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Sandia National Laboratories

Characterizing and Propagating Model Discrepancy in PDE-Constrained Optimization

Joseph Hart and Bart van Bloemen Waanders

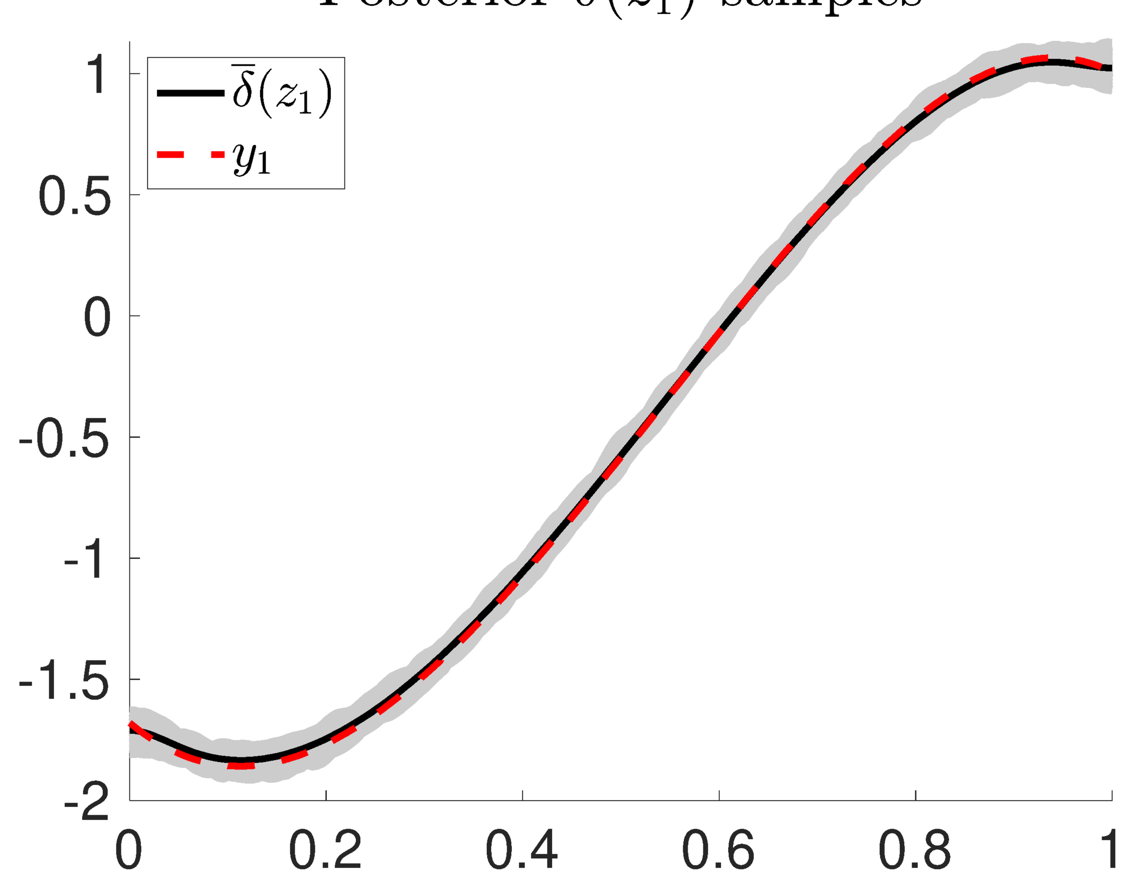
Want to solve:

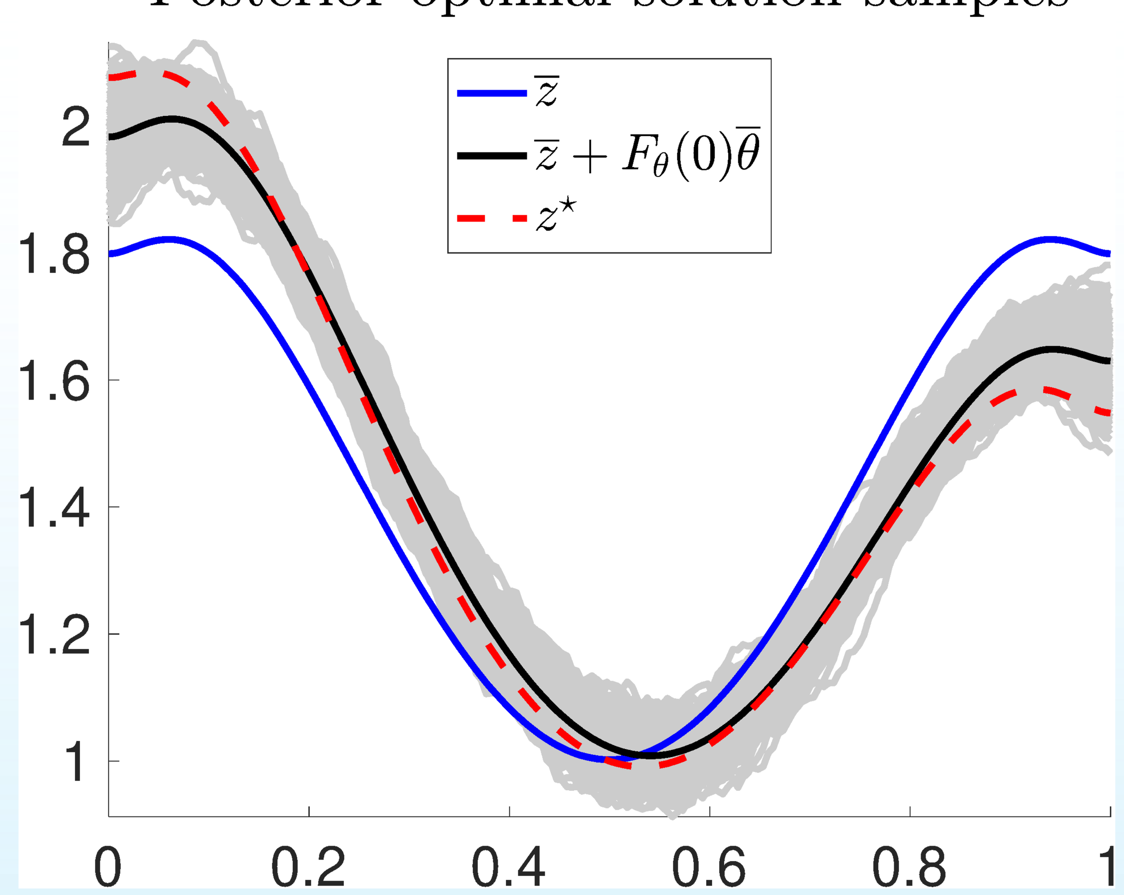
$$\min_{z} J(S(z), z)$$

Actually solve:

$$\min_{z} J(\tilde{S}(z), z)$$

1D Diffusion versus Advection-Diffusion





Low-fidelity Optimization

$$\min_{z} J(\tilde{S}(z) + \delta(z, \theta), z)$$

High-fidelity Data

$$S(z_\ell) - \tilde{S}(z_\ell)$$

Post-Optimality Sensitivity

$$F_\theta'(0) = -H^{-1}B$$

Bayesian Inversion

$$\pi_{\text{post}} \propto \pi_{\text{like}} \pi_{\text{prior}}$$

Post-Optimality Sensitivity

$$\Theta \sim \pi_{\text{post}} \implies z_{\text{post}} \approx F_\theta'(0)\Theta$$

Posterior samples take the form

$$\overline{\theta} + \hat{\theta} + \tilde{\theta}$$

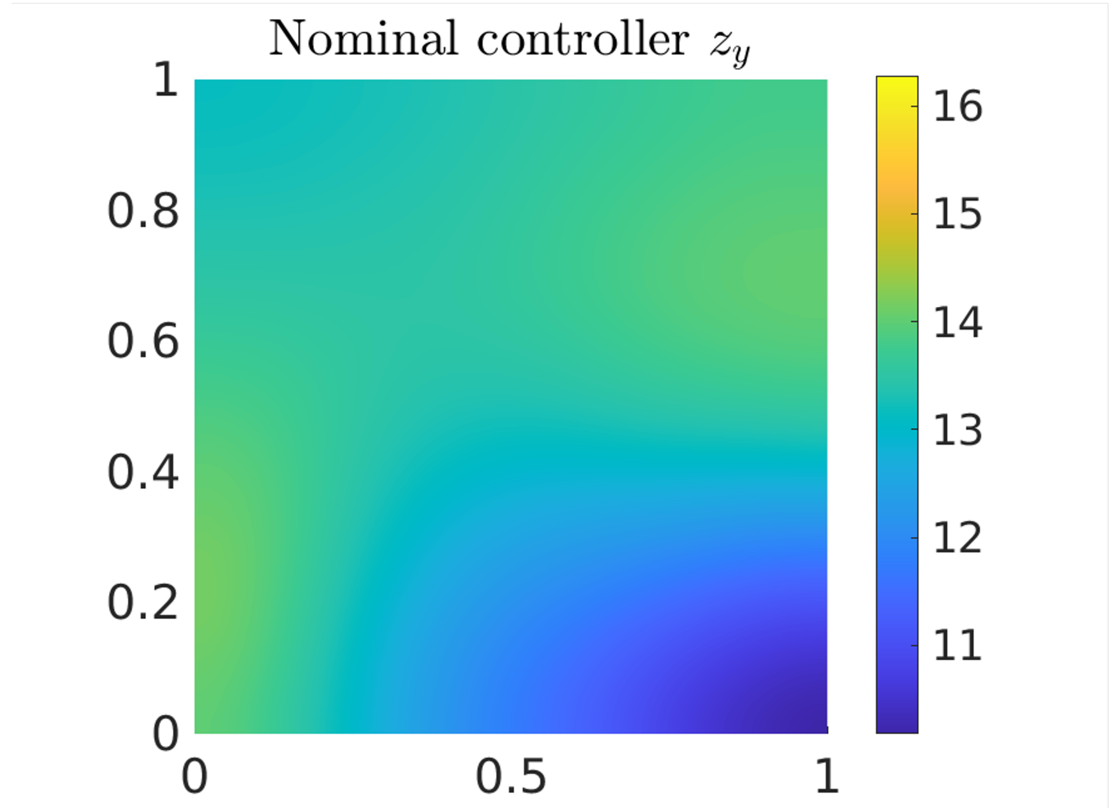
where the mean is

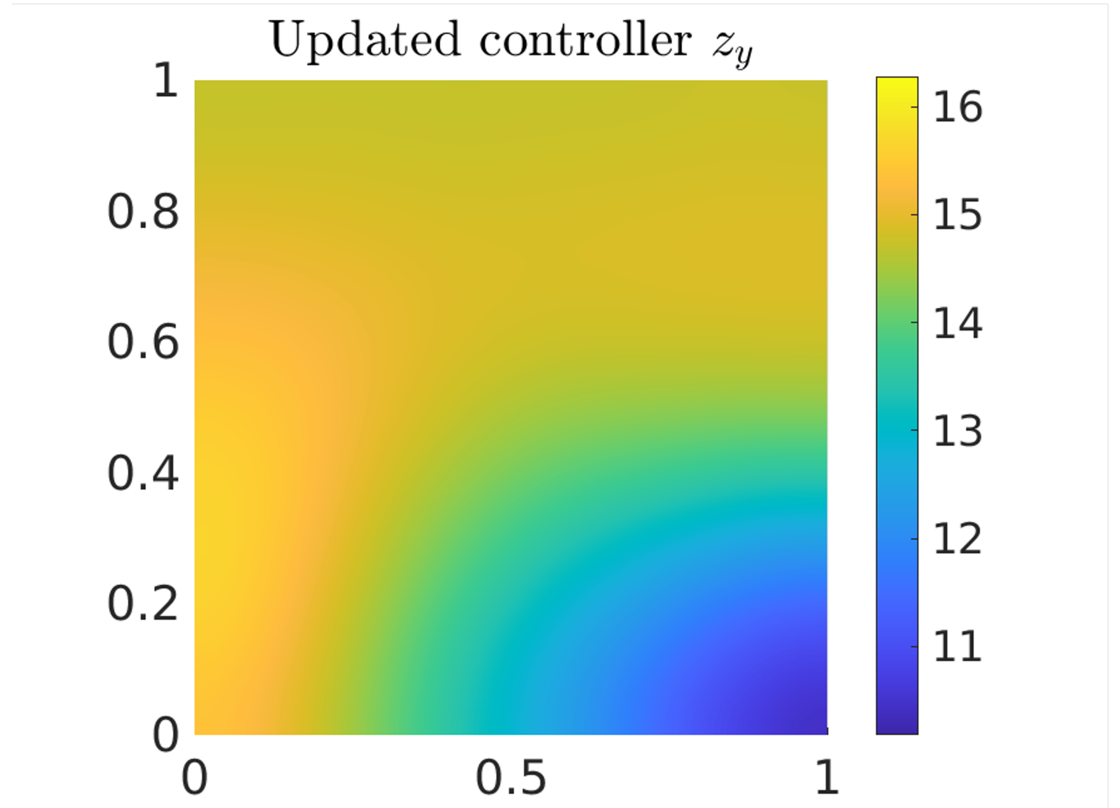
$$\overline{\theta} = \frac{1}{\alpha} \sum_{\ell=1}^{N} \left[\begin{pmatrix} a_\ell u_\ell \\ u_\ell \otimes \mathbf{M}_z^{-1} \mathbf{\Gamma}^{-1} (z_\ell - \overline{z}) \end{pmatrix} - \sum_{i=1}^{N} b_{i,\ell} \begin{pmatrix} s_i \boldsymbol{u}_{i,\ell} \\ \boldsymbol{u}_{i,\ell} \otimes \mathbf{M}_z^{-1} \mathbf{\Gamma}^{-1} \boldsymbol{w}_i \end{pmatrix} \right]$$

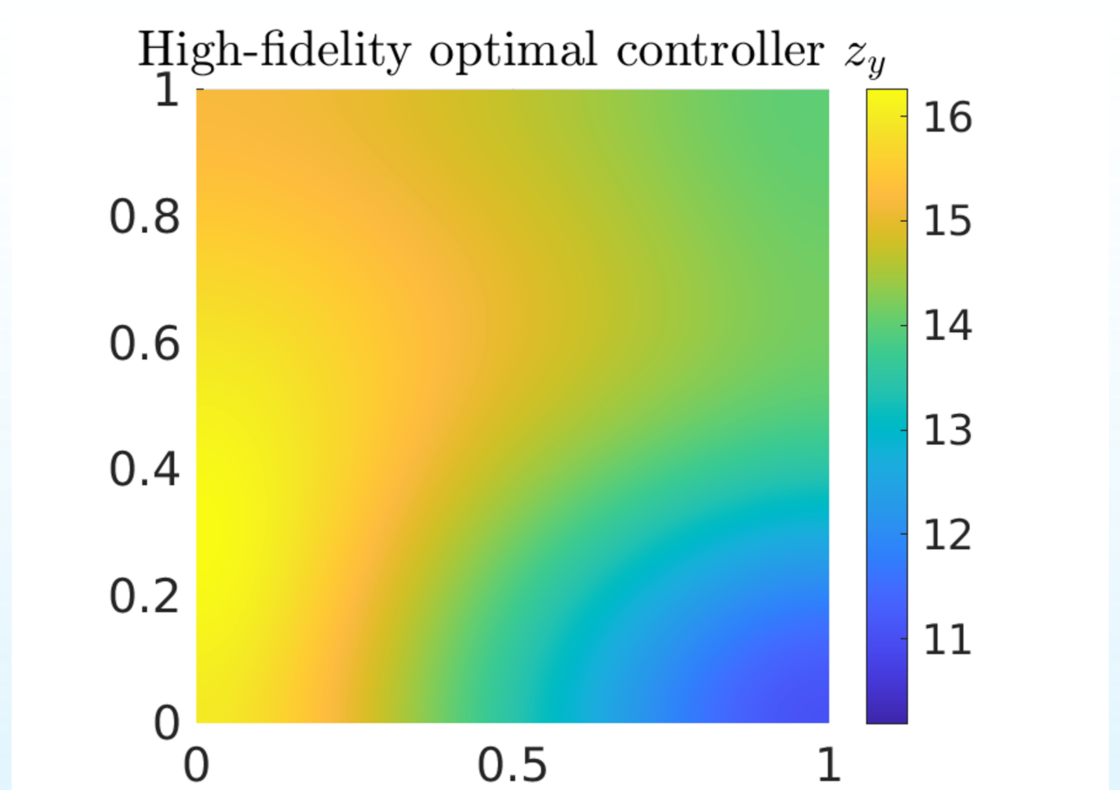
and the uncertainty is modeled by

$$\hat{\theta} = \sqrt{\alpha} \sum_{i=1}^{N} \frac{1}{\sqrt{\lambda_i}} \begin{pmatrix} s_i \hat{u}_i \\ \hat{u}_i \otimes \mathbf{M}_z^{-1} \mathbf{\Gamma}^{-1} \boldsymbol{w}_i \end{pmatrix} \quad \text{and} \quad \tilde{\theta} = \sum_{k=1}^{n-N+1} \begin{pmatrix} \tilde{s}_k \tilde{\boldsymbol{u}}_k \\ \tilde{u}_k \otimes \tilde{\boldsymbol{w}}_k \end{pmatrix}$$

2D Stokes versus Navier-Stokes







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$$\min_{\boldsymbol{z}} \boldsymbol{J}(\boldsymbol{S}(\boldsymbol{z}), \boldsymbol{z})$$ ← The problem we want to solve

The problem we actually solve → $$\min_{\boldsymbol{z}} \boldsymbol{J}(\tilde{\boldsymbol{S}}(\boldsymbol{z}), \boldsymbol{z})$$

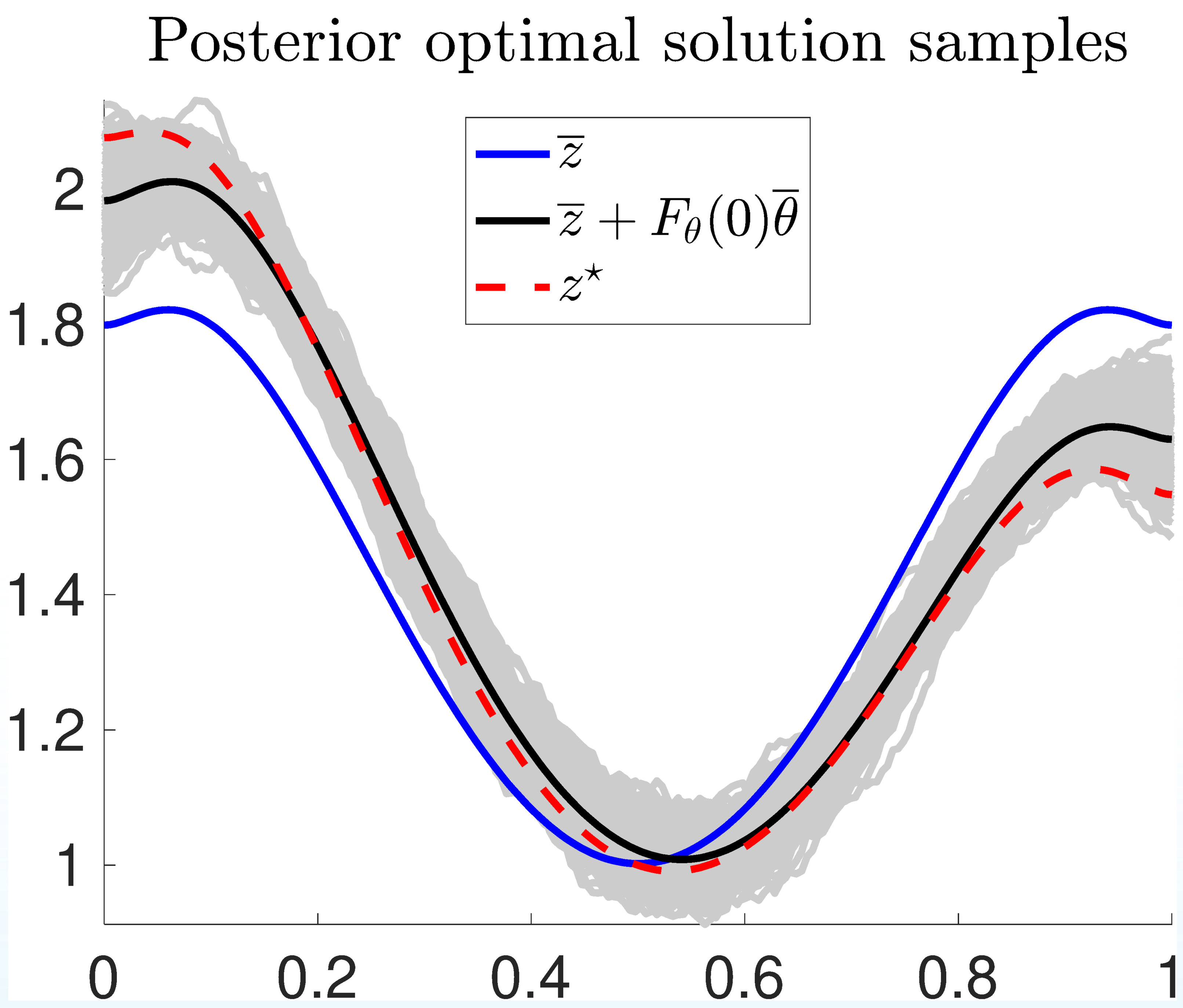
- J is the objective
- z is a design, control, or inversion parameter
- $S(z)$ is an high-fidelity model
- $\tilde{S}(z)$ is an approximate model

Assume that we can

- solve the optimization problem constrained by $\tilde{S}$
- evaluate a high-fidelity model $S(z)$ at a small number of inputs z

Our goals are:

- Use the limited high-fidelity evaluations to improve the solution
- Characterize uncertainty in the optimal solution due to $S - \tilde{S}$



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