

Lecture 23: Bayesian global optimization

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Overview of Bayesian global optimization applications

Problem definition

Deterministic:

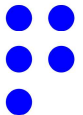
$$\max_x \underline{f(x)}$$

— objective function
[$f(x)$ is expensive
don't have gradients

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

Stochastic:

$$\max_x \mathbb{E}[y | x]$$
$$y = f(x) + \varepsilon$$

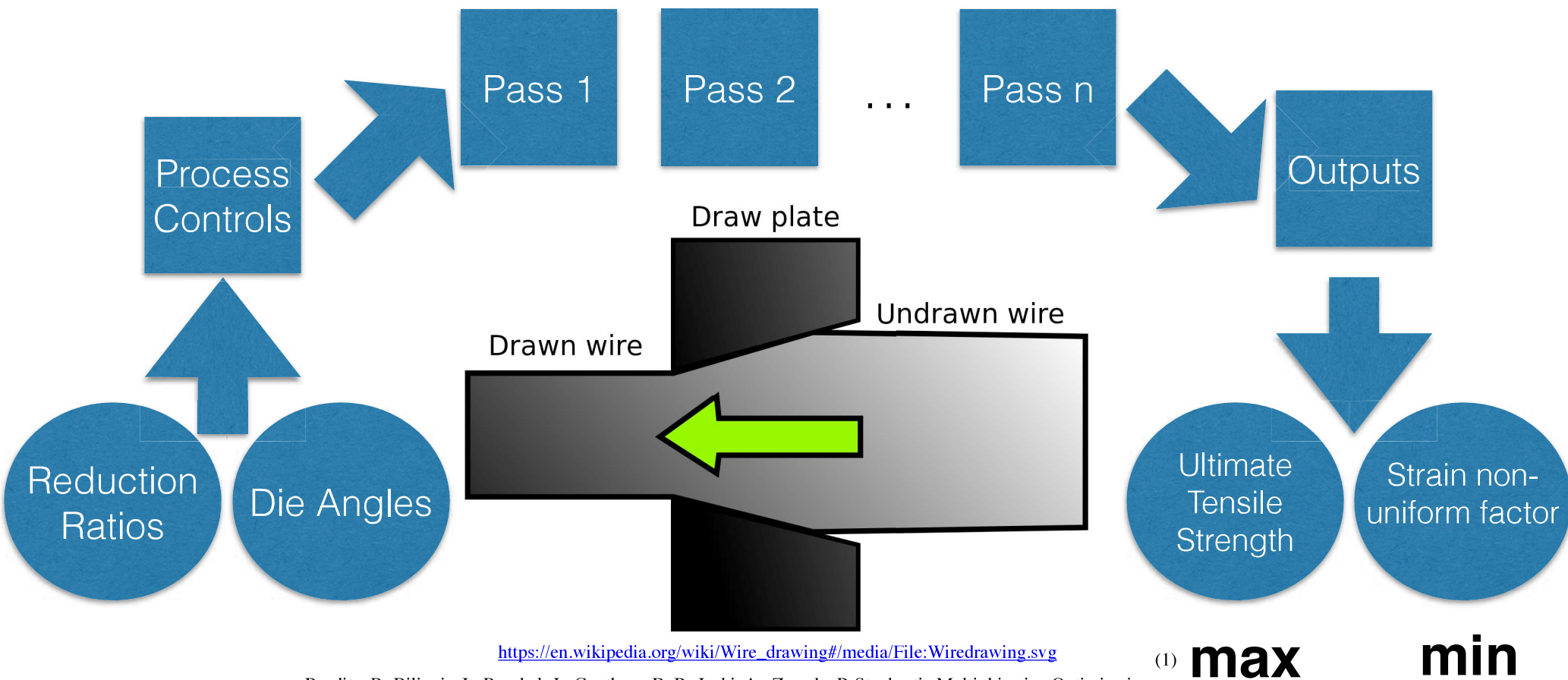


Dynamic vs myopic information acquisition

- Optimal information acquisition policies...
- \Rightarrow 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)

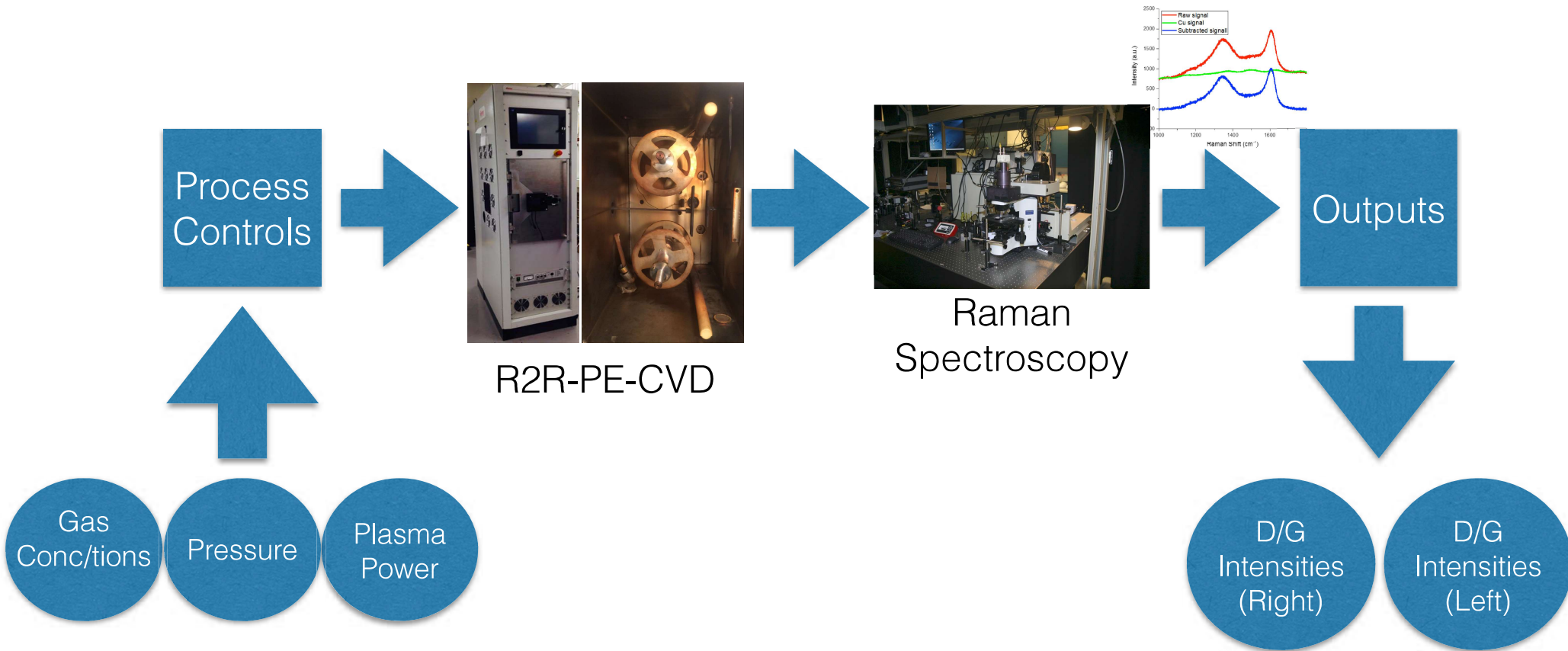


https://en.wikipedia.org/wiki/Wire_drawing#/media/File:Wiredrawing.svg

Pandita, P.; Bilonis, 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>.

Example: Design experiments

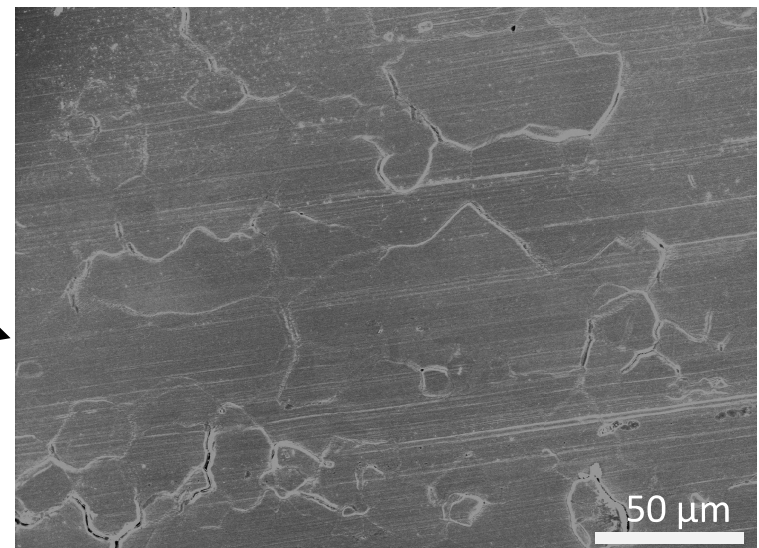
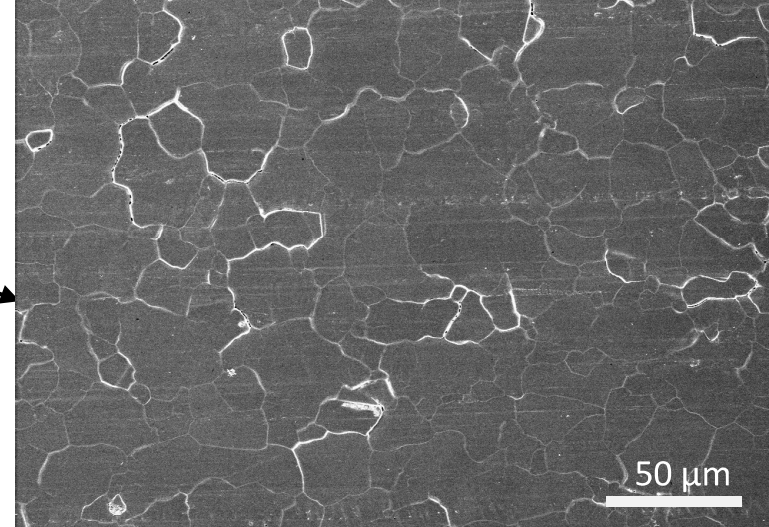
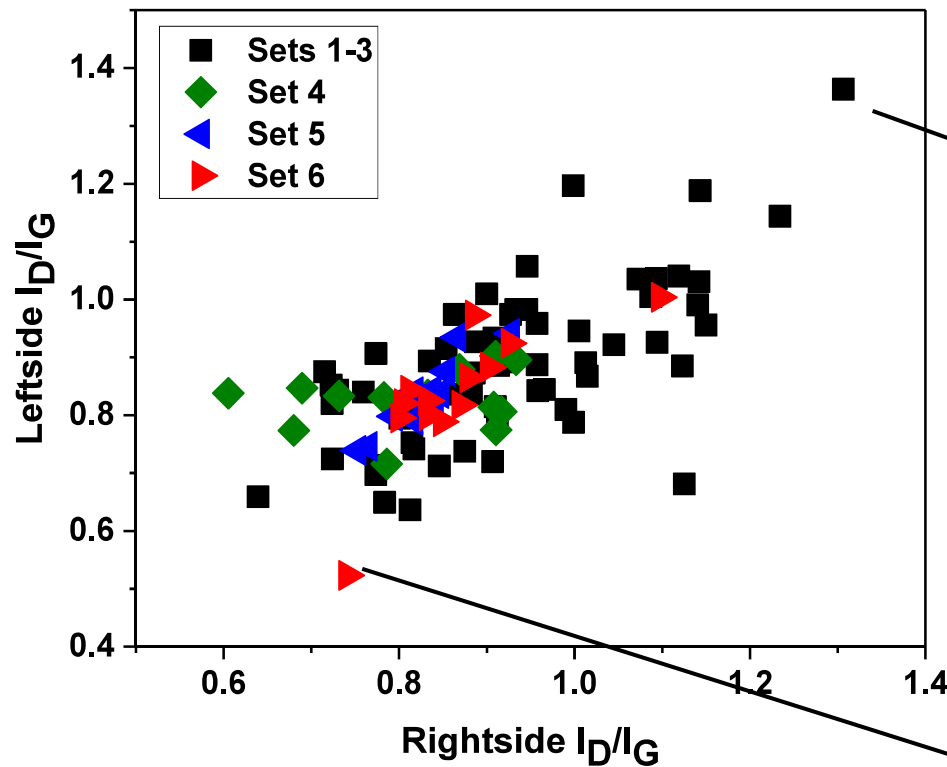
- Graphene manufacturing



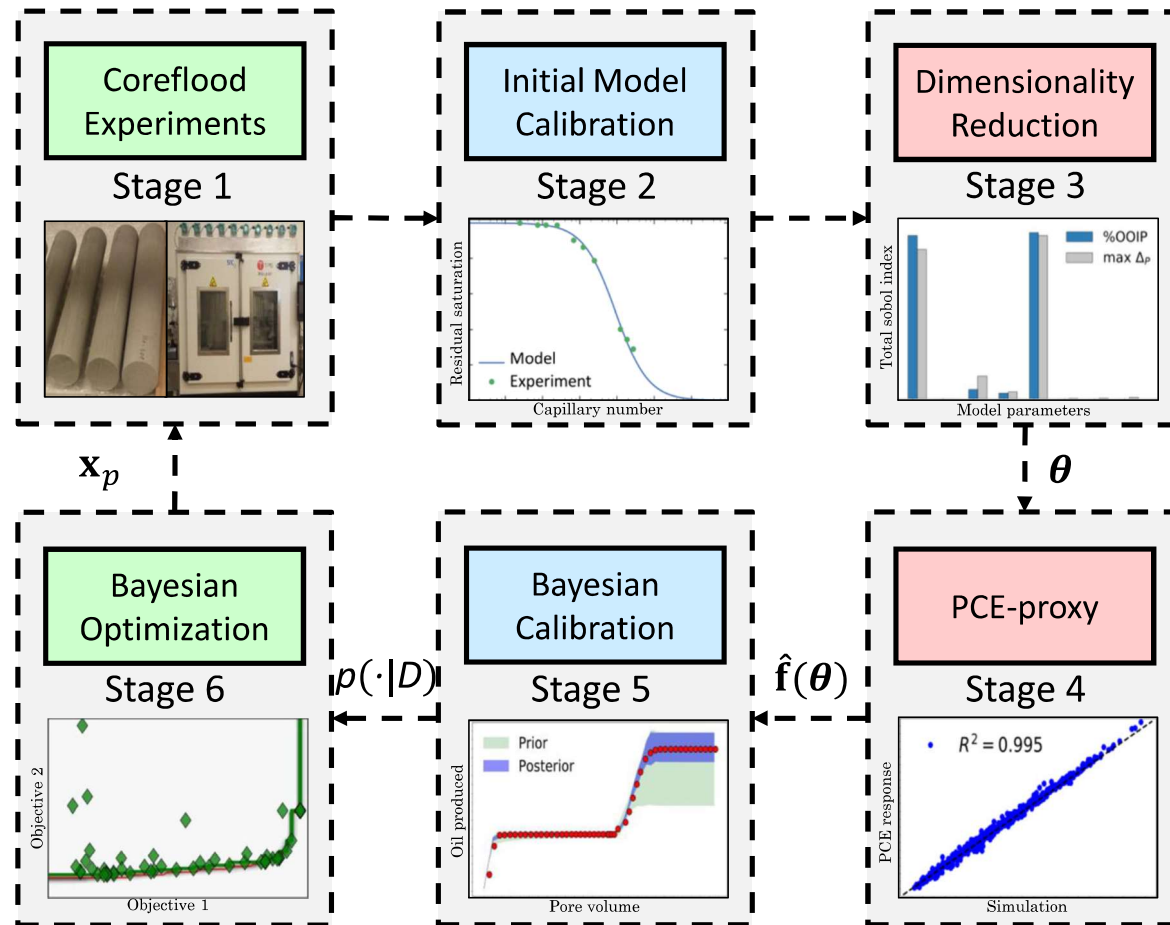
Alrefae, M. A.; Kumar, A.; Pandita, P.; Candadai, A.; Bilonis, I.; Fisher, T. S. Process Optimization of Graphene Growth in a Roll-to-Roll Plasma CVD System. *AIP Advances* **2017**, 7 (11), 115102. <https://doi.org/10.1063/1.4998770>.

Example: Design experiments

- Graphene manufacturing



Example: Calibrating expensive physical models



Naik, P.; Pandita, P.; Aramideh, S.; Bilonis, 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>.

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.** Niranjana 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.; Bilonis, 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.; Bilonis, 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>.
- ...

