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Sandia National Laboratories

A Bayesian Framework for Coupling Optimal Experimental Design and Optimal Control

Rebekah White†, Bart van Bloemen Waanders†, Arvind Saibaba‡, and Alen Alexanderian‡

† Sandia National Laboratories, Machine Learning org. 1441

‡ North Carolina State University

Robust Interpretable Scalable Efficient
RISE

U.S. Department of Energy NNSA

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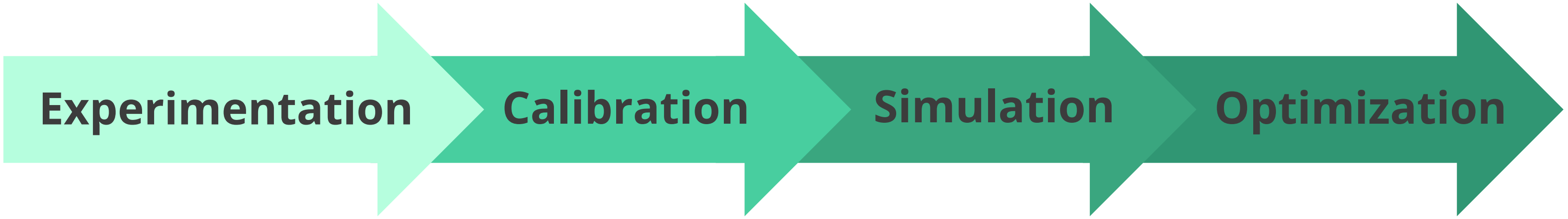
Optimal experimental design (OED)

What data is informative

Optimal experimental design (OED)

Workflow for how experimental data is utilized



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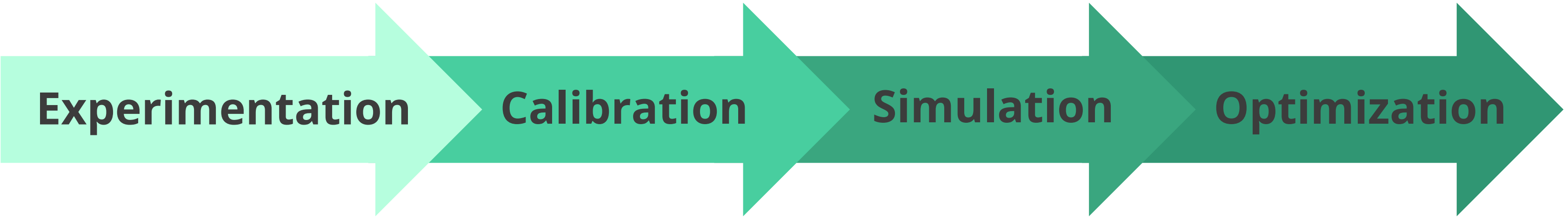

How informative data is, depends on the modeling goals

Optimal experimental design (OED)

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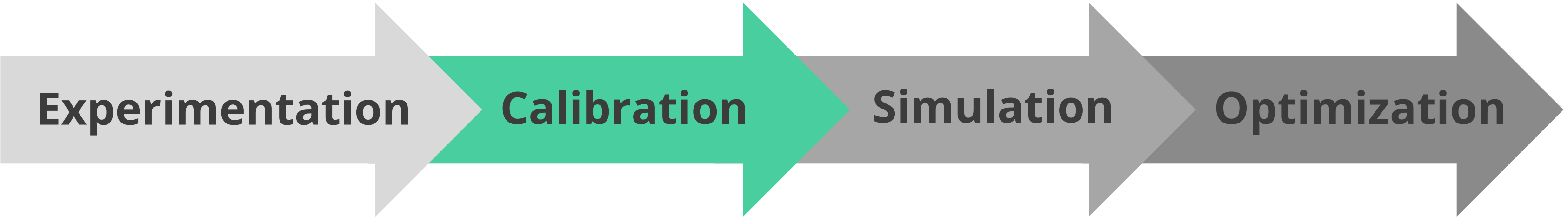
Workflow for how experimental data is utilized



Classical approaches focus on model calibration

↓

Reduce uncertainties in the inverse problem solution

Optimal experimental design (OED)

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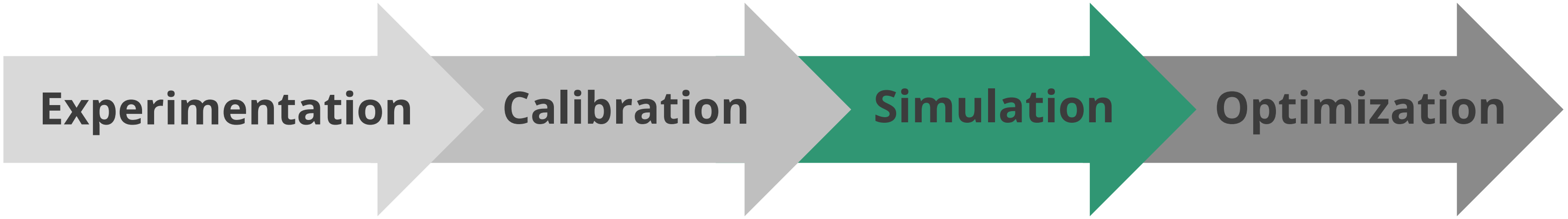

Goal-oriented approaches focus on reducing uncertainty in model predictions directly

↓

Shown to be very beneficial

What data is **informative**

Optimal experimental design (OED)

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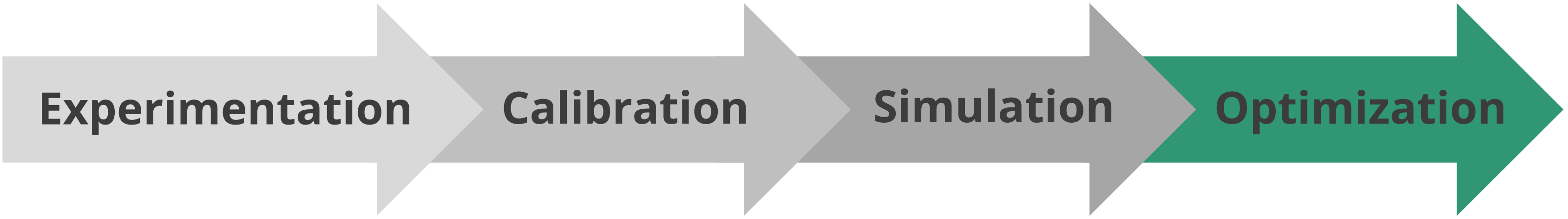

Consider how those uncertainties propagate to optimization

↓

Reduce uncertainties related to an optimal control objective

What data is **informative**

Goals for this presentation

Show how we can derive OED criteria to relate the informativeness of data to optimal control goals

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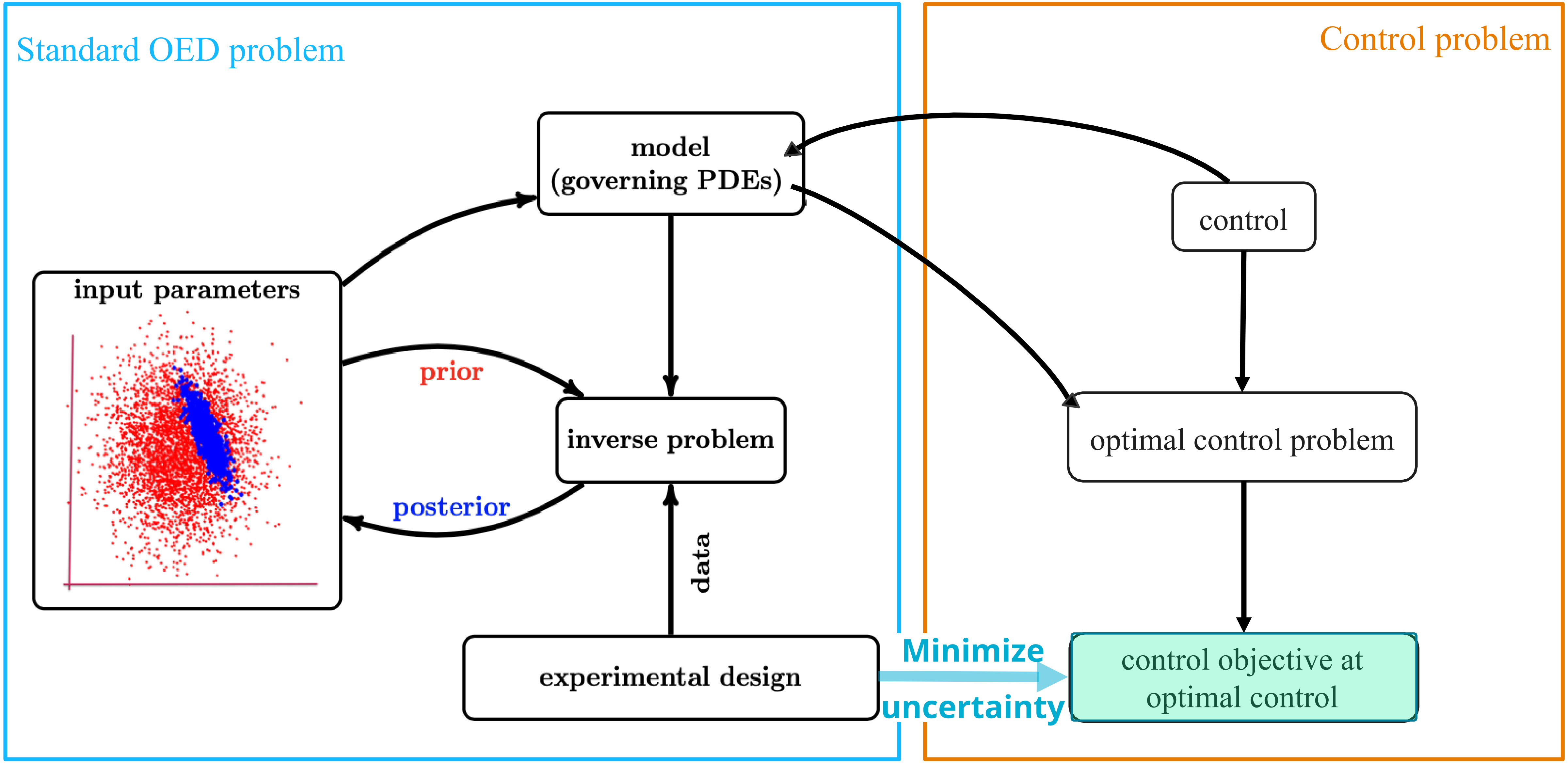
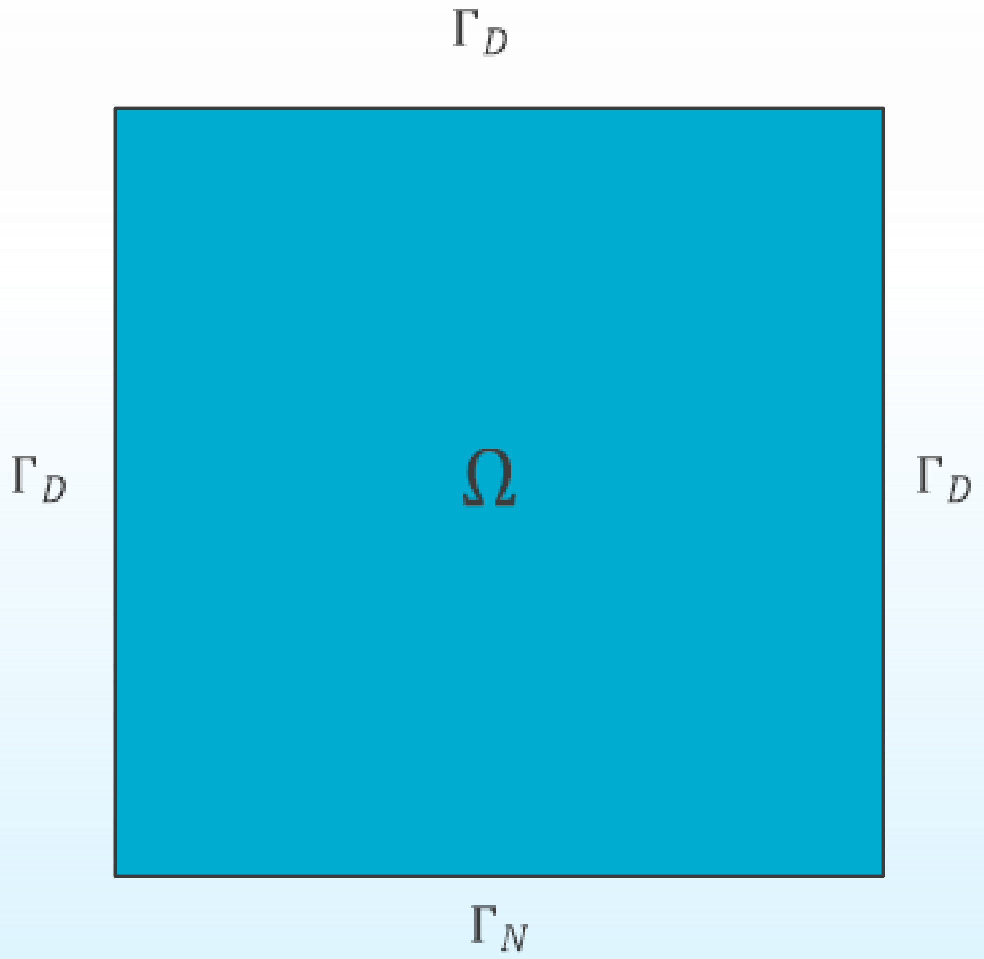
Do this using a simple problem formulation looking at contaminant diffusion across a 2D domain

How can determine optimal experimental designs when the modeling objective is optimal control?



We model contaminant spread using steady-state diffusion equations

$$
\begin{aligned}
-\kappa \Delta u(x,y) &= z(x,y) && \text{in } \Omega \\
u(x,y) &= 0 && \text{on } \Gamma_D \\
-\kappa \nabla u(x,y) \cdot \boldsymbol{n} &= p(x) && \text{on } \Gamma_\mathrm{N}
\end{aligned}
$$



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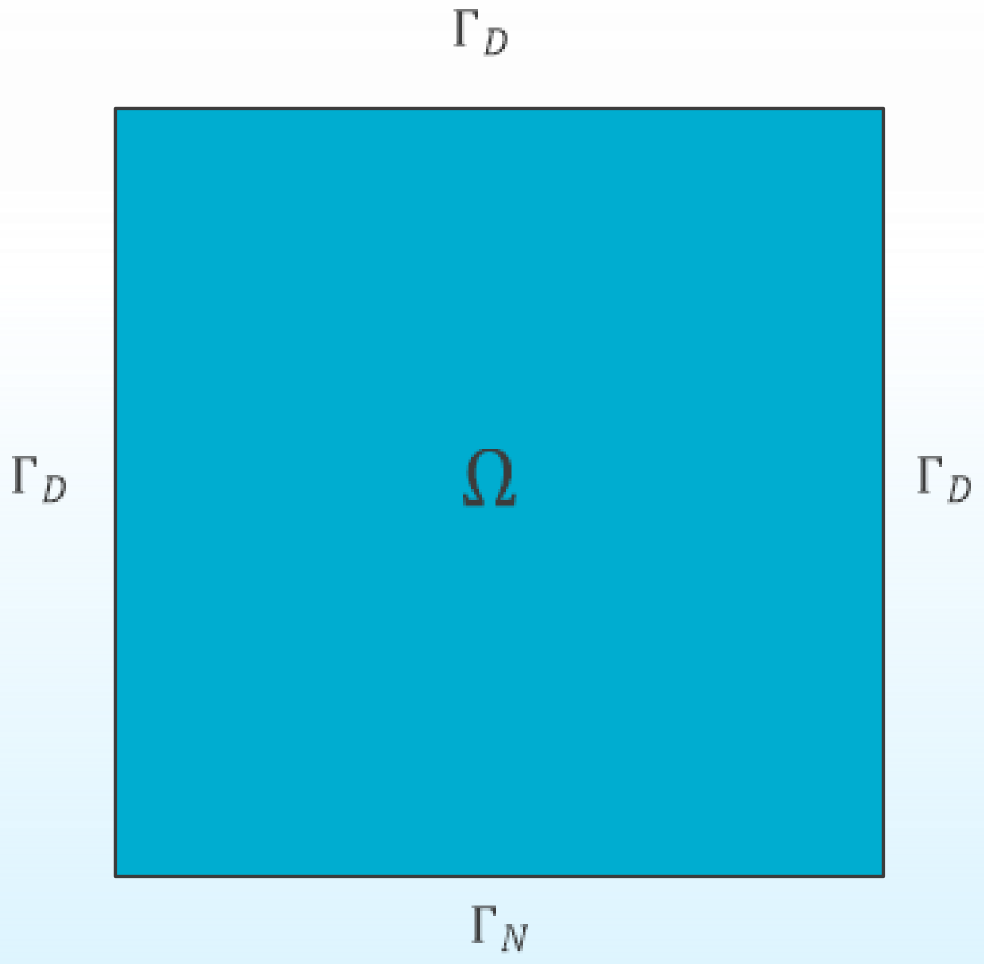
Contaminant concentration



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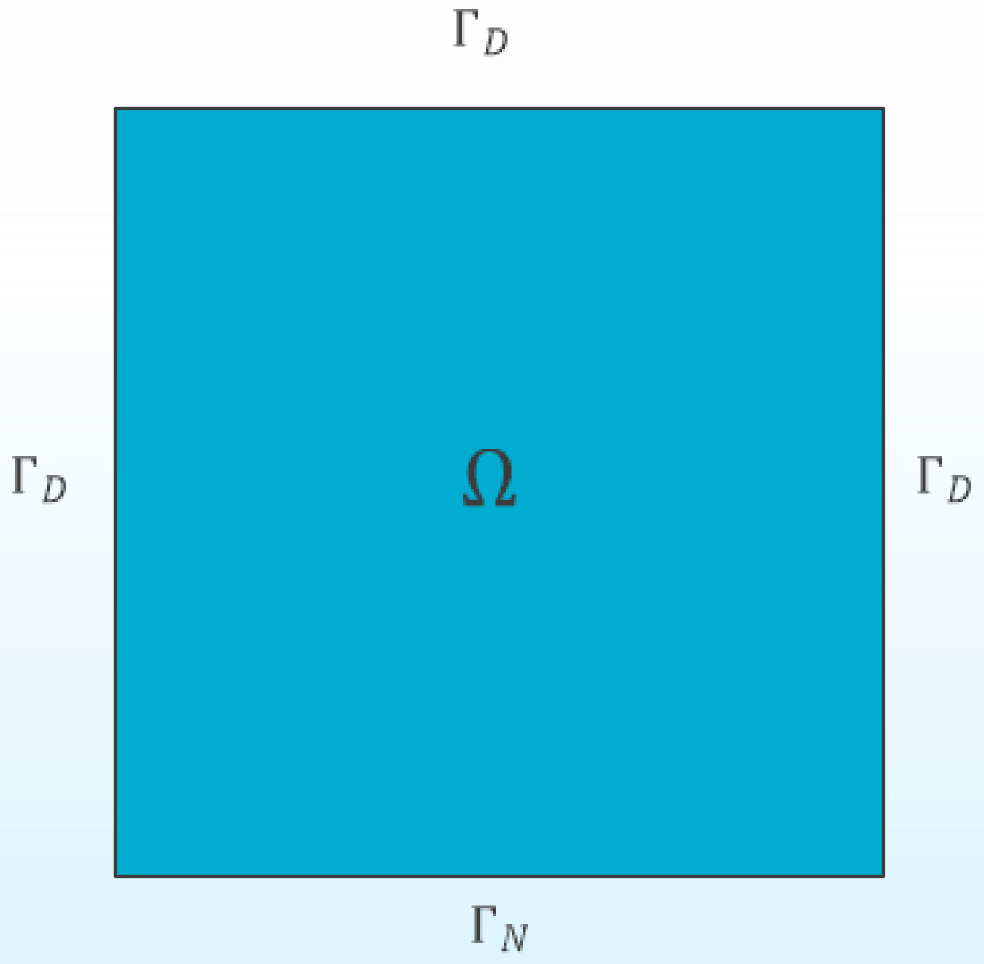
Control



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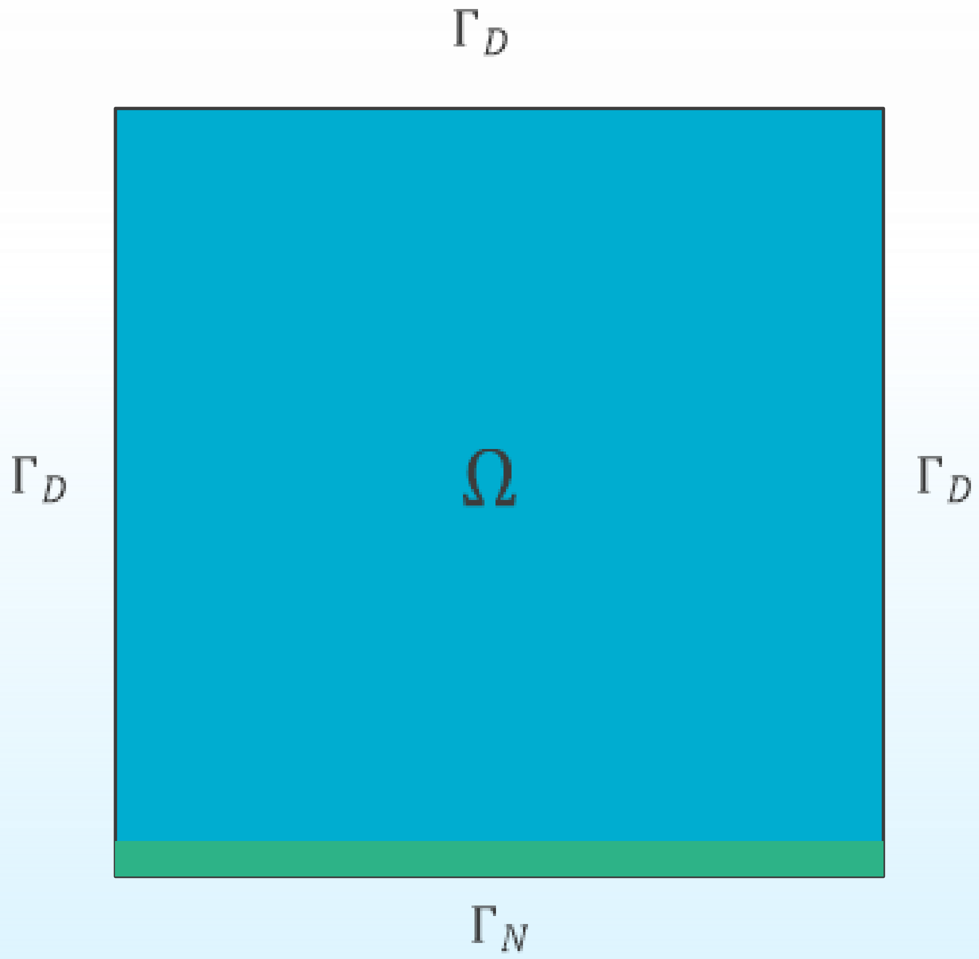
\end{aligned}
$$

Uncertain Neuman boundary condition



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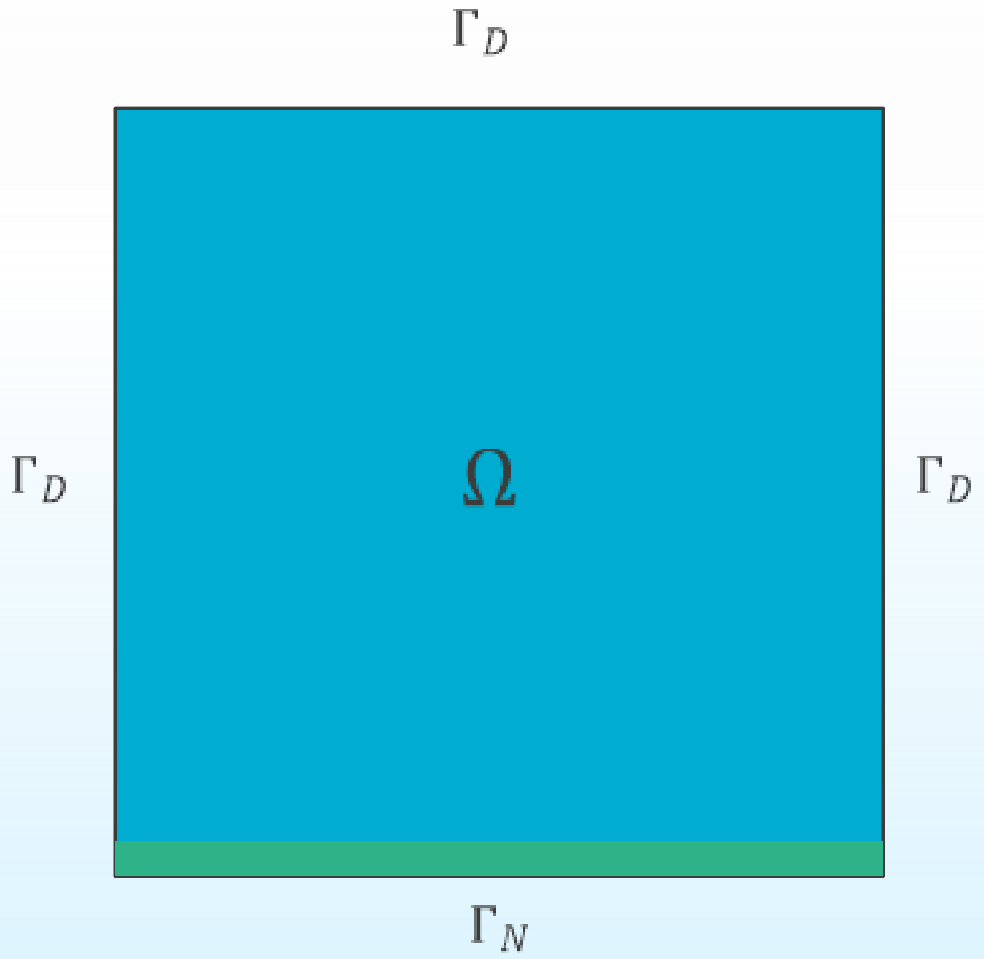
$$

Discretized PDE

$$\boldsymbol{u} = \boldsymbol{A}\boldsymbol{z} + \boldsymbol{B}\boldsymbol{p} + \boldsymbol{c}$$

Parameter-to-observable map

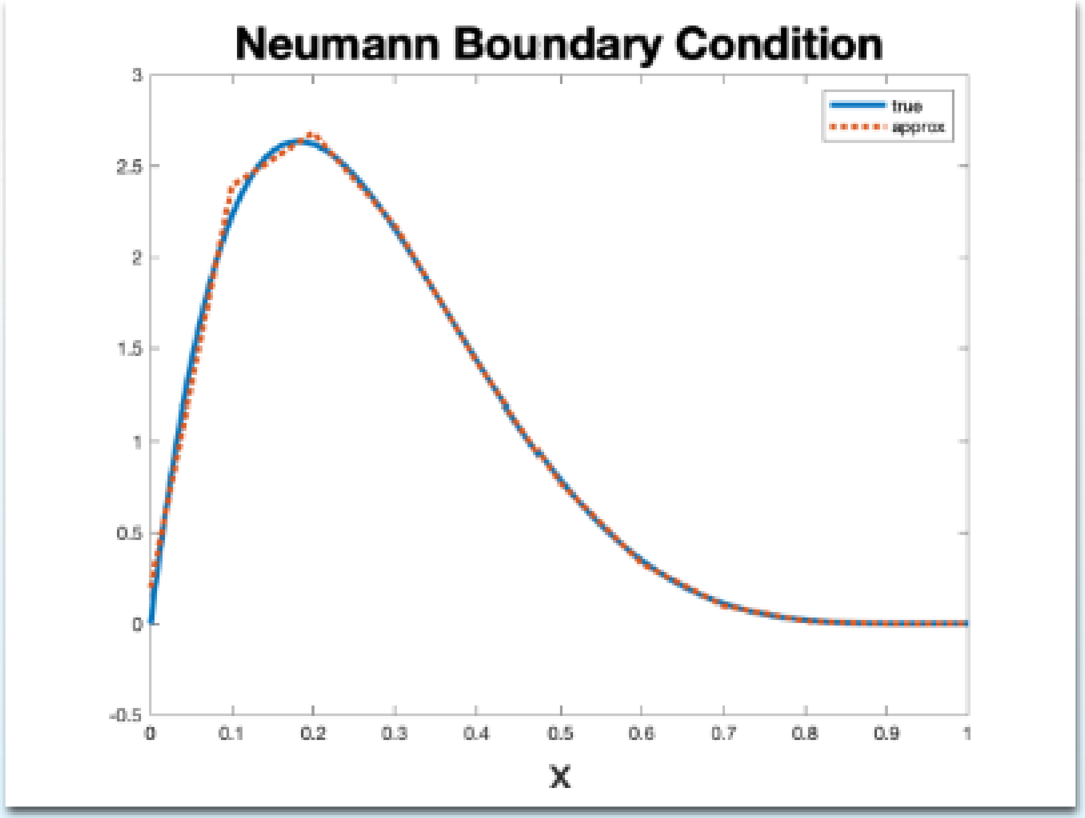
$$\boldsymbol{y} = \mathcal{O}\boldsymbol{u} + \boldsymbol{\eta}$$



The boundary flux is the uncertain model parameter

Assumption – finite dimensional parameters

$$p(x) = \sum_{i=1}^{n_p} p_{i_\phi}{}^{i}(x)$$



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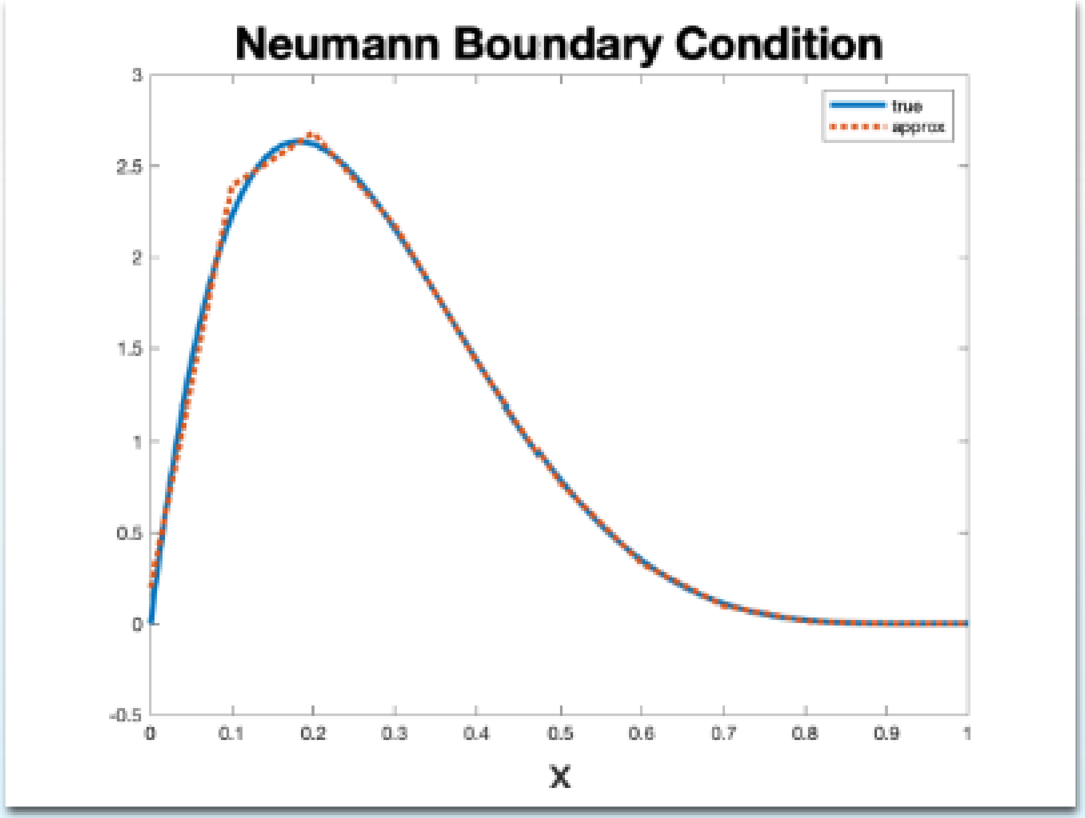
$$p(x) = \sum_{i=1}^{n_p} p_{i_\phi}{}^{i}(x)$$

estimate coefficients $\boldsymbol{p} = \{p_i\}$ from data $\boldsymbol{y}$

$$\pi(\boldsymbol{p}|\boldsymbol{y}) \propto \pi(\boldsymbol{y}\,|\boldsymbol{p})\,\pi_{\text{pri}}(\boldsymbol{p})$$



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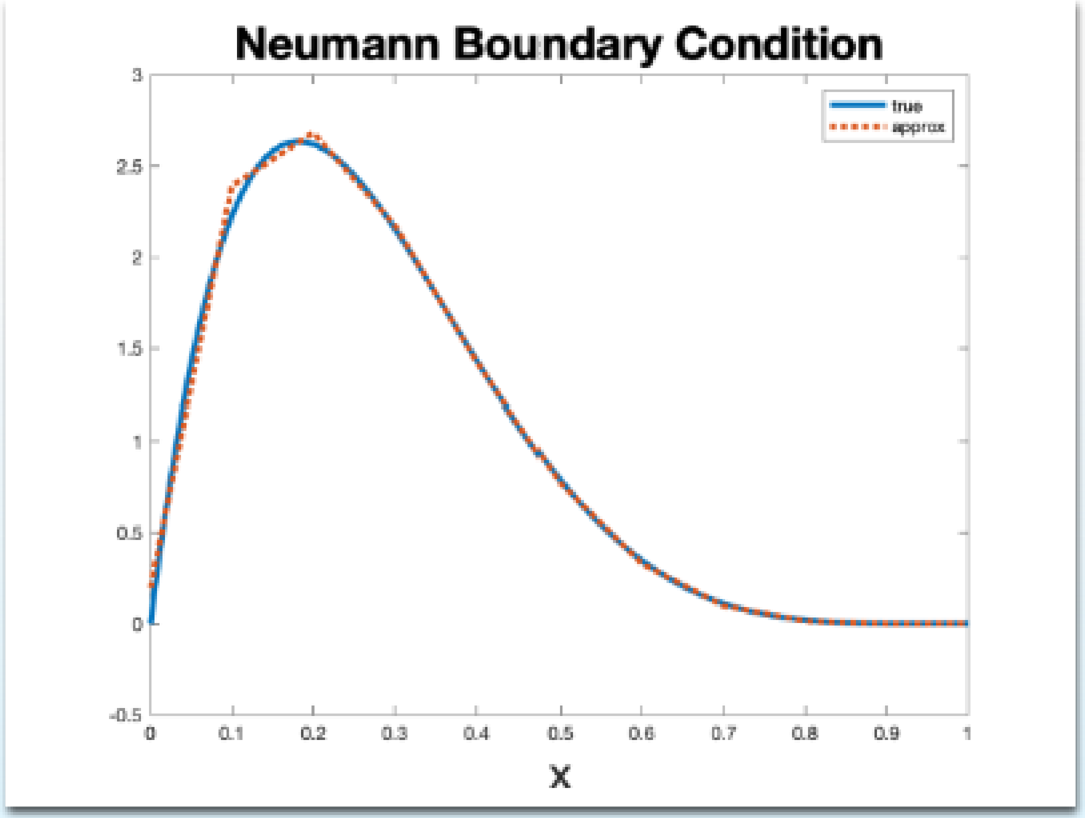
posterior



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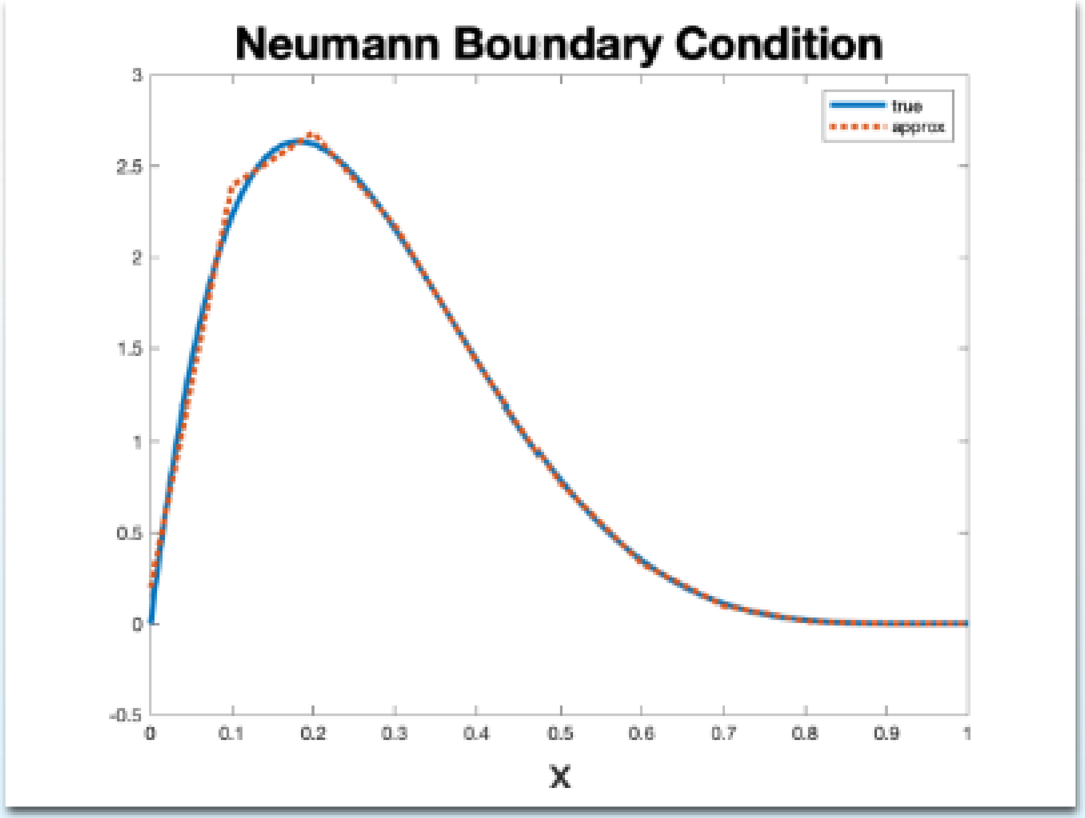
likelihood



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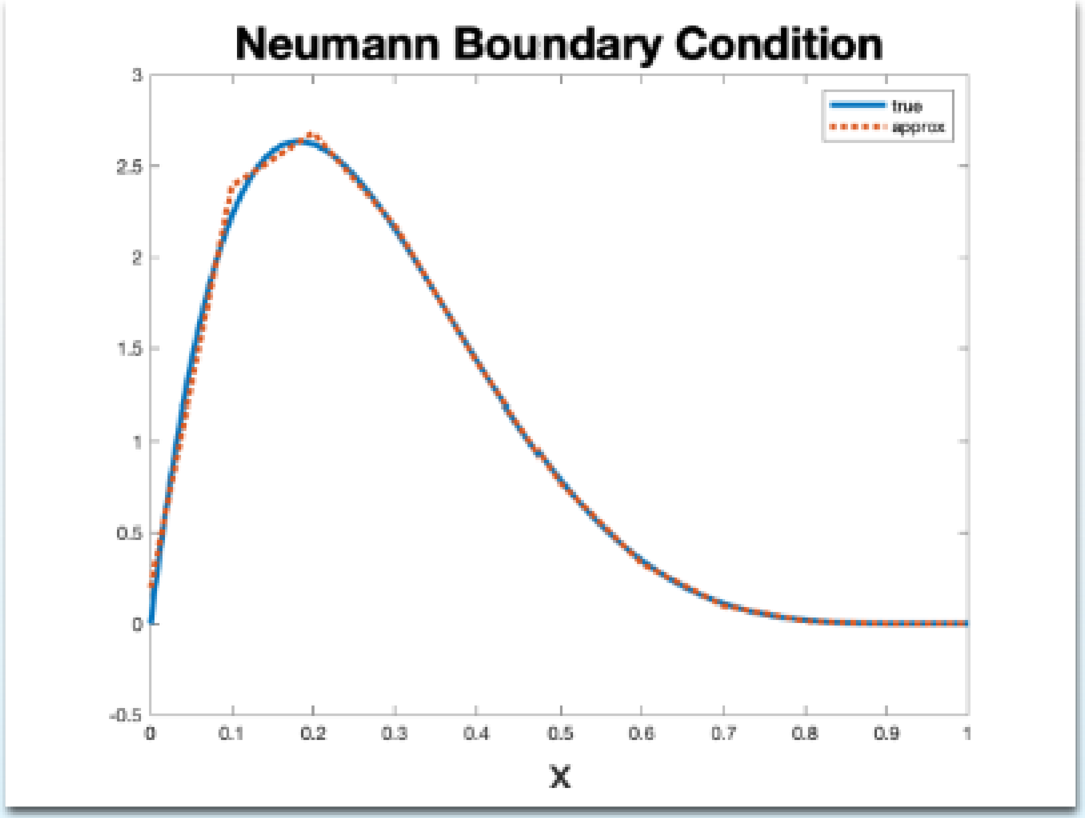
prior



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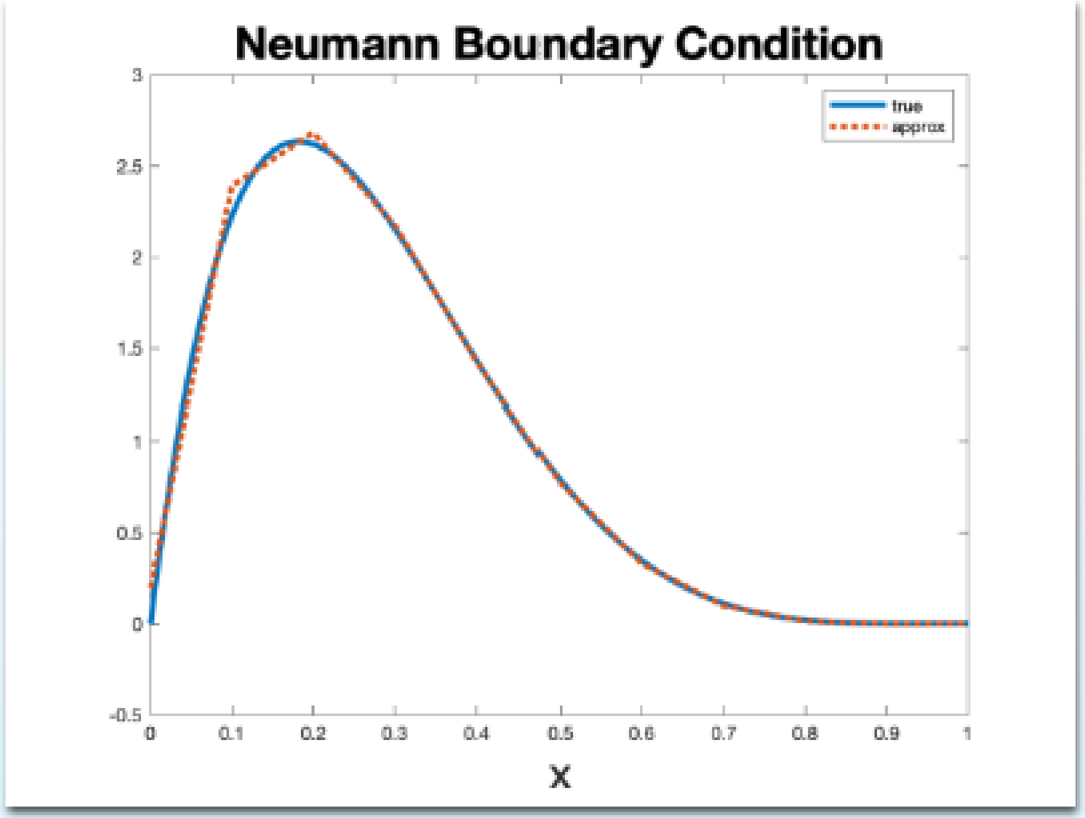
estimate coefficients $\boldsymbol{p} = \{p_i\}$ from data $\boldsymbol{y}$

$$\pi(\boldsymbol{p}|\boldsymbol{y}) \propto \pi(\boldsymbol{y}\,|\boldsymbol{p})\,\pi_{\text{pri}}(\boldsymbol{p})$$

$$\pi(\boldsymbol{y}\,|\boldsymbol{p}) \propto \exp\left(-\frac{1}{2}\,\|f(\boldsymbol{p}) - \boldsymbol{y}\|_{\Gamma}^{2}\right)$$



We consider binary optimal experimental designs

Experimental design

$$\xi = \begin{Bmatrix} \boldsymbol{x}_1, \ldots, \boldsymbol{x}_k \\ w_1, \ldots, w_k \end{Bmatrix}$$

- $\boldsymbol{x}_i \in [0,1] \cup [0,1]$ – Fixed spatial design candidates
- $w_i \in \{0,1\}$ – Binary weights
- $\sum w_i = N$ – Budget

Bayesian OED for inverse problems – minimize uncertainty in boundary coefficients

OED objective function – average variance in parameters

$$U(\xi) = \mathrm{trace}\left(\boldsymbol{\Gamma}_{\mathbf{post}}(\xi)\right)$$

Gaussian prior + linear parameter-to-observable map → Gaussian posterior

$$\pi_{\mathrm{post}} \sim \mathcal{N}\left(\boldsymbol{m}_{\mathrm{post}}, \boldsymbol{\Gamma}_{\mathbf{post}}\right)$$

Analytic expression for the posterior covariance → Analytically evaluate objective function

$$\boldsymbol{\Gamma}_{\mathbf{post}} = \left(\boldsymbol{F}_2^T \boldsymbol{\Gamma}_{\mathrm{noise}}^{-1}(\xi) \boldsymbol{F}_2 + \boldsymbol{\Gamma}_{\mathrm{pr}}^{-1}\right)^{-1}$$

The optimal control problem is to maintain a target concentration across the domain

Optimal control

$$\boldsymbol{z}^* = \underset{z}{\operatorname{argmin}} \frac{1}{2} \int_{[0,1]\times[0,1]} (u(\boldsymbol{z}) - \bar{u})^2 dx\, dy + \frac{\gamma}{2} \|\boldsymbol{z}\|_2^2$$

Target concentration

$$\bar{u}(x, y) = -1$$

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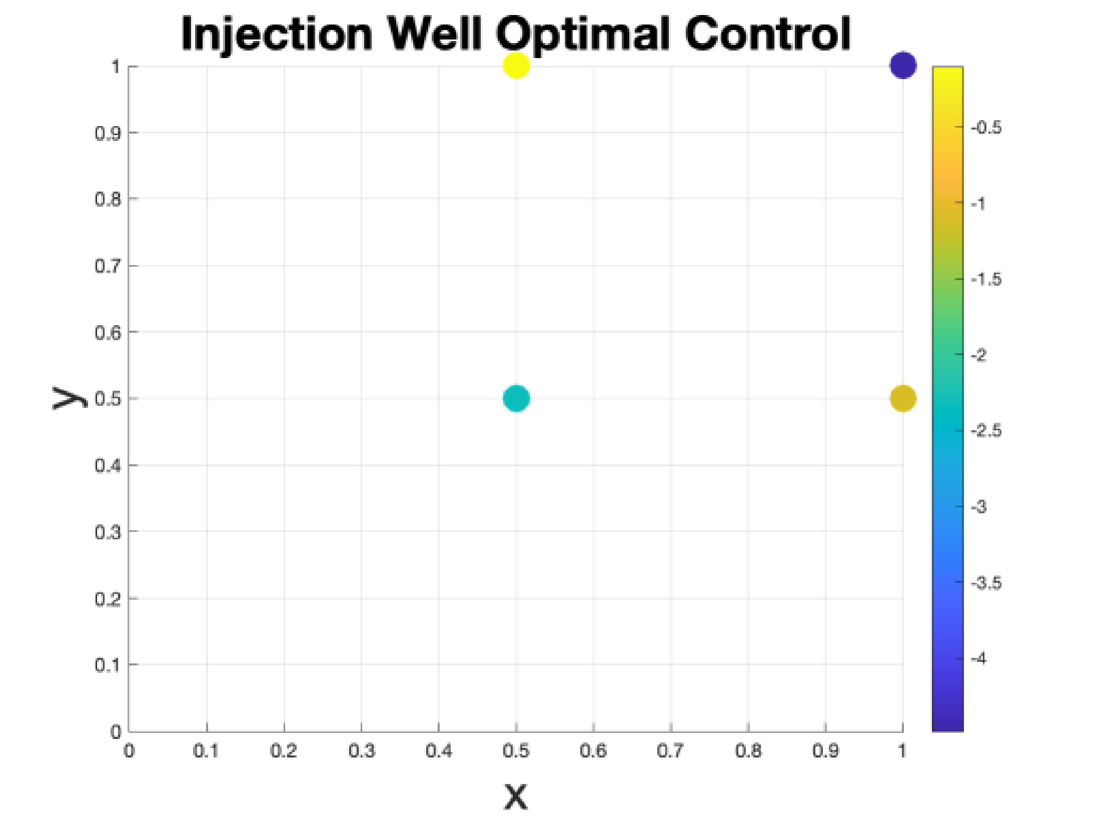
Discrete injection/reuptake wells

$$z = [z_1, z_2, z_3, z_4]$$



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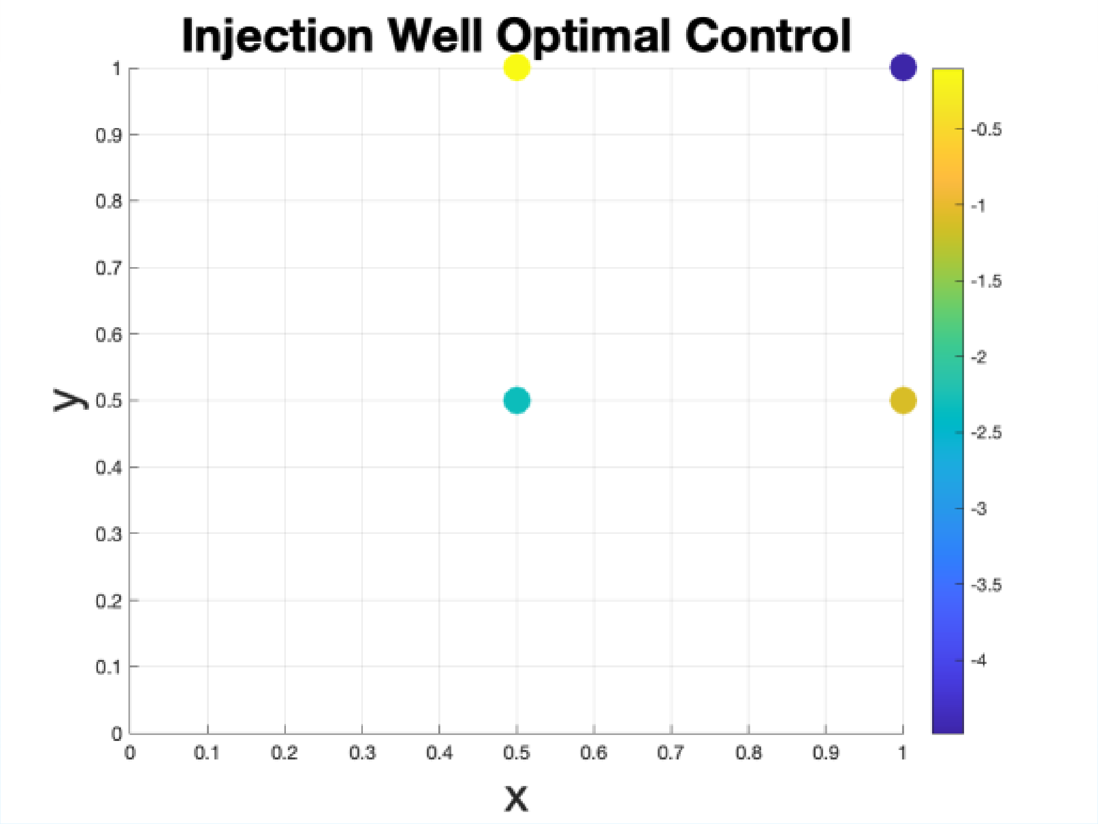
$$z = [z_1, z_2, z_3, z_4]$$

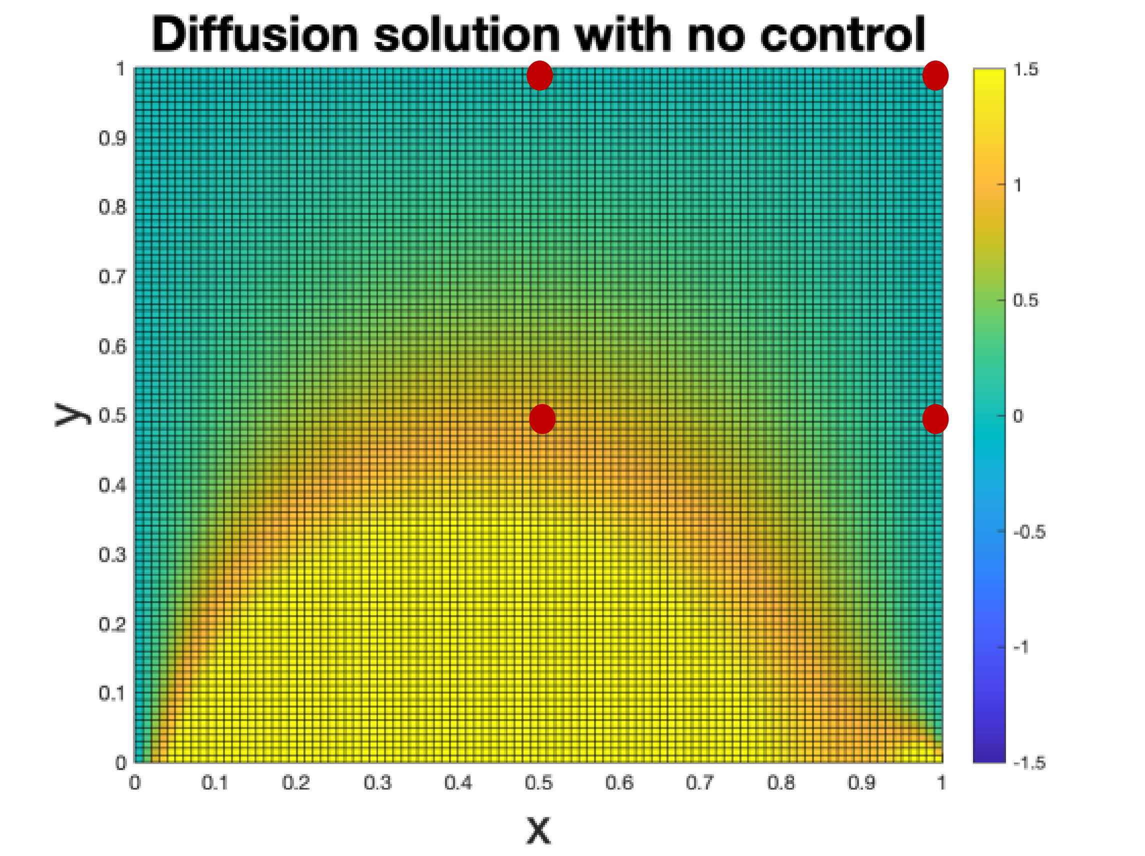
$$z^*(p) = \hat{A}p + \hat{c}$$

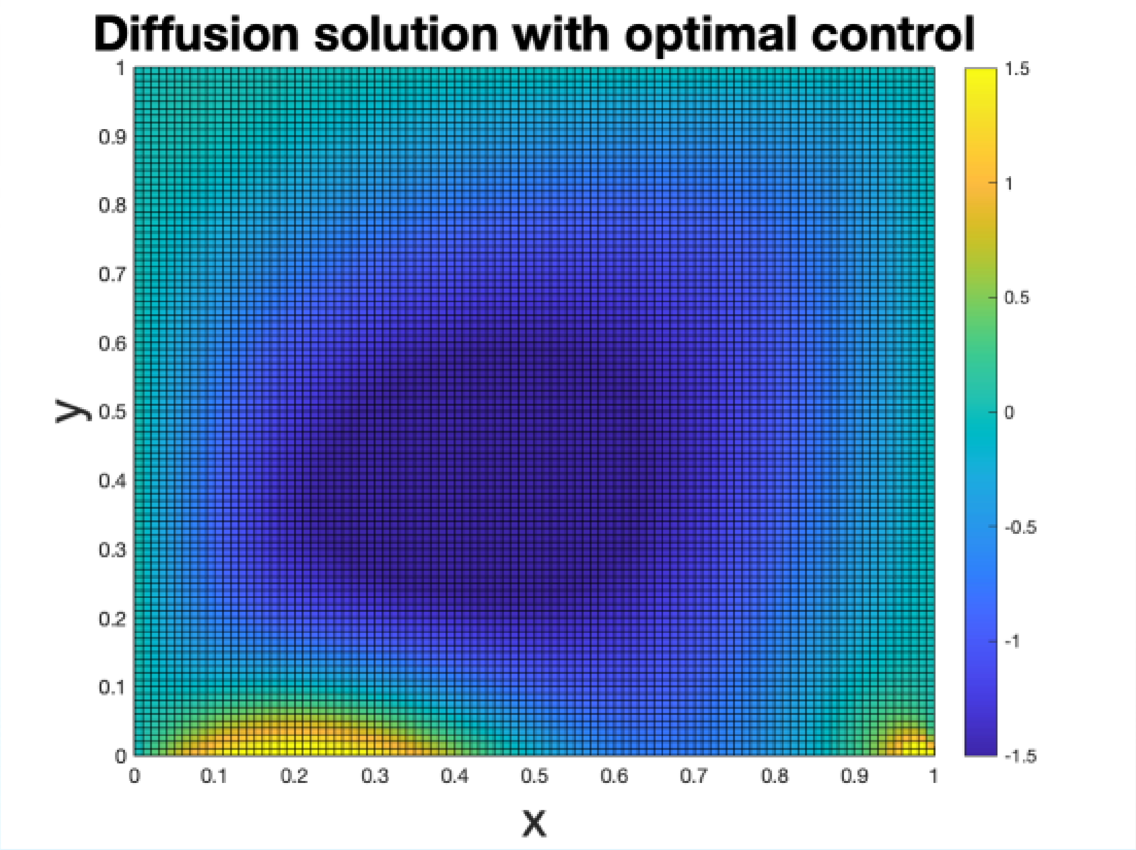


Injection/reuptake wells control the contaminant concentration

● Injection/reuptake wells

■ Target concentration





Bayesian control-oriented OED – minimize uncertainty in control objective

Control objective is quadratic in the model parameter

$$\phi(\mathbf{z}^*(\mathbf{p})) = \frac{1}{2}\int_\Omega (u(\mathbf{z}^*(\mathbf{p})) \; - \bar{u})^2 dxdy \approx \frac{1}{2}\langle \boldsymbol{F}\boldsymbol{p} + \boldsymbol{d}, \boldsymbol{Q}(\boldsymbol{F}\boldsymbol{p} + \boldsymbol{d})\rangle \,,$$

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Analytic expressions for the variance of quadratic functionals of Gaussian random vectors

$$\psi(\boldsymbol{y}, \xi) := \operatorname{Var}\left[\frac{1}{2}\langle \boldsymbol{Fp} + \boldsymbol{d}, \boldsymbol{Q}(\boldsymbol{Fp} + \boldsymbol{d})\rangle\right]$$

$$= \frac{1}{2}\operatorname{tr}\left[\left(\widetilde{\boldsymbol{A}}\boldsymbol{\Gamma}_{\text{post}}\right)^2\right] + \langle \widetilde{\boldsymbol{A}}\boldsymbol{m}_{\text{post}} + \widetilde{\boldsymbol{b}}, \boldsymbol{\Gamma}_{\text{post}}(\widetilde{\boldsymbol{A}}\boldsymbol{m}_{\text{post}} + \widetilde{\boldsymbol{b}})\rangle$$

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↓

$$\boldsymbol{F}^T\boldsymbol{Q}\boldsymbol{F}$$

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↓

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Bayesian control-oriented OED – minimize uncertainty in control objective

OED control-oriented objective function – variance in control objective

$$U(\xi) = E_{\boldsymbol{y}}\left[\psi(\boldsymbol{y}, \xi)\right], \quad \boldsymbol{y} \sim \pi(\boldsymbol{y}|\xi)$$

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Analytically evaluate objective function and compare to OED for inverse problems

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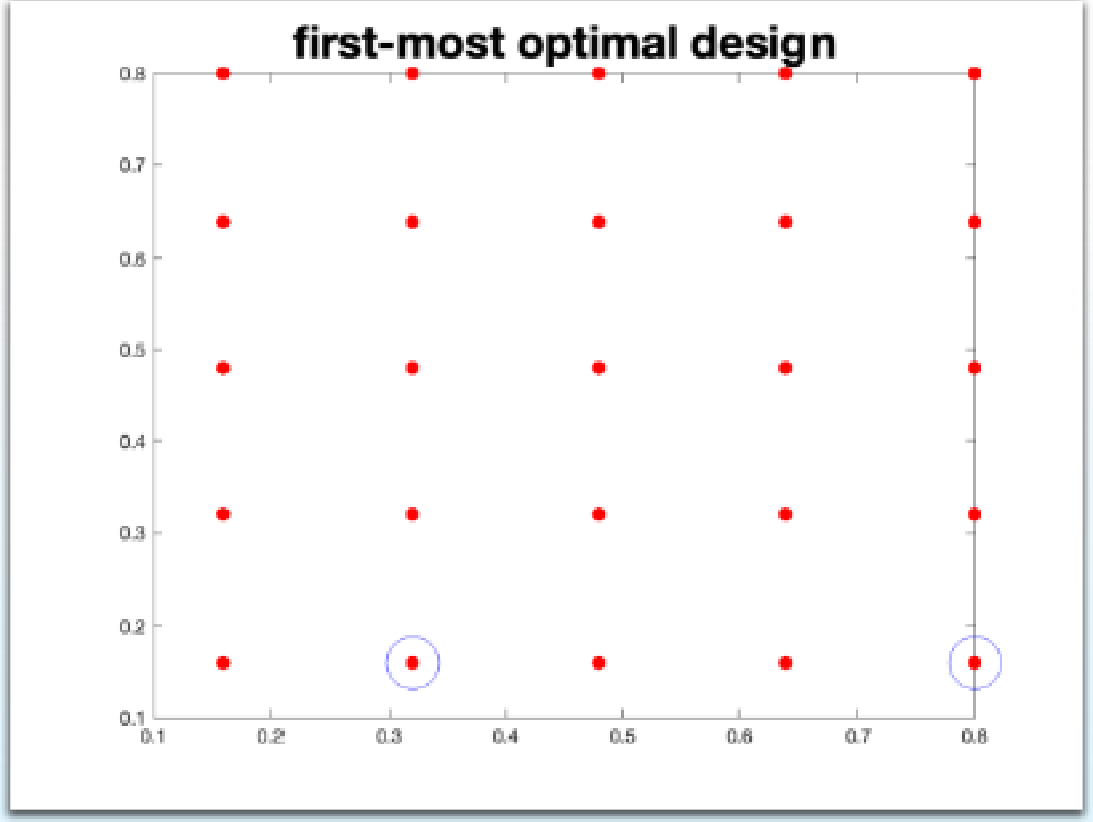
OED objective function – average variance in parameters

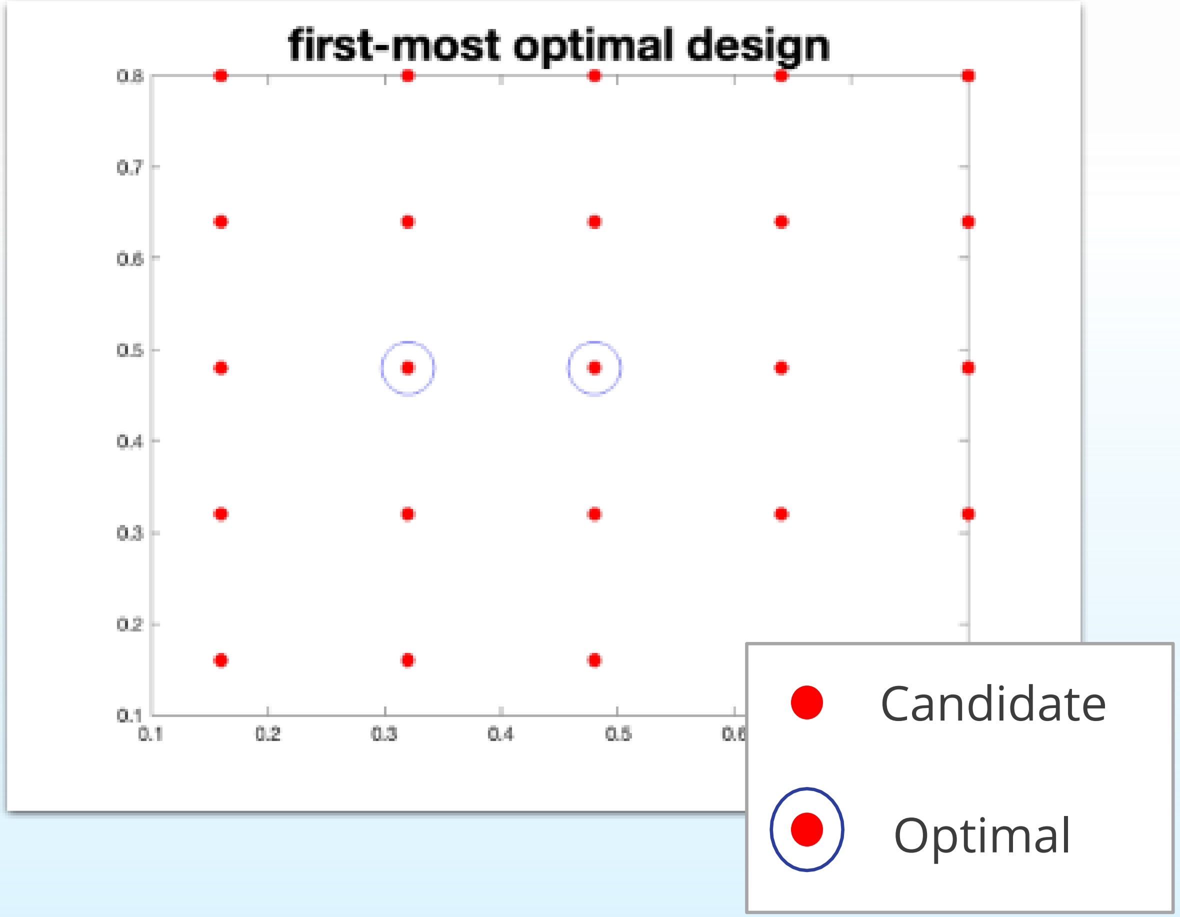
$$U(\xi) = \mathrm{trace}\left(\boldsymbol{\Gamma}_{\mathbf{post}}(\xi)\right)$$

Compare the optimal designs for OED for inverse problems versus control-oriented OED with a budget of 2 sensors

Minimize parameter uncertainty



Minimize control objective uncertainty



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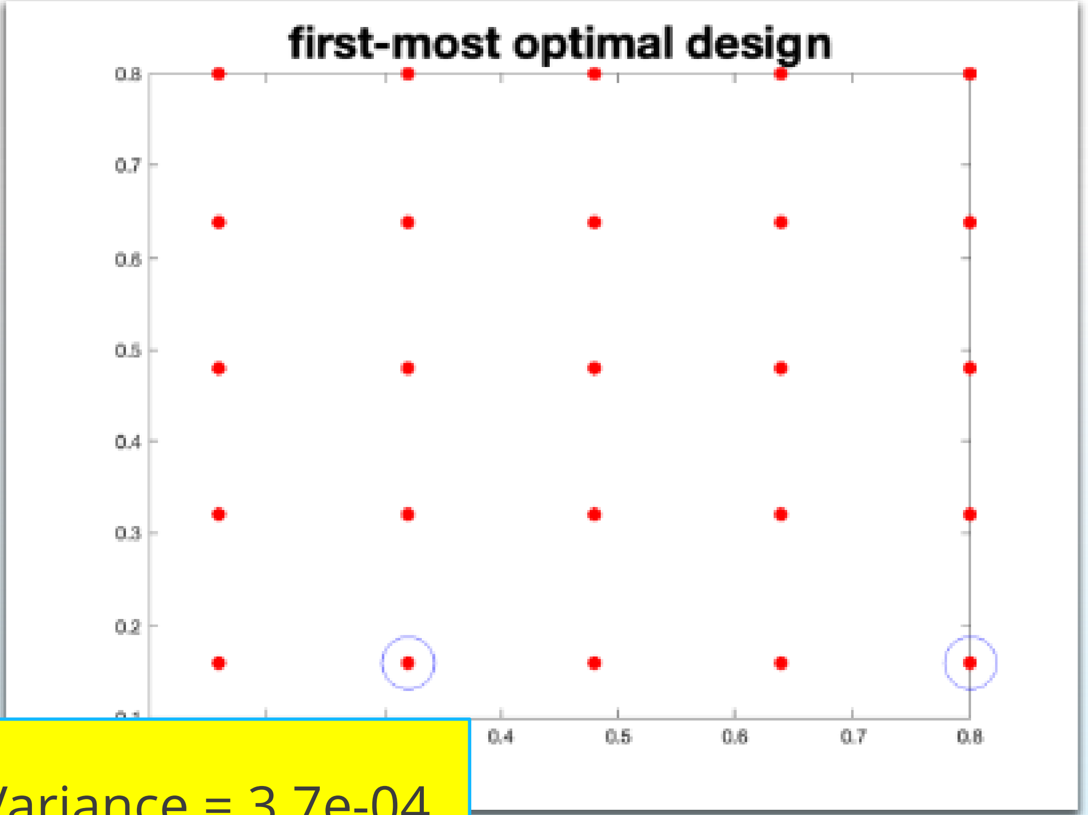
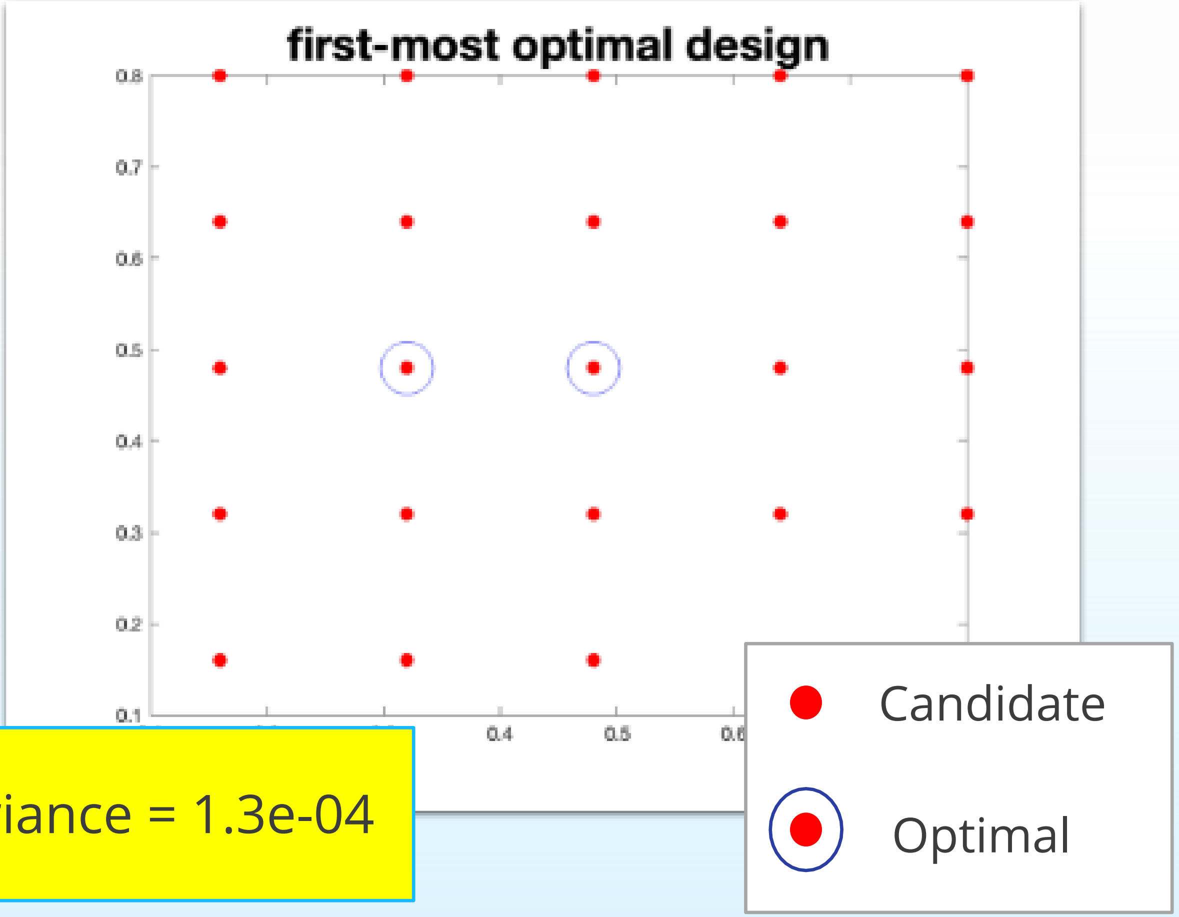


Variance = 3.7e-04

Minimize control objective uncertainty



Variance = 1.3e-04

Conclusions

- Derived a control-oriented OED objective function – reduce uncertainties in an optimization goal

- Control objective uncertainty that is three times smaller than classical OED strategies provide

Future work

Scale this to more complicated problems

- Transient
- Infinite dimensional parameters
- Nonlinear parameter-to-observable maps