TEXAS A&M UNIVERSITY
Department of Materials Science and Engineering

Batch Reification Fusion Optimization (BAREFOOT) Framework

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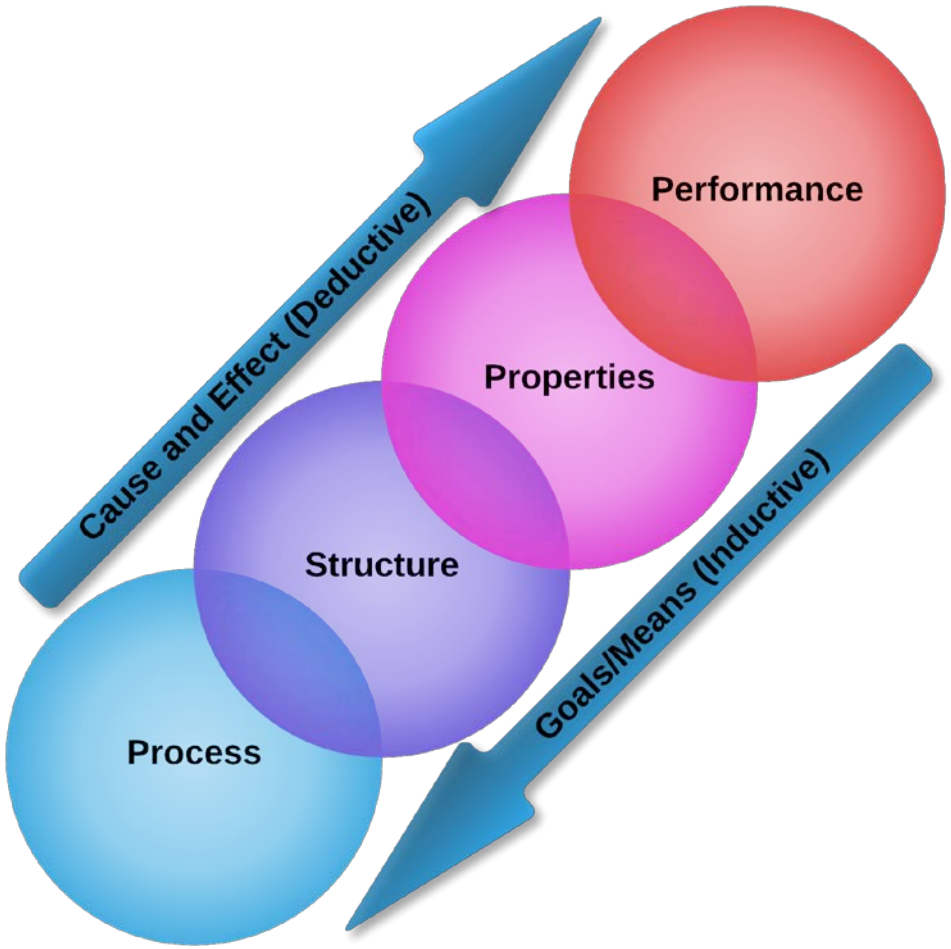
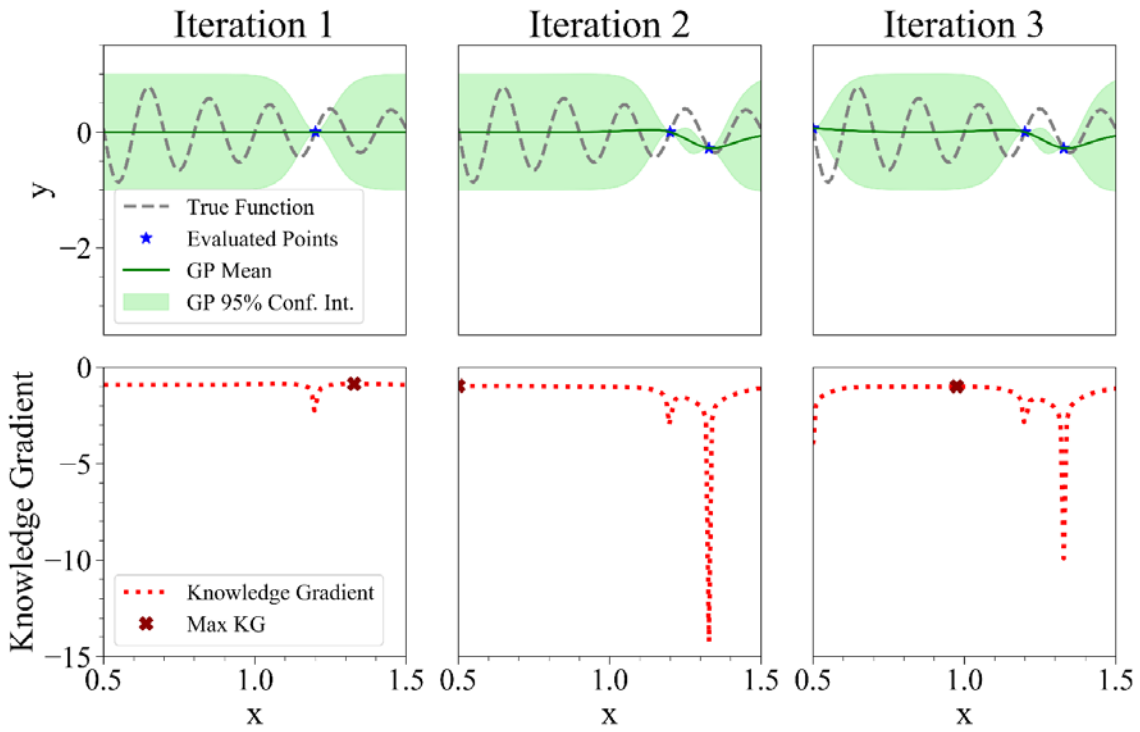
Accelerated Material Design

- One of the primary aims of:
  - Integrated Computational Materials Engineering (ICME)
  - Materials Genome Initiative (MGI)
- Materials as Systems
  - Process-Structure-Property-Performance relationships
  - Many methods available for evaluating these relationships
- Many recent developments
  - High Throughput experiments and computation
    - Thin Film and Additive Manufacturing
- For design:
  - Need to “invert” these relationships
  - Not always simple to do
  - Common Solution:
    - Bayesian Optimization



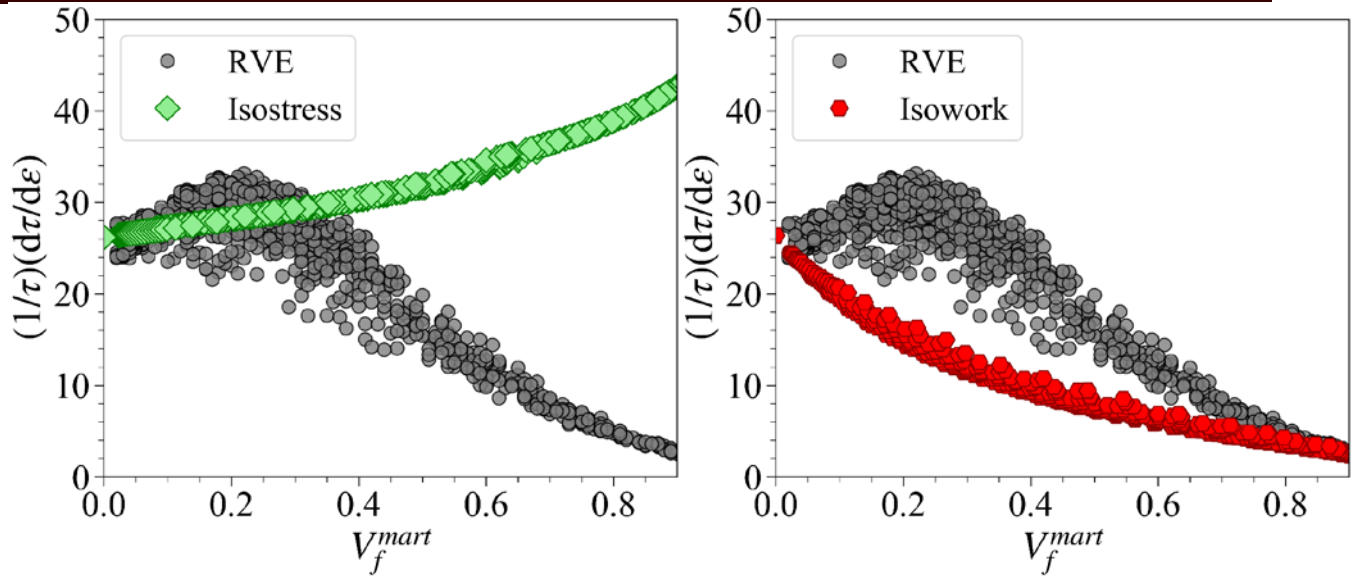
Bayesian Optimization

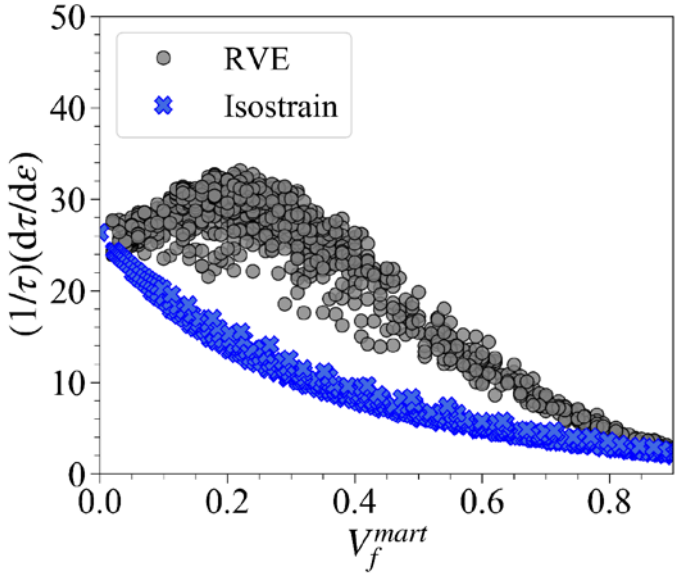
- Black Box optimization approach
  - Surrogate Model used for the unknown function
  - Acquisition function used to determine next point to evaluate
  - Next best point evaluated and posterior of surrogate model recalculated
  - Repeat process
- Why do we use it?
  - Provides reduced cost
  - Generally a good global optimizer
  - Flexibility
    - Surrogate models
    - Acquisition functions



Multi-fidelity Model Fusion

- In many material science applications:
  - More than one model for a property
  - Models differ in accuracy
  - But all hold some information
- Multi-fidelity Model Fusion
  - Aims to utilize information in all models
  - Reduce evaluations of most expensive (most accurate) information source





Notes on the NanoHub Tool

- Due to limitations with Jupyter Notebook
  - Incompatibility with mutli-processing and Notebooks
  - Implementation uses multi-threading with limited threads
- For multiprocessing code
  - Github Repository
    - Most recent code can be found here
- The Nanohub tool demonstrates
  - Reification/Fusion
    - Multi-fidelity model approach
  - Batch and Sequential BO
  - Barefoot approach
    - Combined Reification/Batch
  - These approaches are all implemented in the Framework

Concluding Remarks

- BAREFOOT
  - Flexible, easy to implement
  - Provides multiple calculation approaches
  - Provides almost all acquisition functions
  - Maximization or minimization
  - Multi-objective
  - Implemented in parallel code
    - Makes calculations quite efficient
  - Open source
    - And under active development

- Calculations Approaches:
  - Barefoot
  - Batch only
  - Reification only
- Acquisition Functions:
  - Probability of improvement
  - Expected Improvement
  - Upper Confidence Bound
  - Thompson Sampling
  - Knowledge Gradient
  - Greedy Sampling
  - GP-Hedge Portfolio Optimization

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https://github.com/RichardCouperthwaite/BAREFOOT-Framework