Lecture 23: Bayesian global optimization

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Overview of Bayesian global optimization applications

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Problem definition

Deterministic: $\max_x f(x)$ — objective function

- $f(x)$ is expensive
- don't have gradients

How do you solve this problem with a limited budget of evaluations?

Stochastic: $\max_x \mathbb{E}[y \mid x]$

$y = f(x) + \varepsilon$

- expensive
- challenging to evaluate analytically

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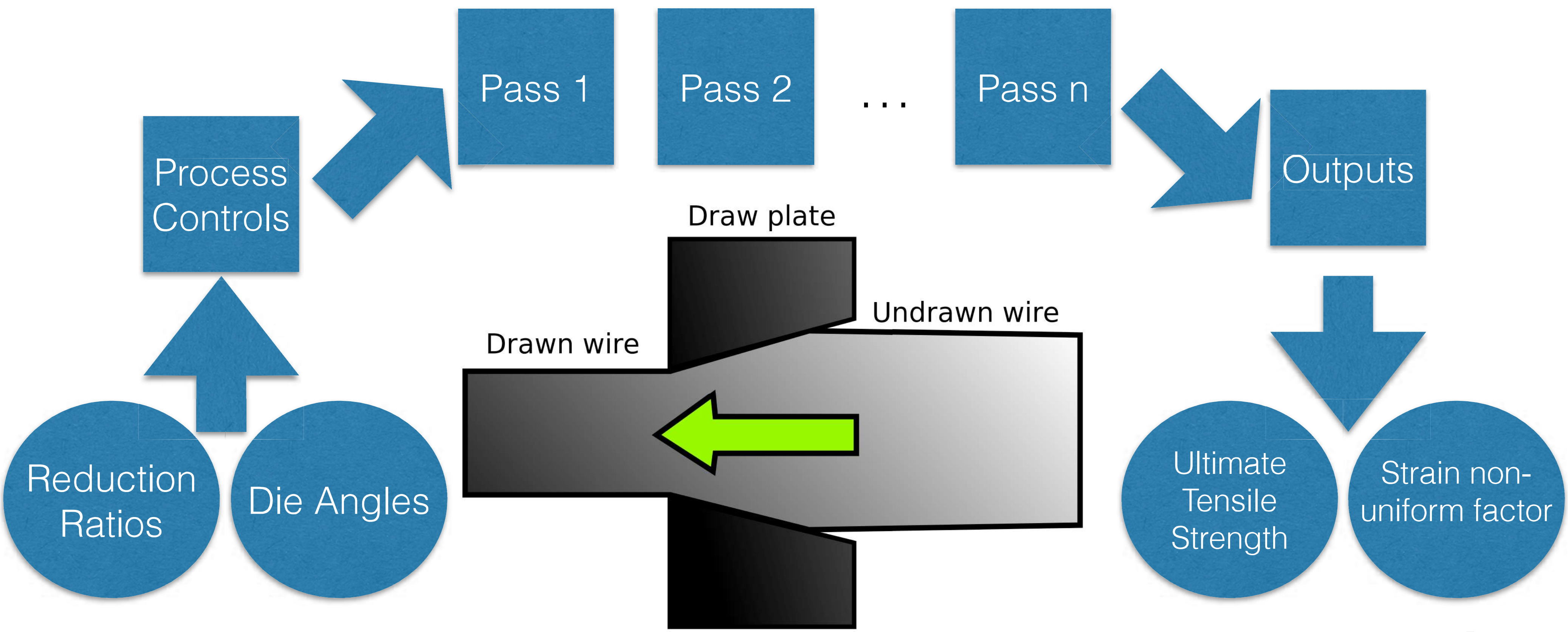
Dynamic vs myopic information acquisition

- Optimal information acquisition policies…
- => Dynamic programming/control theory.
- Too hard mathematical/computational problems.
- What if, we just pick one piece of information at a time?
- Myopic (one-step-look-ahead) policies.

Example: Design with expensive physical models

f (FEM simulations)



https://en.wikipedia.org/wiki/Wire_drawing#/media/File:Wiredrawing.svg

(1) **max** **min**

Pandita, P.; Bilionis, I.; Panchal, J.; Gautham, B. P.; Joshi, A.; Zagade, P. Stochastic Multiobjective Optimization on a Budget: Application to Multipass Wire Drawing with Quantified Uncertainties. *IJUQ* **2018**, *8* (3). https://doi.org/10.1615/Int.J.UncertaintyQuantification.2018021315.

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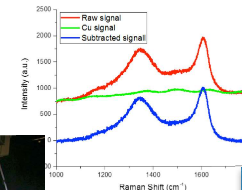
Example: Design experiments - Graphene manufacturing

Process Controls

R2R-PE-CVD

Raman Spectroscopy



Outputs

Gas Conc/tions

Pressure

Plasma Power

D/G Intensities (Right)

D/G Intensities (Left)

Alrefae, M. A.; Kumar, A.; Pandita, P.; Candadai, A.; Bilionis, I.; Fisher, T. S. Process Optimization of Graphene Growth in a Roll-to-Roll Plasma CVD System. *AIP Advances* **2017**, *7* (11), 115102. https://doi.org/10.1063/1.4998770.

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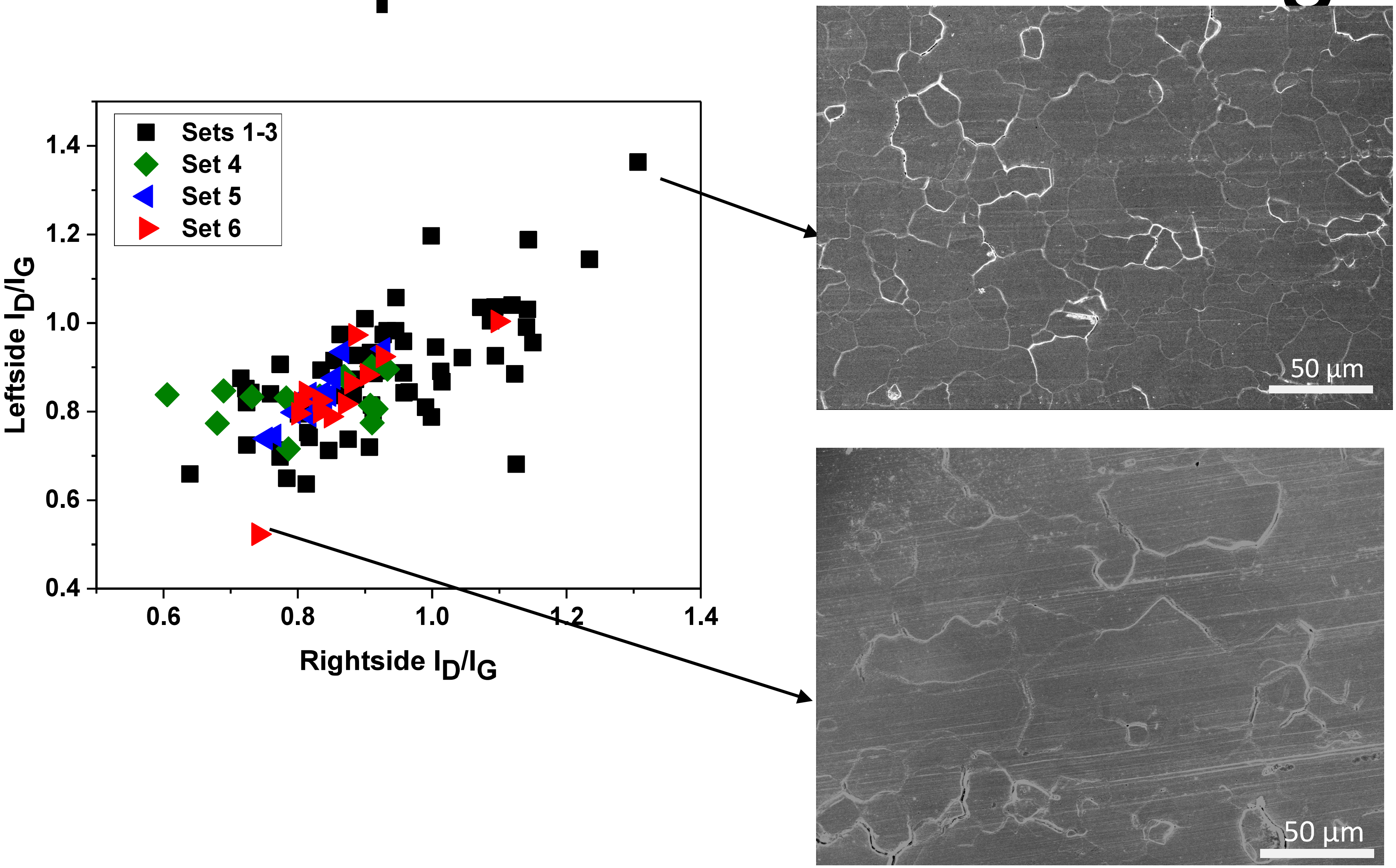
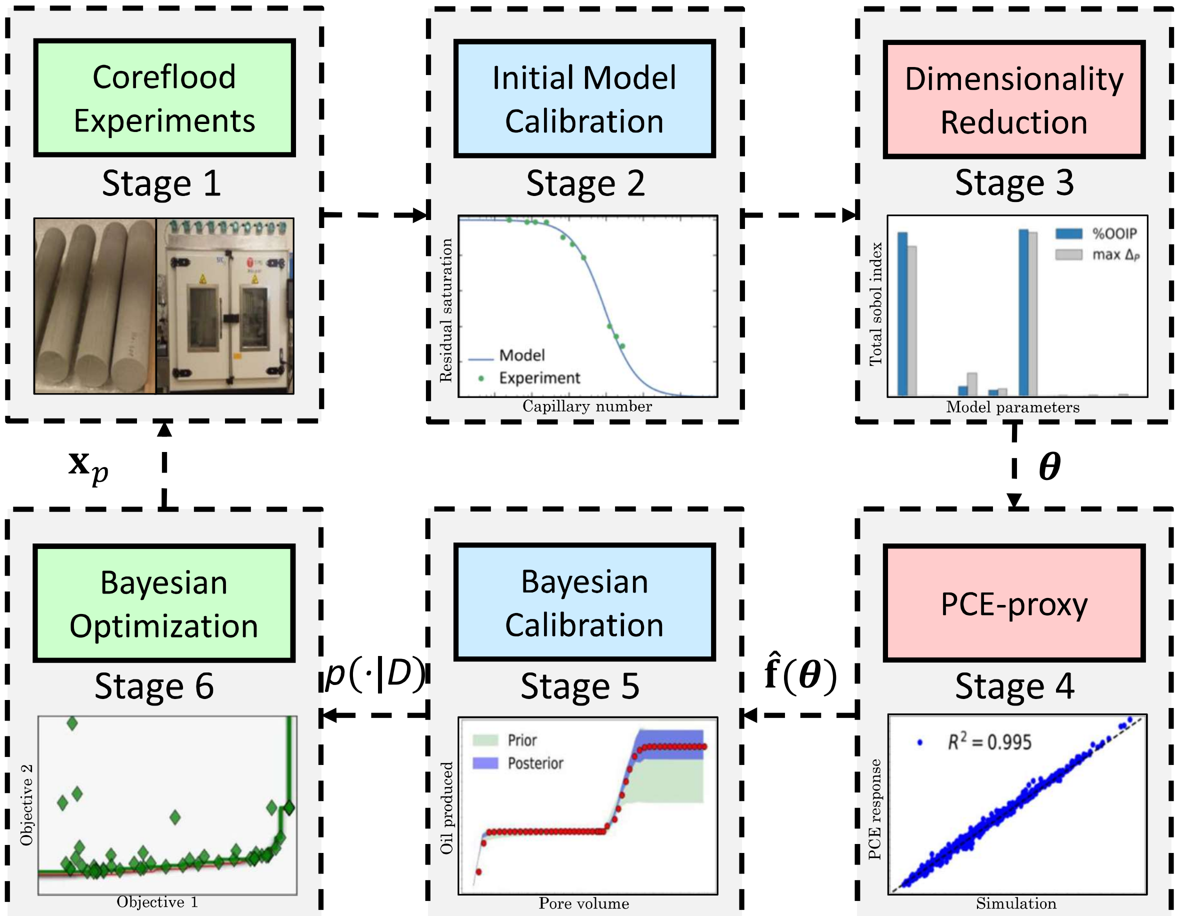
Example: Design experiments - Graphene manufacturing



Example: Calibrating expensive physical models



Naik, P.; Pandita, P.; Aramideh, S.; Bilionis, I.; Ardekani, A. M. Bayesian Model Calibration and Optimization of Surfactant-Polymer Flooding. *Comput Geosci* **2019**, *23* (5), 981–996. https://doi.org/10.1007/s10596-019-09858-z.

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Other examples

- Robotics. Ruben Martinez-Cantin, Nando de Freitas, Eric Brochu, Jose Castellanos and Arnaud Doucet. A Bayesian exploration-exploitation approach for optimal online sensing and planning with a visually guided mobile robot. Autonomous Robots. Volume 27, Issue 2, pp 93–103 (2009)

- Sensor placement. Niranjan Srinivas, Andreas Krause, Sham M. Kakade, Matthias W. Seeger: Information-Theoretic Regret Bounds for Gaussian Process Optimization in the Bandit Setting. IEEE Transactions on Information Theory 58(5):3250–3265 (2012)

- Discovery of materials. Kristensen, J.; Bilionis, I.; Zabaras, N. Adaptive Simulation Selection for the Discovery of the Ground State Line of Binary Alloys with a Limited Computational Budget. In *Recent Progress and Modern Challenges in Applied Mathematics, Modeling and Computational Science*; Melnik, R., Makarov, R., Belair, J., Eds.; Springer New York: New York, NY, 2017; pp 185–211. https://doi.org/10.1007/978-1-4939-6969-2_6.

- Tuning hyper-parameters of deep neural networks. Tripathy, R. K.; Bilionis, I. Deep UQ: Learning Deep Neural Network Surrogate Models for High Dimensional Uncertainty Quantification. *Journal of Computational Physics* **2018**, *375*, 565–588. https://doi.org/10.1016/j.jcp.2018.08.036.

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