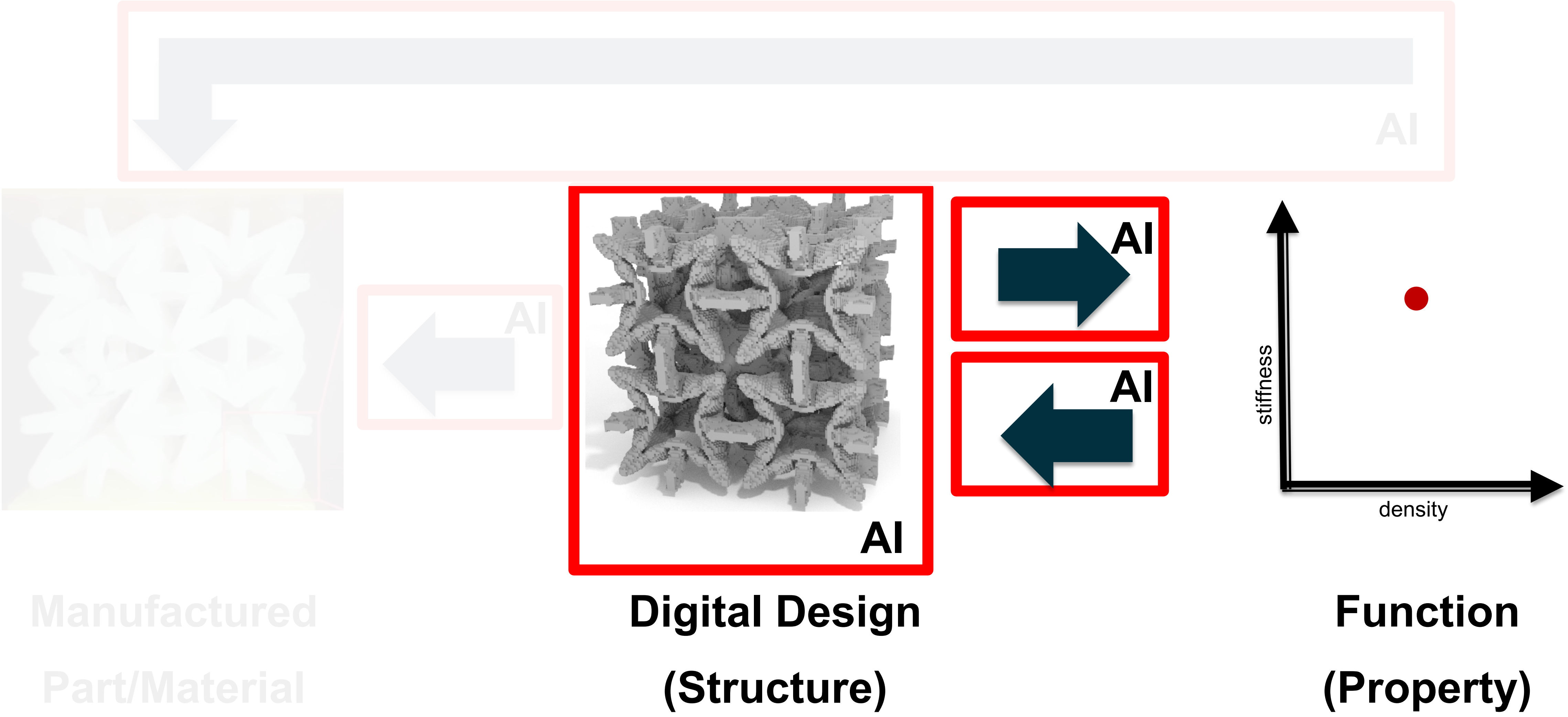
Optimal Experiment Design Platform



- Open-source
- Easy-to-use GUI
- Built-in visualization
- Human-in-the-loop optimization

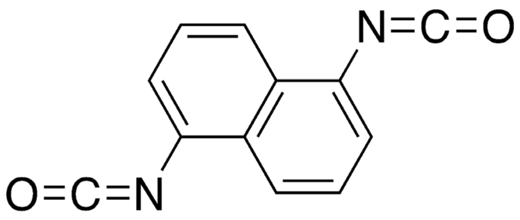
https://www.autooed.org/

AI-based Design Workflow

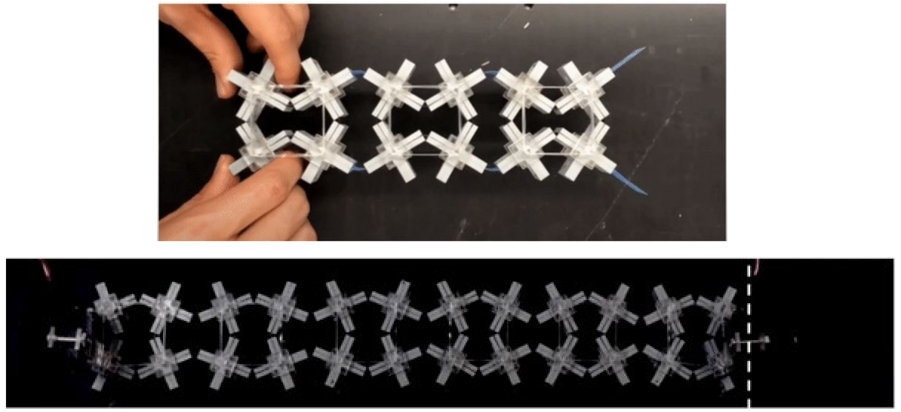


Representing Designs using Graphs

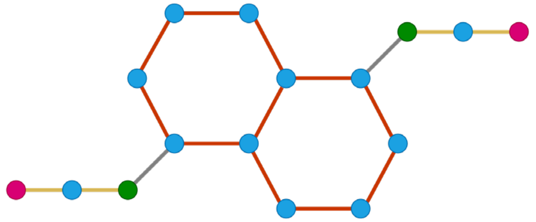
Molecule

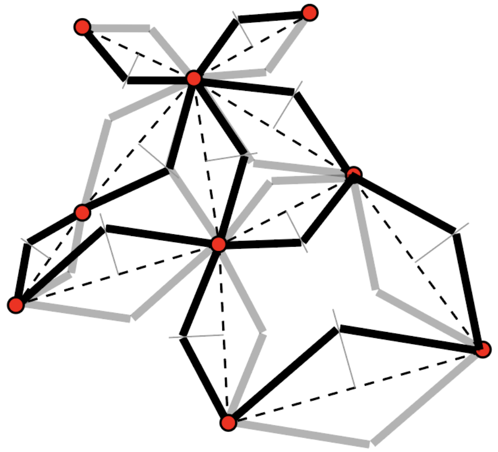


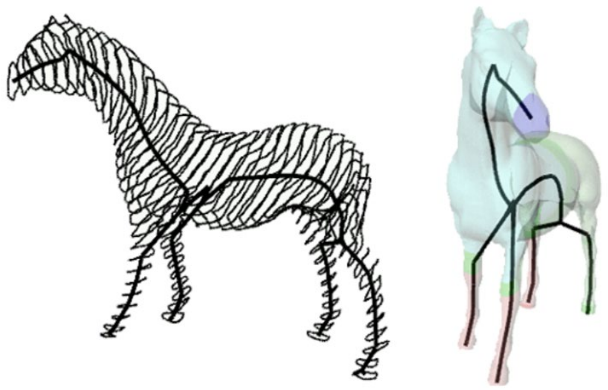
Meta-Material



3D Shape

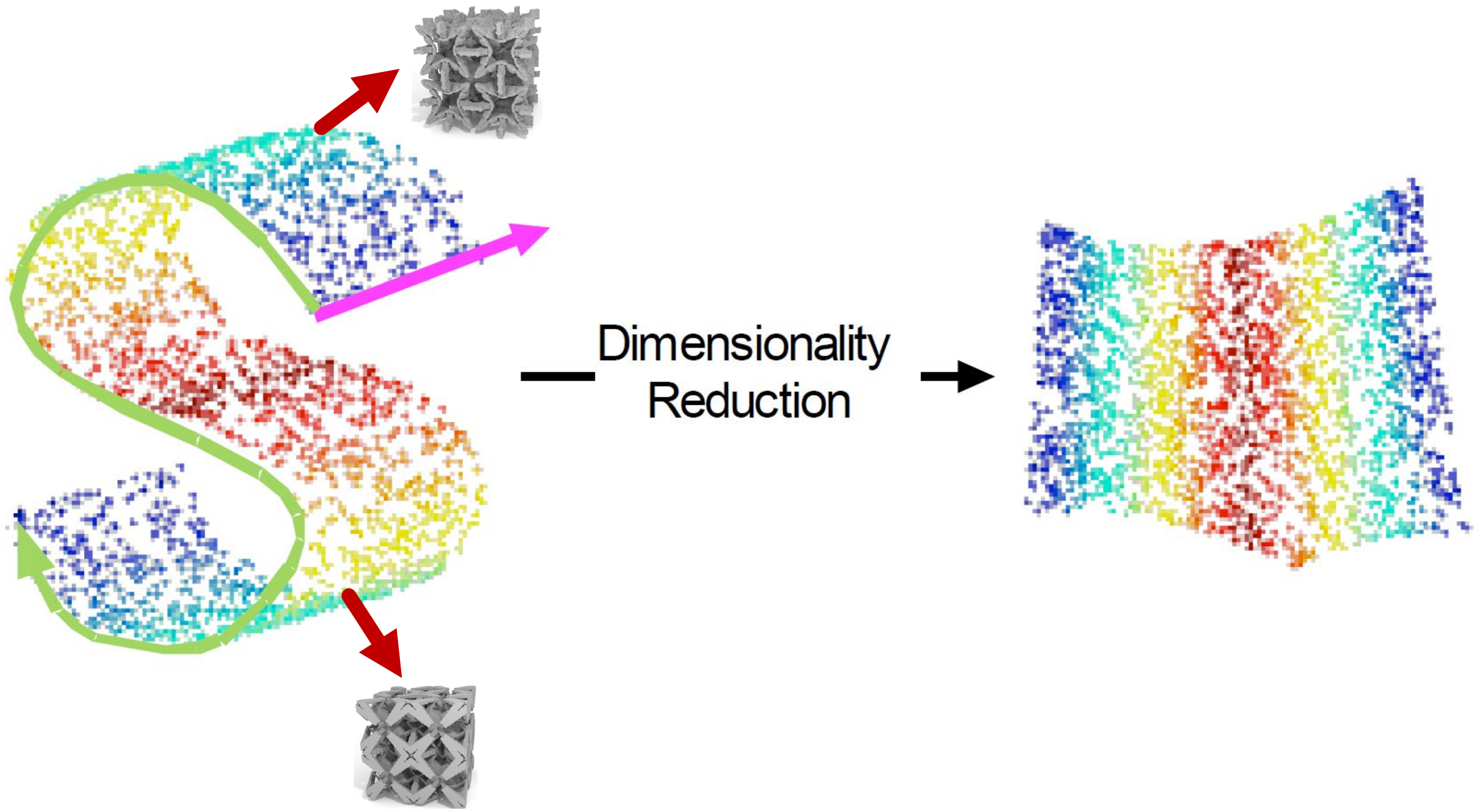






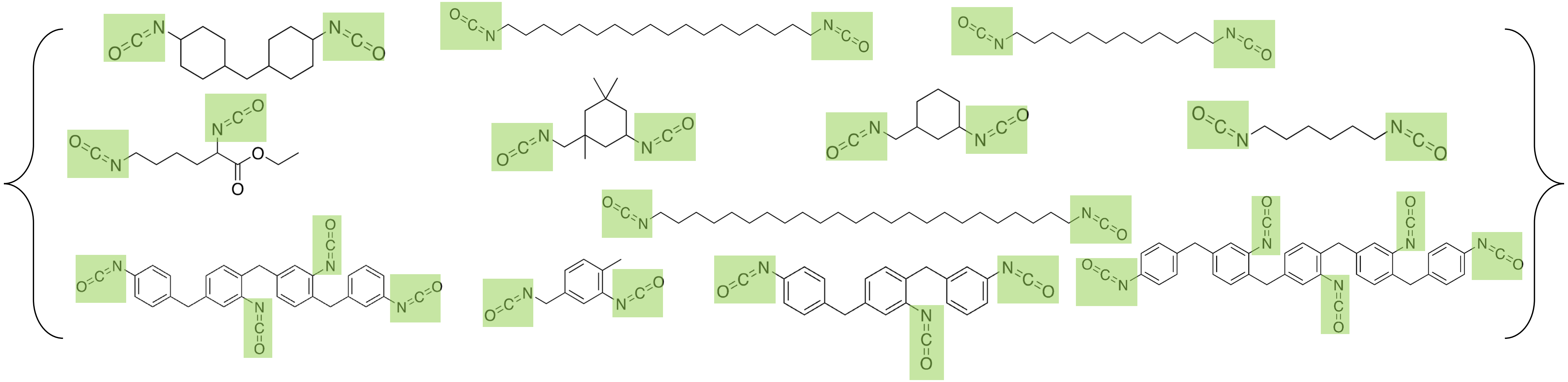
Representing Design Space

- Use a dataset of materials to generate more materials in each class
  - Examples: molecules, engineered materials, batteries, …
- Generative model is required to construct a search space for computational design



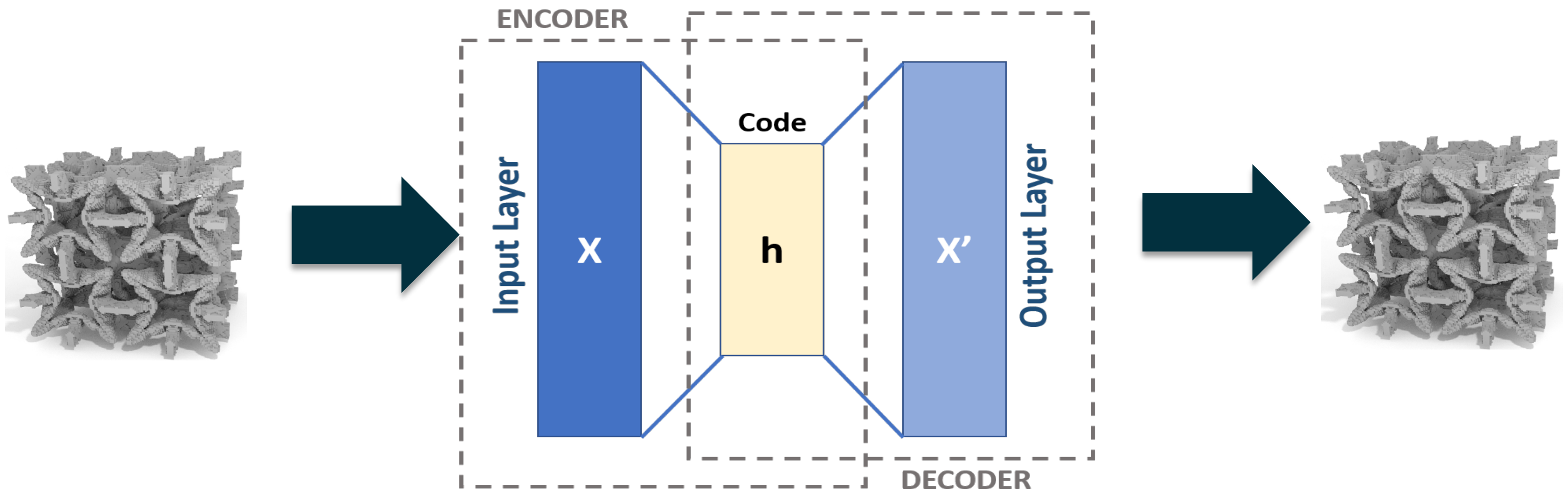
A Key Challenge for Molecular Design

- Literature provides only **tens of examples** for specific classes of molecules



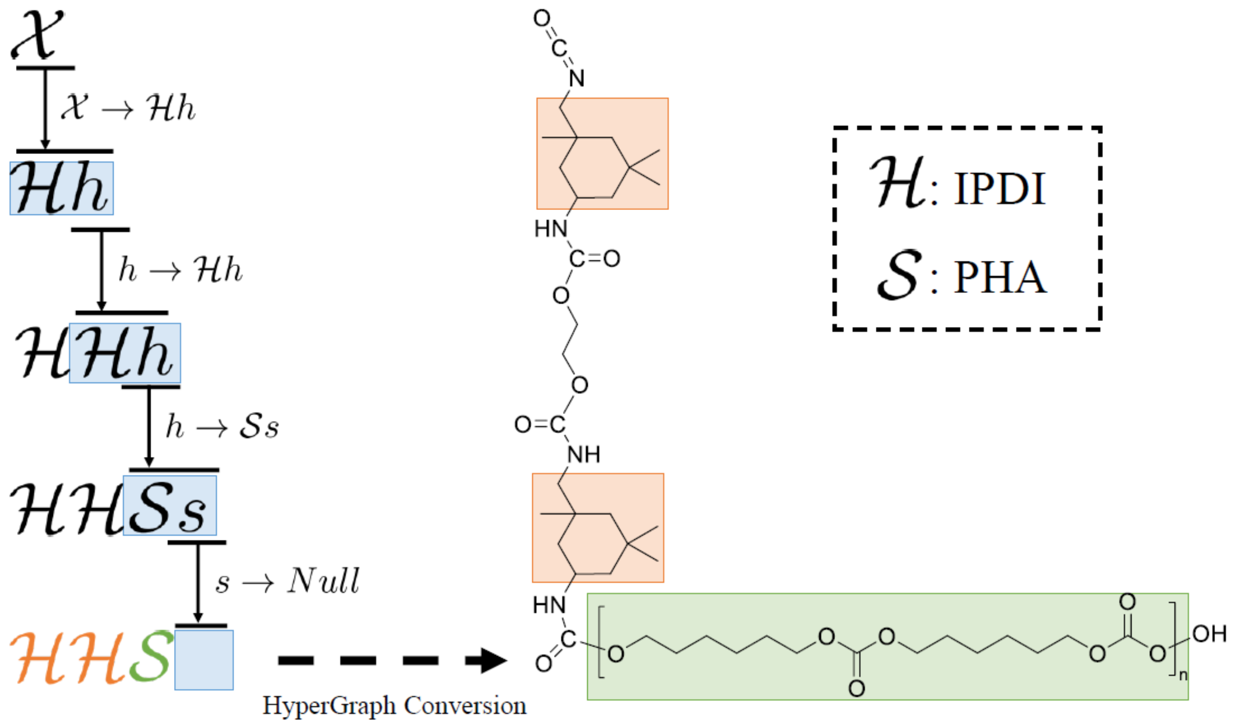
Deep Learning Solutions

- Feed-forward neural network learns to copy input to output
- Encoder maps input to code
- Decoder maps code to reconstruction of original input
- Autoencoder, Variational Autoencoder (VAE), Generative Adversarial Network (GAN) require large amount of data (10K+)

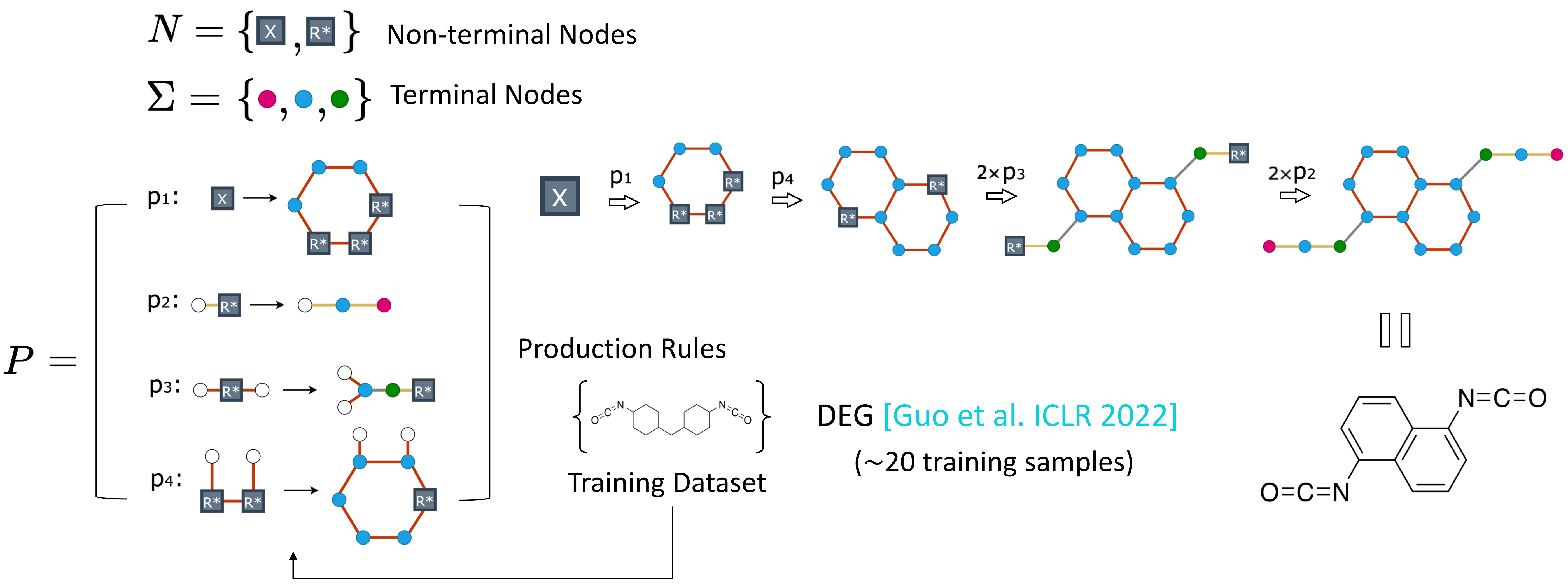


Symbolic Generative Models

- Designs are represented as a custom symbolic language called grammar
- Much more data efficient compared to deep learning
- Symbolic grammars are explainable

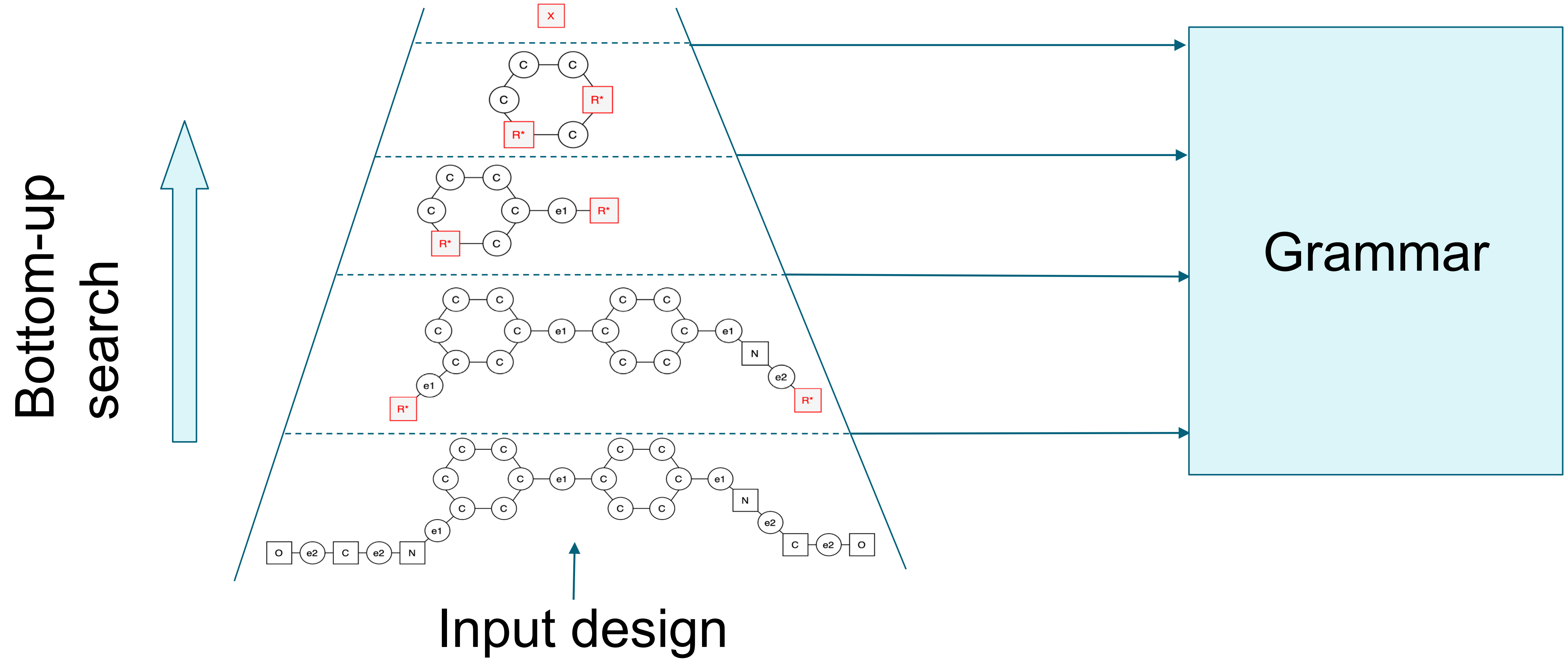


Graph Grammar

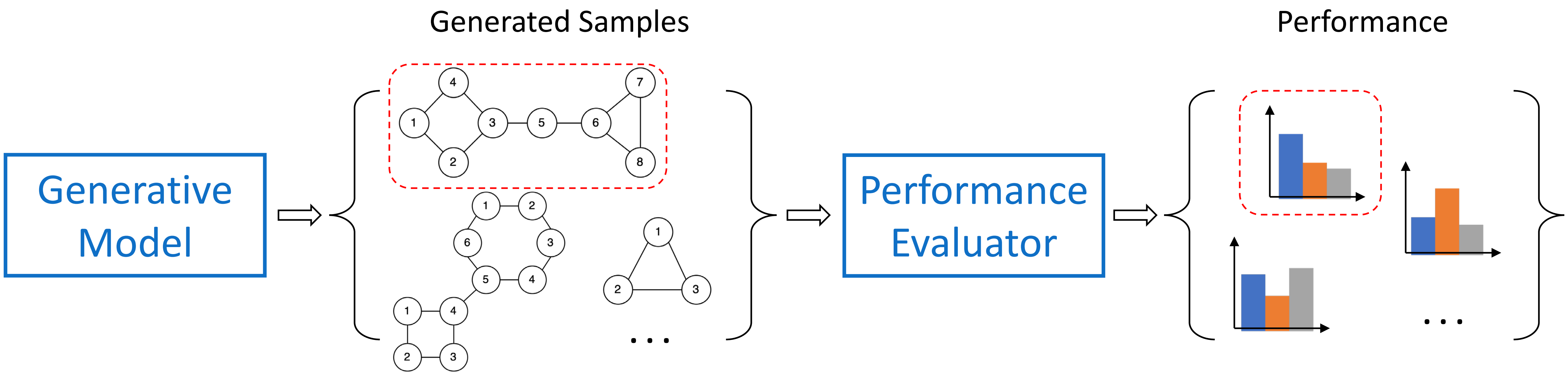


Learning Symbolic Generative Model

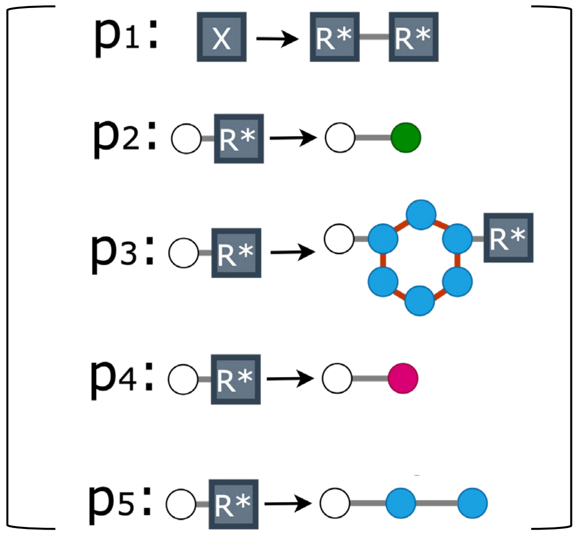
- We use **bottom-up search** to automatically generate the grammar



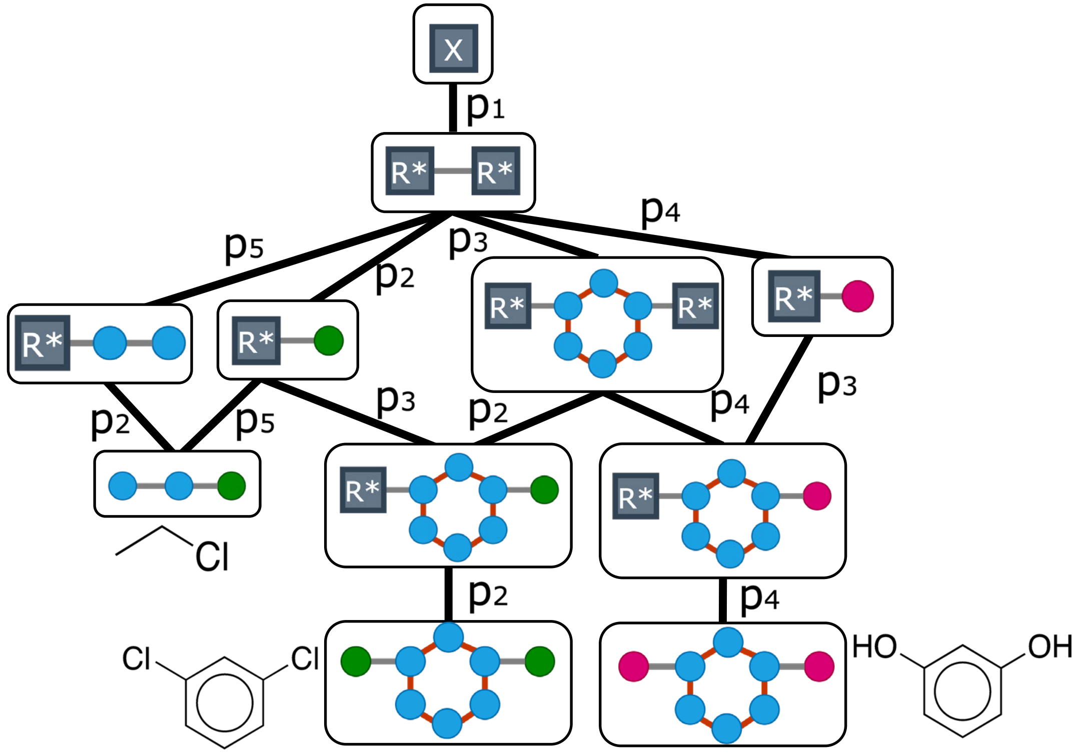
General Pipeline of Computational Design



Similarity Metric for Designs

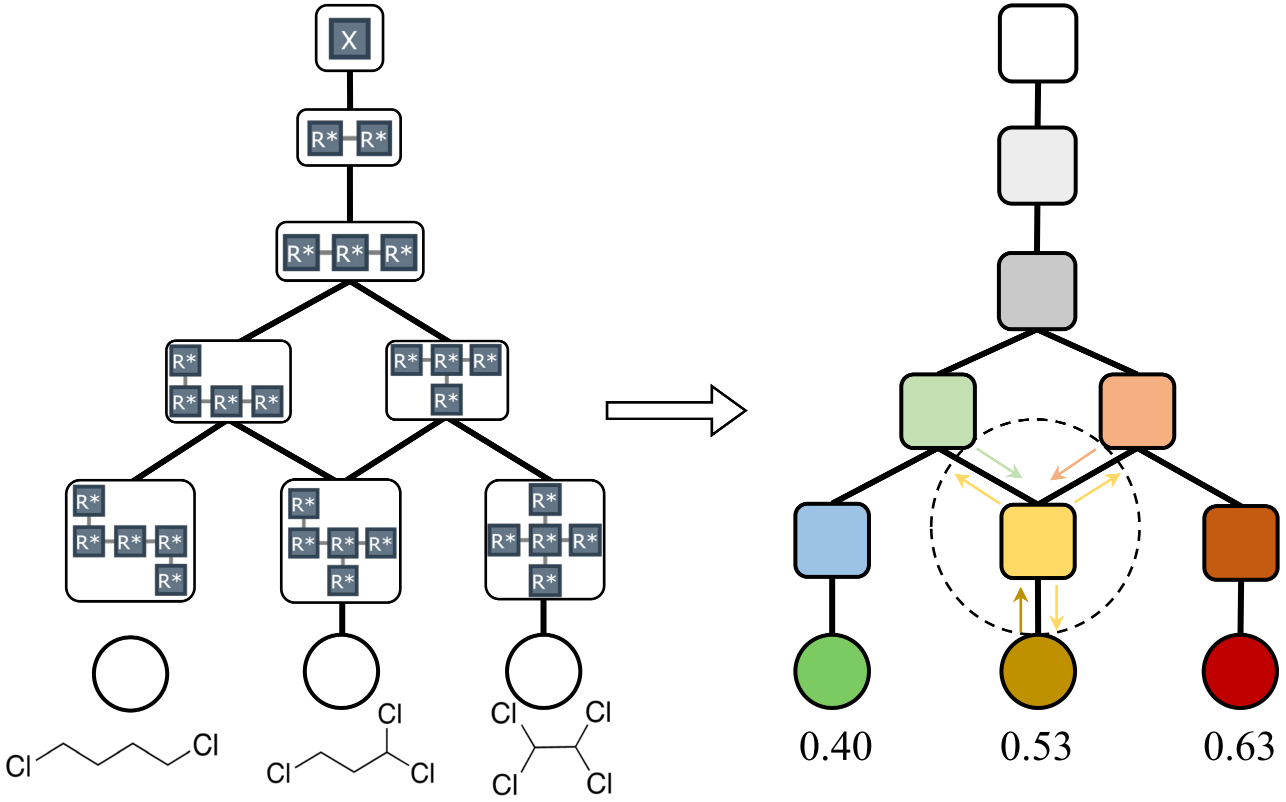


Graph Grammar



Grammar-induced Geometry

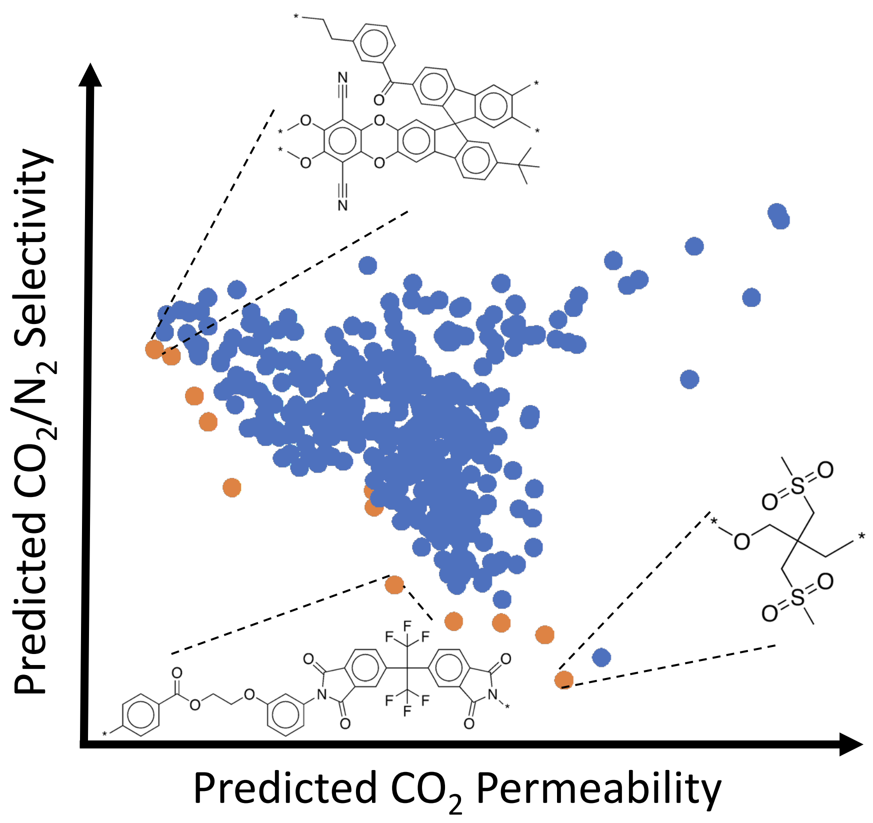
Molecular Property Prediction



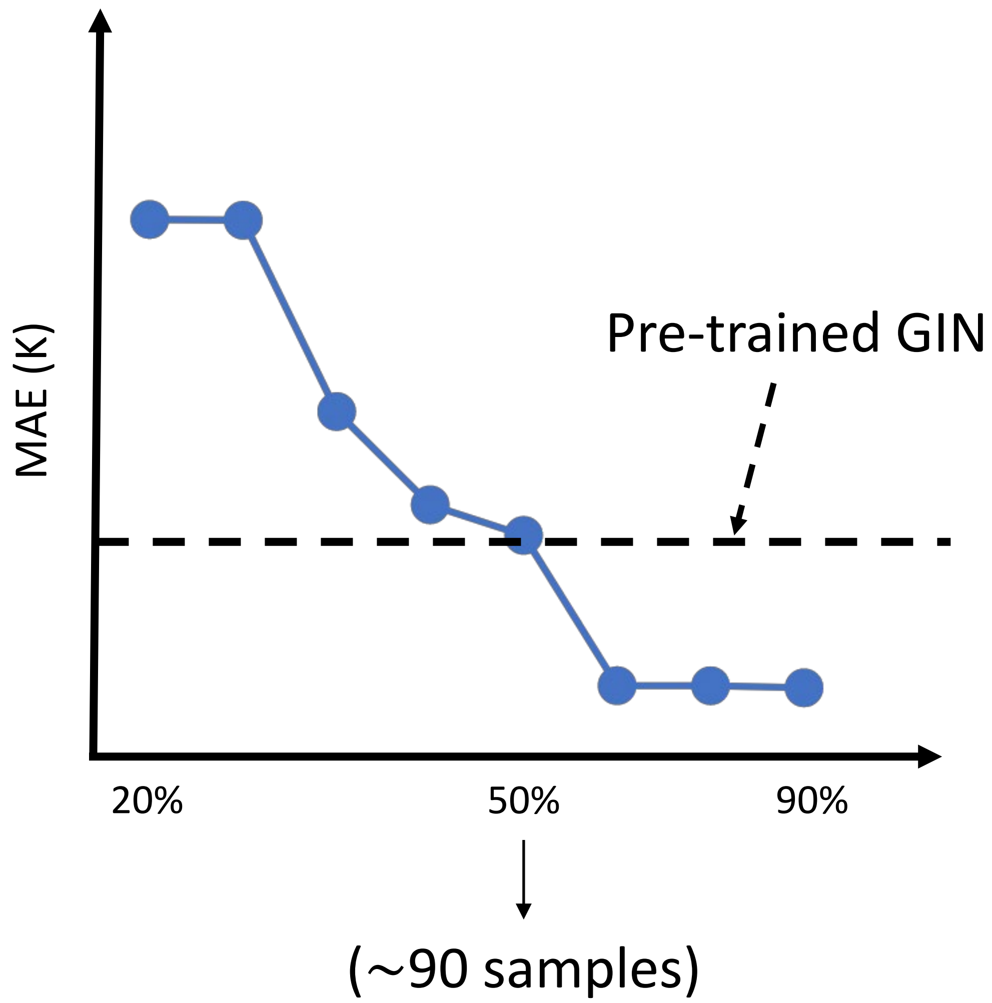
Graph Neural Diffusion

[Chamberlain et al. 2021]

Results



Predicted CO_2/N_2 Selectivity
Predicted CO_2 Permeability

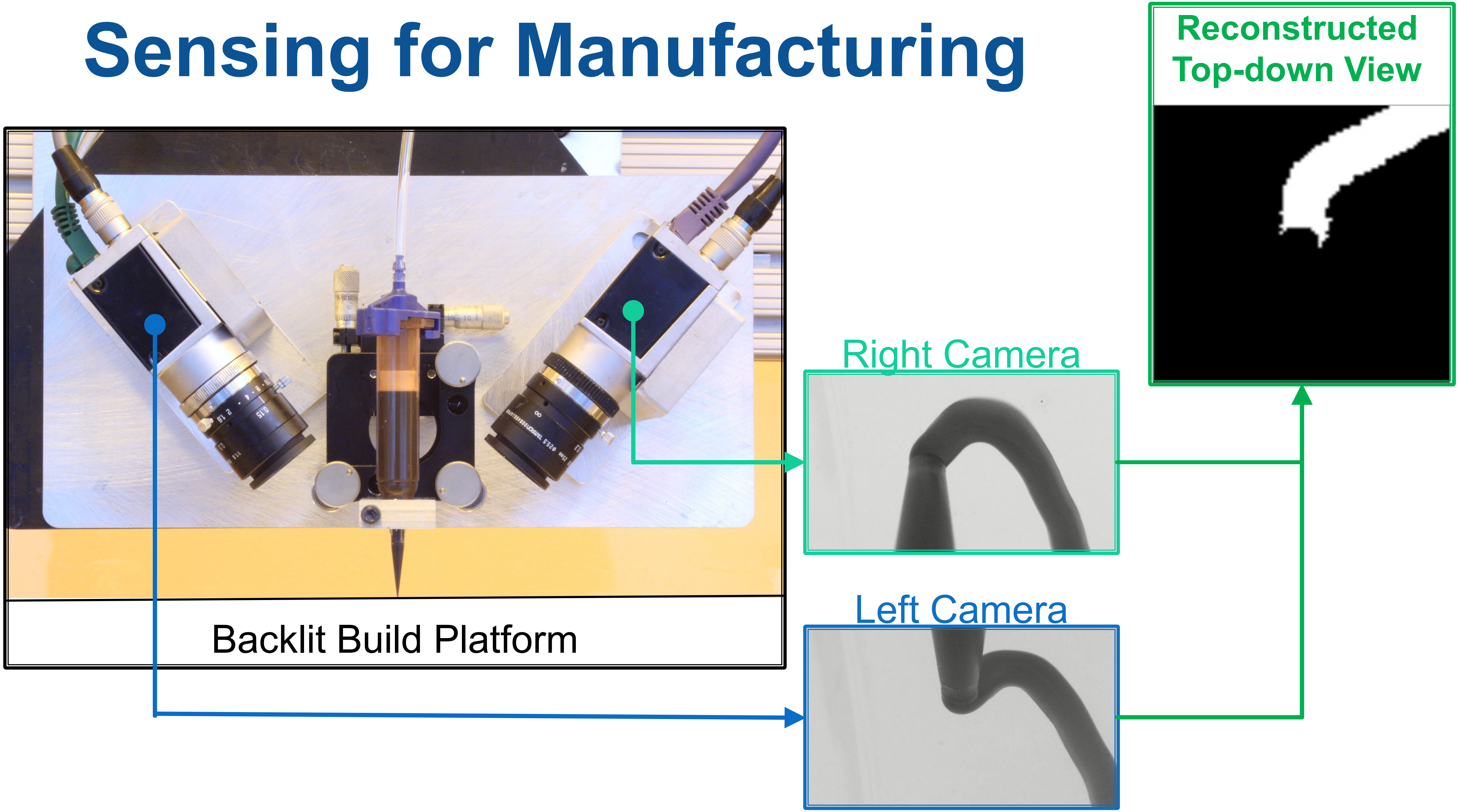


MAE (K)
Pre-trained GIN
20%
50%
90%
(~90 samples)

Why AI for R&D and Manufacturing?

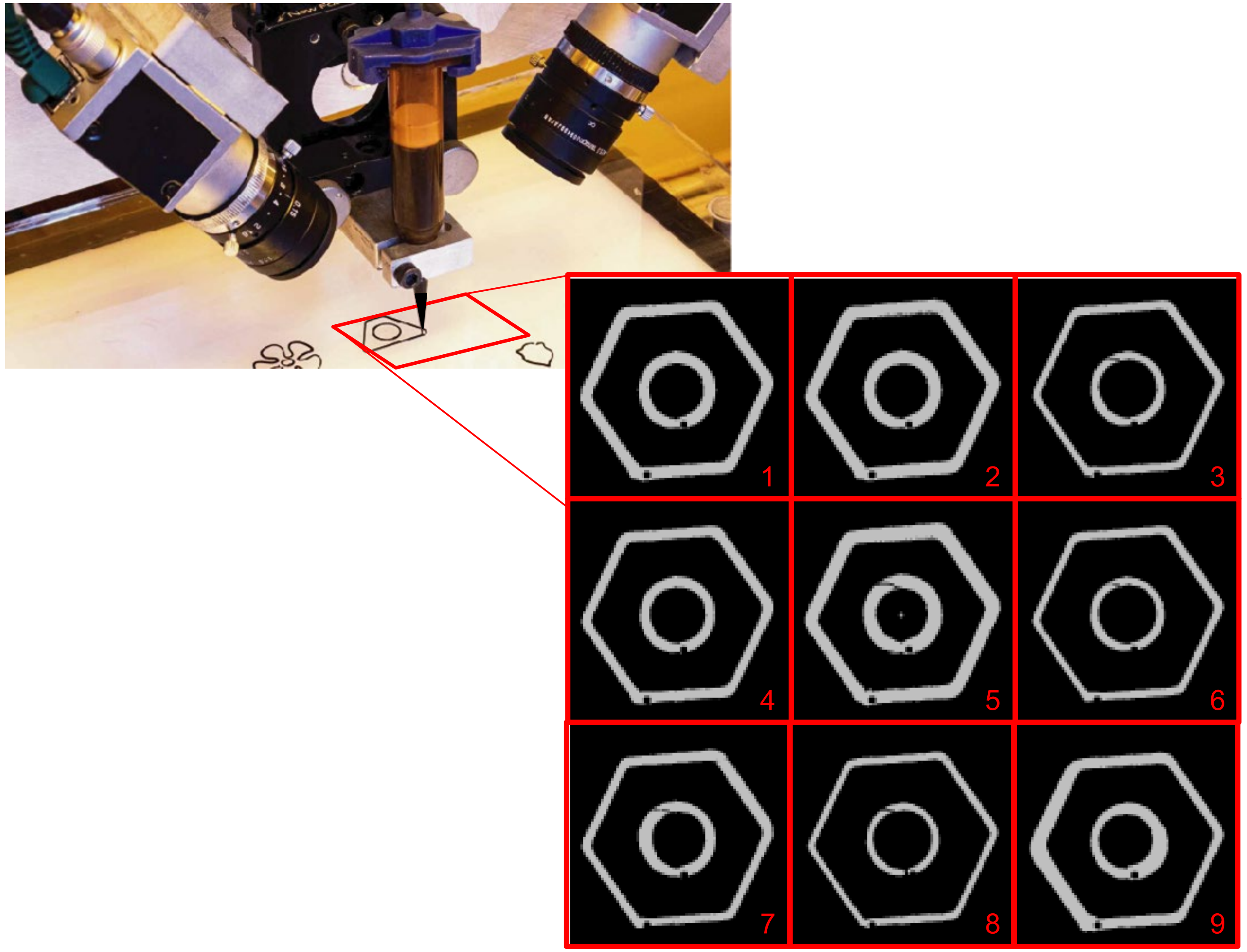
- Automatically evaluate many more designs than a human can do manually
  - Accelerate product design process
  - Reduce R&D costs
  - Generate higher performing products
- **Provide a layer of intelligence for manufacturing processes**
  - Automatically tune manufacturing process
  - Improve yield and accuracy
  - Predict and schedule maintenance

Sensing for Manufacturing



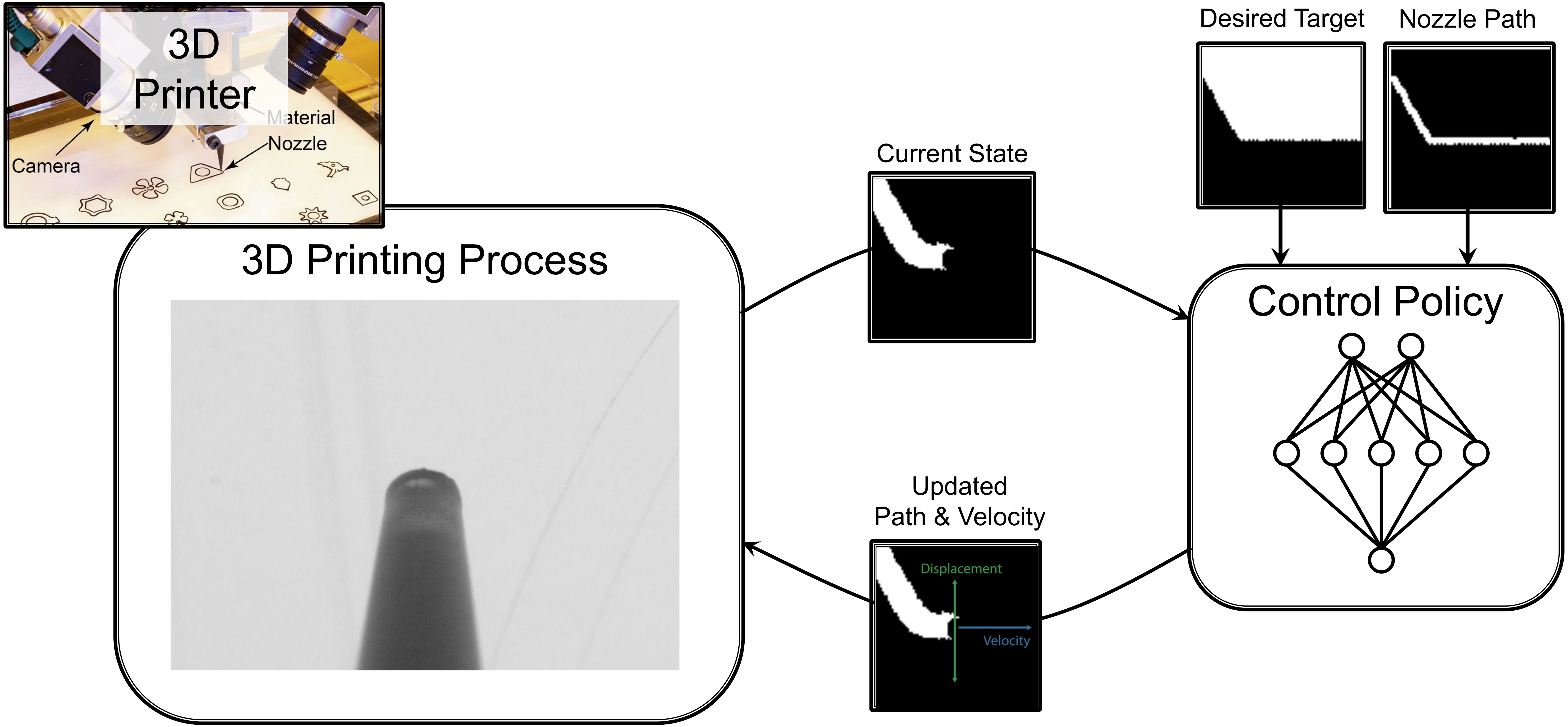
Control for Manufacturing

- AM is prone to **random changes** in materials and process
- AM lacks **closed-loop** control limiting **accuracy**
- **Controllers are hand designed and** use no (or limited) sensing



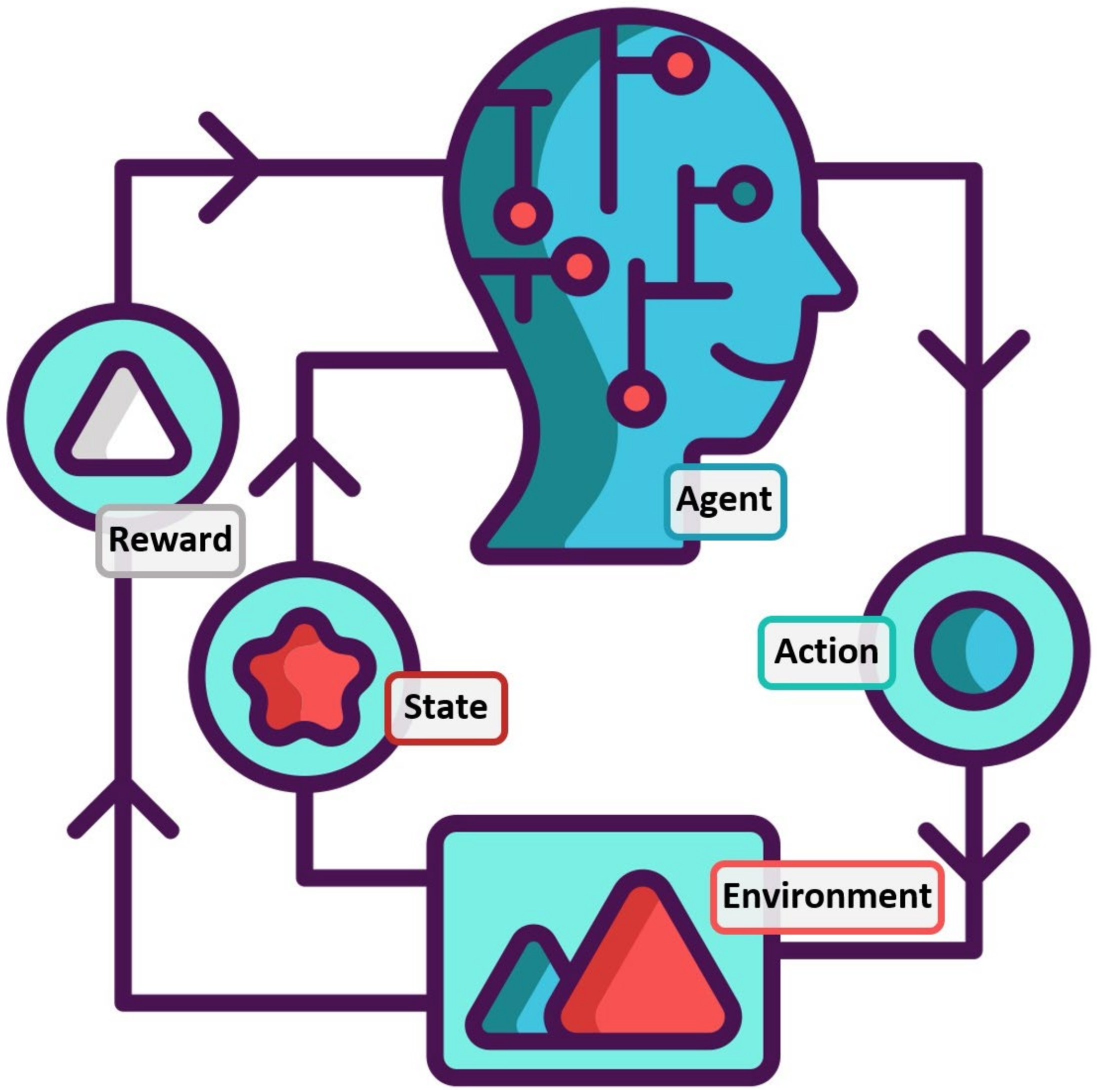
Random Variation

Manufacturing with Control Policy



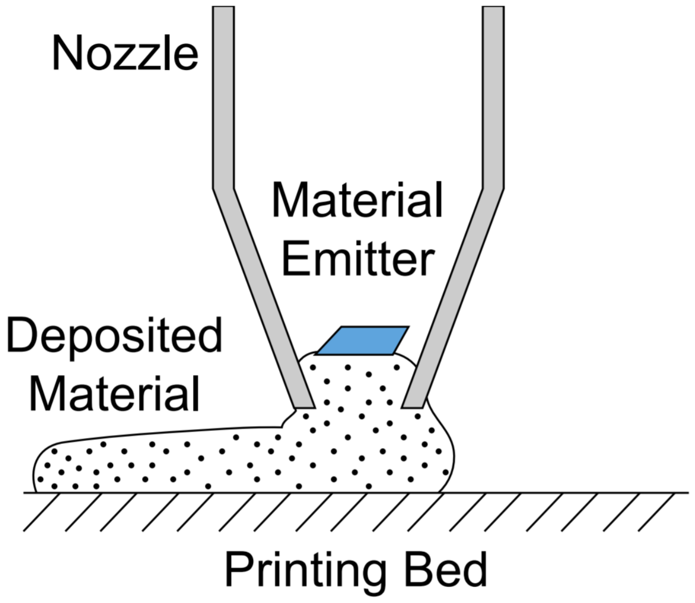
Learning to Control for Manufacturing

- Reinforcement learning (RL) emerges as a promising methods to optimize control in robotics
- RL requires real-time observations/sensing of the environment
- RL requires lots of training data (e.g., 100K experiments)
- High-performance RL controllers can beat human-designed controllers

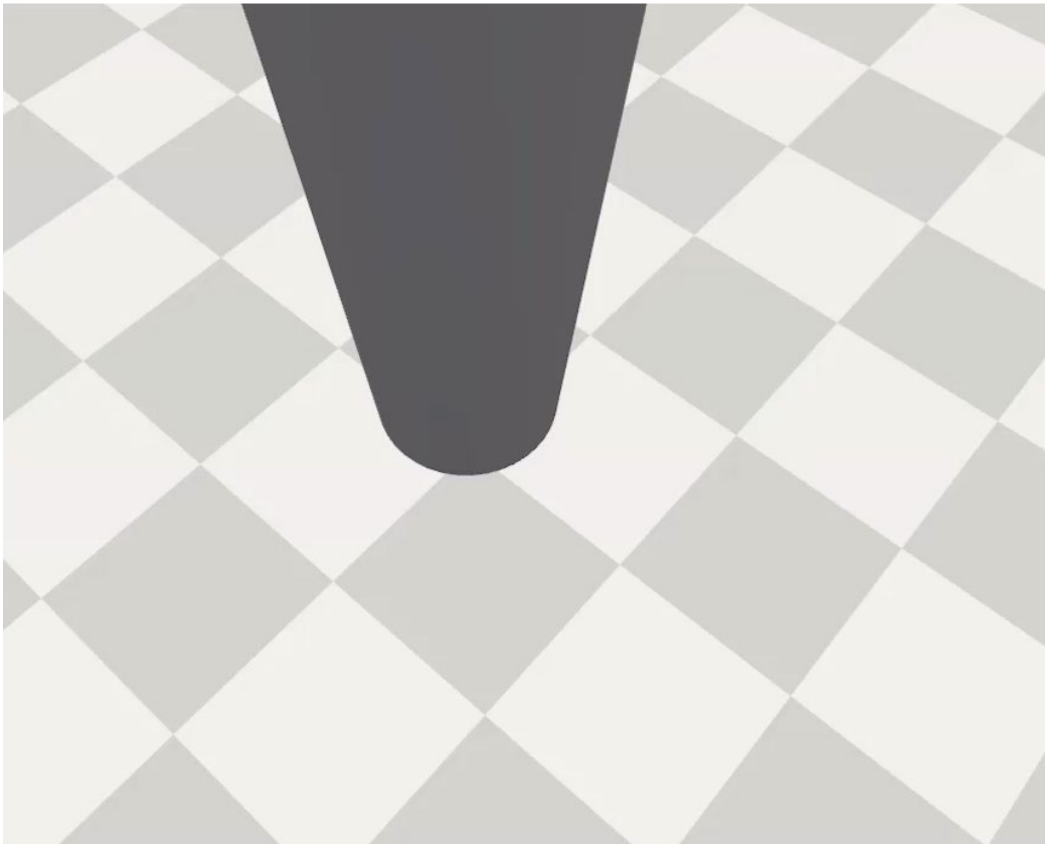


Process Simulation

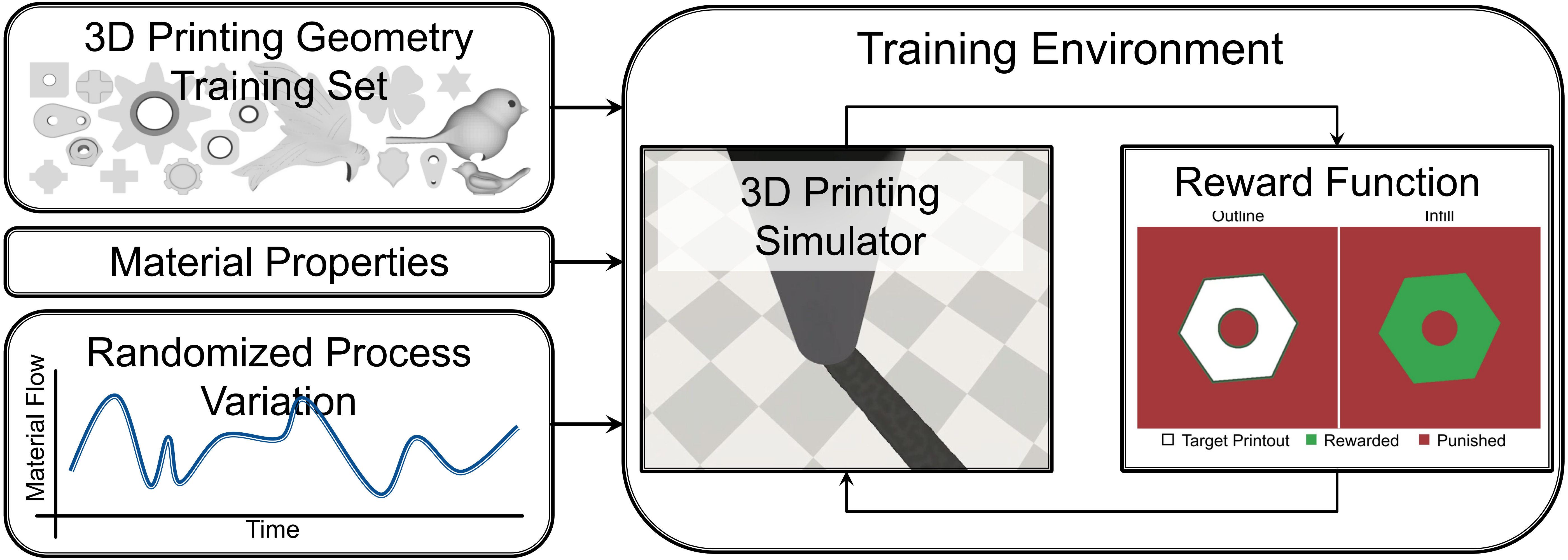
- 3D printer simulation
  - Particle based simulation
  - Simulates in real-time
  - Easily parallelizable making training possible in short period of time.



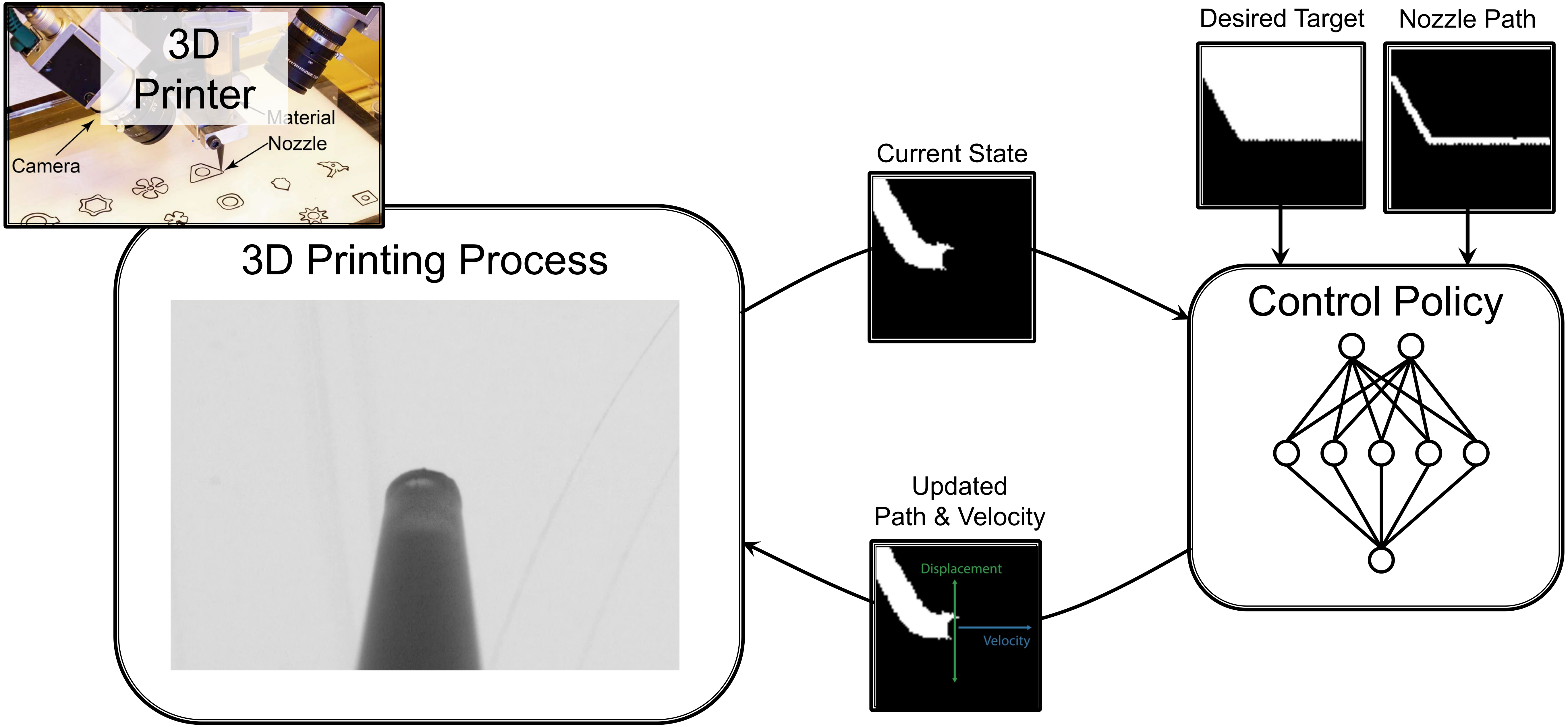
3D Printing Simulation



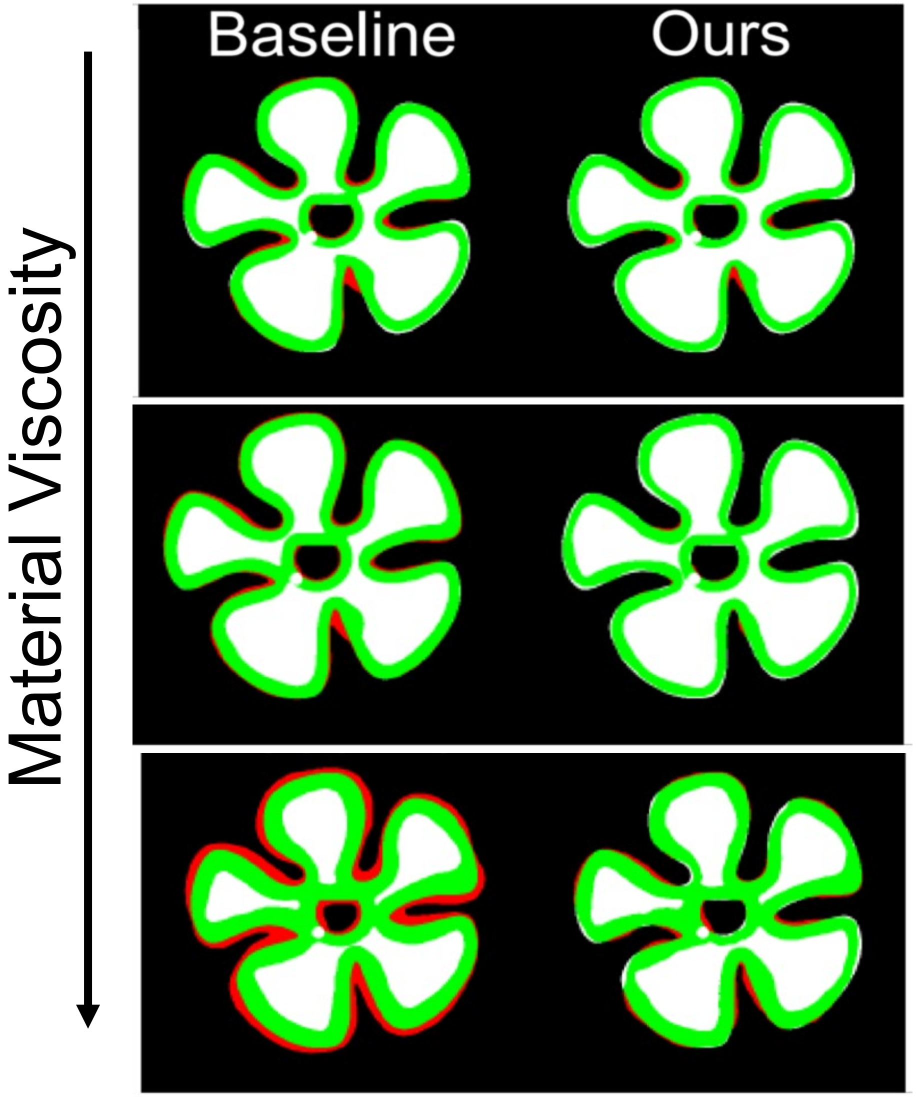
Training Robust Control Policy

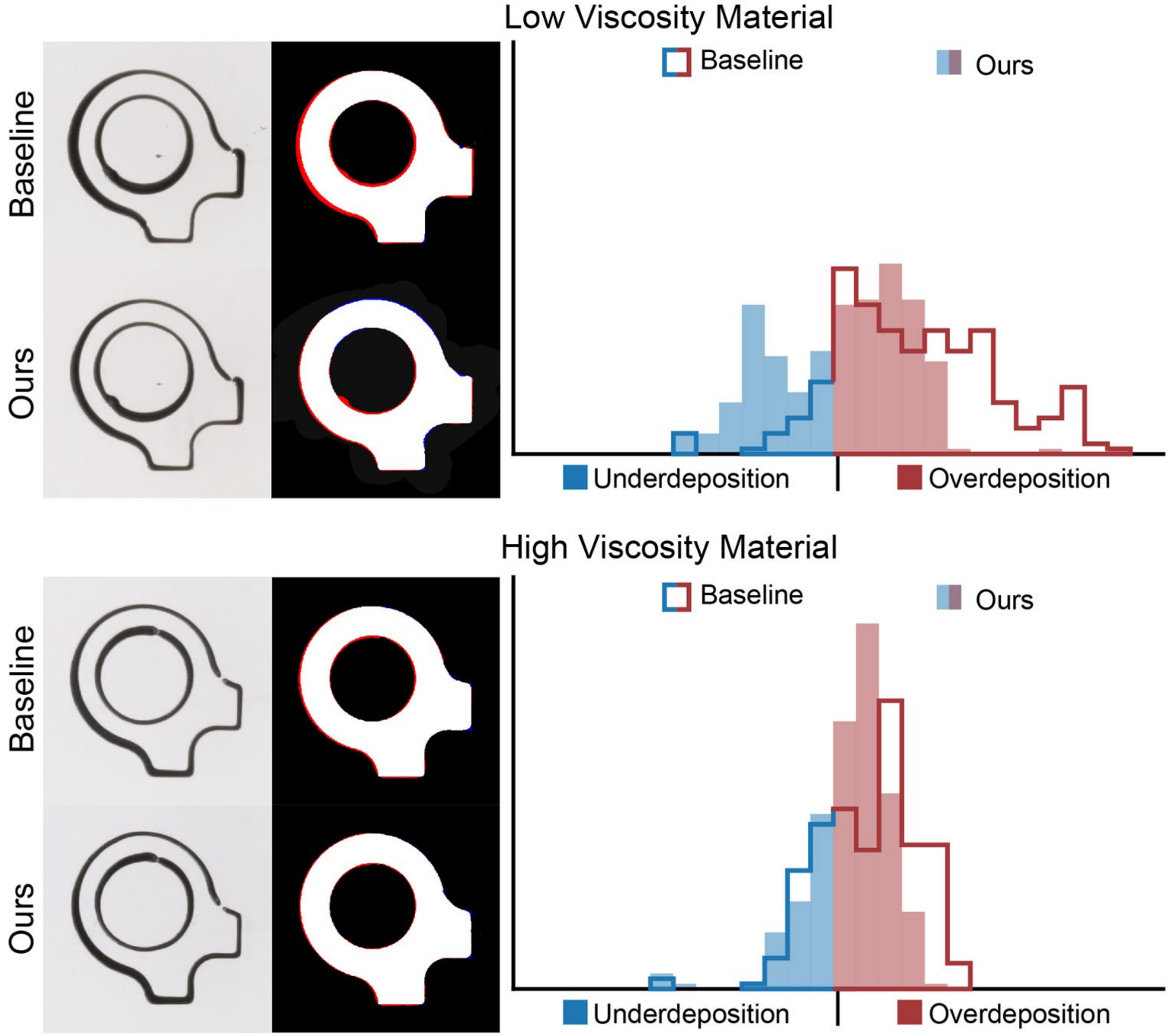


Control Transferred to Real System



Process is Robust to Material Changes



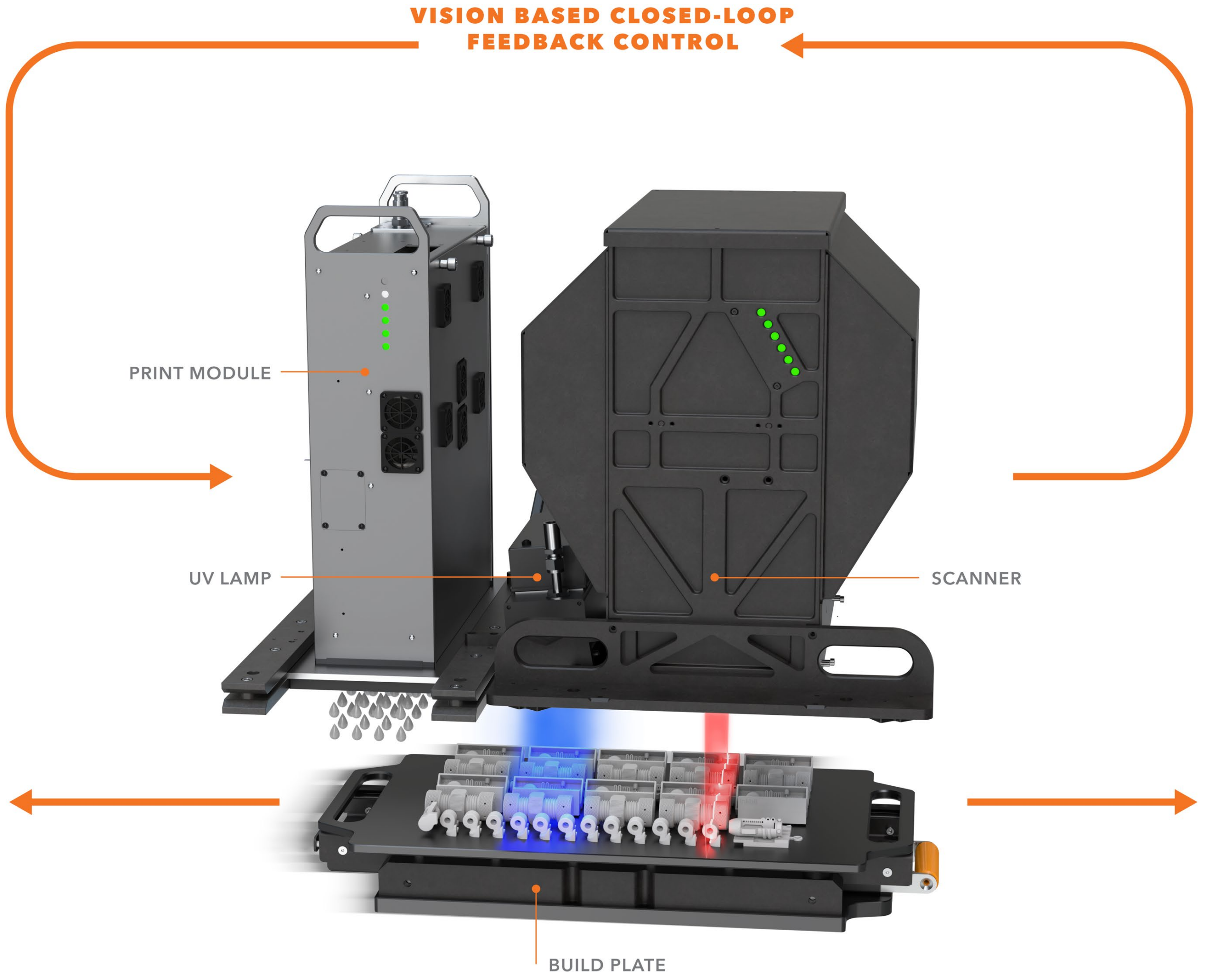



inkbit

Vision Controlled Jetting (VCJ) unlocks high-precision 3DP with functional materials at scale

Adaptive 3D Vision Process Control Unlocks **High Accuracy and Precision**

Non-contact Process Unlocks **Functional End-Use Materials**



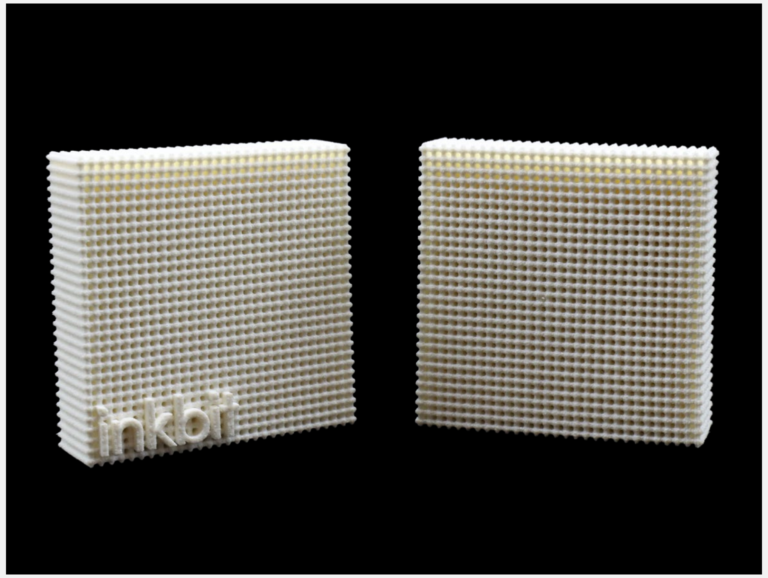
VCJ Enables End Use Materials

Titan Tough Epoxy 75

Rigid, durable general use material

Vulcan Soft Elastomer 30

Soft, elastomeric material with good elongation and rebound



Titan Chem Epoxy

Chemical resistant material with high heat deflection temperature

Titan Tough Epoxy 85

New material available end of year
Featuring higher elongation and HDT

Vulcan Soft Elastomer 50

New material available end of year
Featuring a durometer of Shore 50A

VCJ Enables True Production Additive Manufacturing

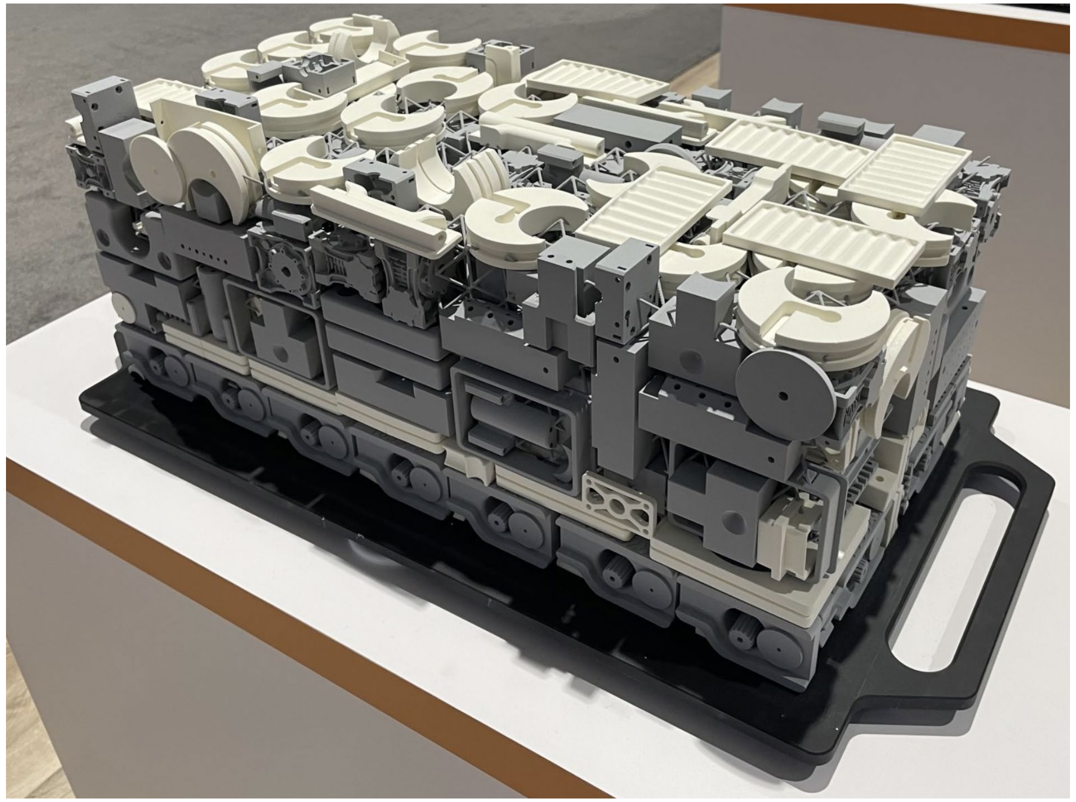
HIGH
THROUGHPUT

LOW
LABOR

ACCURATE AND
PRECISE PARTS

HIGH PERFORMANCE
MATERIALS

MULTI-MATERIAL
CAPABILITY



Summary and Outlook

- AI methods in materials science and manufacturing are here to stay
- AI can be used in many different problem domains
- AI can be used for different components of the design workflow
- Lack of data, highly proprietary nature of data are the main roadblocks
- Growing commercial deployment