Scalable algorithms for PDE-constrained optimization under uncertainty

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PDE-constrained optimization under uncertainty

Decision-making under uncertainty is often the ultimate goal of UQ:

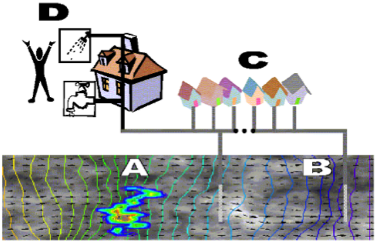
- Inverse problem: Infer uncertain model parameters given data
- Optimal experimental design problem: How should we acquire data to reduce uncertainty in inferred parameters?
- Forward problem: Propagate uncertain parameters through forward model
- Optimal design/control problem: Find design/control variables that optimize a desired uncertain objective

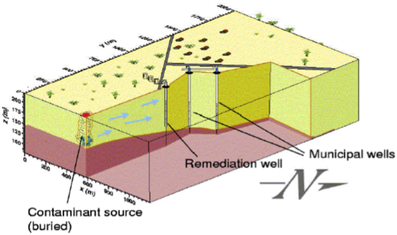
Fundamental difficulty: OUU amounts to many forward UQ problems

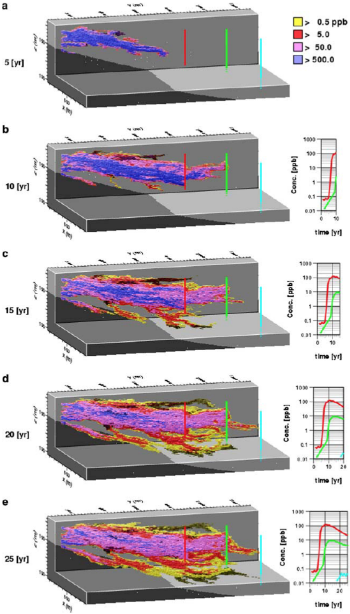
Sessions here at UQ18:

- IP8: Johannes Royset: *Good and bad uncertainty: Consequences in UQ and design*
- MT8: Drew Kouri: *Optimization and control under uncertainty*
- OED sessions: MS2/15, MS31/37, MS51/64/77
- OUU sessions: MS11/24, CP9, MS46/60, MS73, MS97/110

Example: Groundwater contaminant remediation







Source: Reed Maxwell, CSM

Classes of PDE-constrained optimization under uncertainty

- Inverse problem
  - Infer initial contaminant field from measurements of pressure at wells and from a model of subsurface flow and transport with random log permeability field
- Optimal experimental design problem
  - Where should new observation wells be placed so that initial condition is “best” inferred? (alphabetic optimality criteria, Bayes risk, expected information gain)
- Optimal design problem
  - Where should remediation wells be placed so that (uncertain) contaminant concentrations at municipal wells are minimized?
- Optimal control problem
  - What should the rates of pumping/injection at remediation wells be so that (uncertain) contaminant concentrations at municipal wells are minimized?

PDE-constrained optimal control under uncertainty

Find control/design variables z (pumping rates $q_j^z(t)$ and locations $\boldsymbol{x}_j^z$ of remediation wells) so that the expected value of the contaminant concentration c at the drinking wells is minimized:

$$\min_{z \in Z} \mathcal{J}(z) := \sum_i \int_X \int_0^T \int_\Omega w\, c(m, z)\, \delta_\varepsilon(\boldsymbol{x}_i^w)\, d\boldsymbol{x}\, dt\, d\mu(m) + \sum_j \beta_j \int_0^T (q_j^z)^2\, dt$$

where concentration c depends on random log permeability field m, control variables $q_j^z(t)$, and design variables $\boldsymbol{x}_j^z$ through the coupled groundwater flow and contaminant transport equations

$$\phi \rho c_t \frac{\partial p}{\partial t} - \boldsymbol{\nabla} \cdot (\rho \boldsymbol{v}) = -\sum_i q_i^w\, \delta_\varepsilon(\boldsymbol{x}_i^w) - \sum_j q_j^z\, \delta_\varepsilon(\boldsymbol{x}_j^z)$$

$$\frac{\mu \phi}{\exp(m)} \boldsymbol{v} + \boldsymbol{\nabla} p = \boldsymbol{0}$$

$$\frac{\partial (R \phi c)}{\partial t} + \boldsymbol{\nabla} \cdot (\phi c \boldsymbol{v}) - \boldsymbol{\nabla} \cdot (\phi \boldsymbol{D} \boldsymbol{\nabla} c) = -\sum_i c(\boldsymbol{x}_i^w)\, q_i^w \delta_\varepsilon(\boldsymbol{x}_i^w) - \sum_j c(\boldsymbol{x}_j^z)\, q_j^z\, \delta_\varepsilon(\boldsymbol{x}_j^z)$$

$$\boldsymbol{D} \approx (\alpha_T |\boldsymbol{v}| + \hat{D}) \boldsymbol{I} + (\alpha_L - \alpha_T) \frac{\boldsymbol{v} \otimes \boldsymbol{v}}{|\boldsymbol{v}|}$$

Mean-variance PDE-constrained optimal control

- Weak form of forward PDE model with random and control variables:

$$\text{find } u \in \mathcal{U} \text{ such that } r(u, v, m, z) = 0 \quad \forall v \in \mathcal{V}$$

  where $u \in \mathcal{U}$ is state, $v \in \mathcal{V}$ adjoint, $m \in \mathcal{M}$ random field, $z \in \mathcal{Z}$ control
- Objective function: Consider mean–variance of control functional $Q(\cdot, \cdot) : \mathcal{U} \times \mathcal{M} \to \mathbb{R}$:

$$\mathcal{J}(z) = \mathbb{E}[Q] + \beta \mathrm{Var}[Q] + \mathcal{P}(z)$$

  where $\mathcal{P}(z)$ is cost of controls (or regularization)
- Optimal control problem: find $z^* \in \mathcal{Z}$, s.t.

$$z^* = \arg\min_{z \in \mathcal{Z}} \mathcal{J}(z), \text{ subject to } r(u, v, m, z) = 0$$

- Sample average approximation (SAA) is prohibitive: entails as many (nonlinear) PDE constraints as required for accurate estimation of $\mathbb{E}[Q]$

$$z^* = \arg\min_{z \in \mathcal{Z}} \mathcal{J}^{\mathrm{MC}}(z), \text{ subject to } r(u, v, m_i, z) = 0 \quad i = 1, \ldots, M$$

$\Longrightarrow$ "Many-PDE-constrained optimization"

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Some existing approaches for PDE-constrained OUU

- Schulz & Schillings, *Problem formulations and treatment of uncertainties in aerodynamic design*, AIAA J, 2009.
- Borzì & von Winckel, *Multigrid methods and sparse-grid collocation techniques for parabolic optimal control problems with random coefficients*, SISC, 2009.
- Borzì, Schillings, & von Winckel, *On the treatment of distributed uncertainties in PDE-constrained optimization*, GAMM-Mitt. 2010.
- Borzì & von Winckel, *A POD framework to determine robust controls in PDE optimization*, Computing and Visualization in Science, 2011.
- Gunzburger & Ming, *Optimal control of stochastic flow over a backward-facing step using ROM*, SISC 2011.
- Hou, Lee, & Manouzi, *Finite element approximations of stochastic optimal control problems constrained by stochastic elliptic PDEs*, J Math Anal Appl, 2011.
- Gunzburger, Lee, & Lee, *Error estimates of stochastic optimal Neumann boundary control problems*, SINUM, 2011.
- Rosseel & Wells, *Optimal control with stochastic PDE constraints and uncertain controls*, CMAME, 2012.
- Tiesler, Kirby, Xiu, & Preusser, *Stochastic collocation for optimal control problems with stochastic PDE constraints*, SICON, 2012.
- Kouri, Heinkenschloss, Ridzal, & Van Bloemen Waanders, *A trust-region algorithm with adaptive stochastic collocation for PDE optimization under uncertainty*, SISC, 2013.
- Chen, Quarteroni, & Rozza, *Stochastic optimal Robin boundary control problems of advection-dominated elliptic equations*, SINUM, 2013.
- Kunoth & Schwab, *Analytic regularity and gPC approximation for control problems constrained by linear parametric elliptic and parabolic PDEs*, SICON, 2013.
- Kouri, *A multilevel stochastic collocation algorithm for optimization of PDEs with uncertain coefficients*, JUQ, 2014.
- Chen & Quarteroni, *Weighted reduced basis method for stochastic optimal control problems with elliptic PDE constraint*, JUQ, 2014.
- Ng & Willcox, *Multifidelity approaches for optimization under uncertainty*, IJNME, 2014.
- Kouri, Heinkenschloss, Ridzal, & van Bloemen Waanders, *Inexact objective function evaluations in a trust-region algorithm for PDE-constrained optimization under uncertainty*, SISC, 2014.
- Chen, Quarteroni, & Rozza, *Multilevel and weighted reduced basis method for stochastic optimal control problems constrained by Stokes equations*, Num. Math. 2015.
- Ng & Willcox, *Monte Carlo information-reuse approach to aircraft conceptual design optimization under uncertainty*, J Aircraft, 2015.
- P. Benner, A. Onwunta, and M. Stoll. Block-diagonal preconditioning for optimal control problems constrained by PDEs with uncertain inputs. SIMAX, 2016.
- A.A. Ali, E. Ullmann, & M. Hinze, Multilevel Monte Carlo analysis for optimal control of elliptic PDEs with random coefficients, SIAM/ASA JUQ, 2017.

Quadratic approximation in infinite dimensions

- We approximate Q by a quadratically-truncated Taylor expansion

$$Q(m) \approx Q_{\mathsf{quad}}(m) = Q(\bar{m}) + \langle g_m(\bar{m}), m - \bar{m} \rangle + \frac{1}{2} \langle \mathcal{H}_m(\bar{m})(m - \bar{m}), m - \bar{m} \rangle$$

- For a Gaussian random field m with $m \sim \mathcal{N}(\bar{m}, \mathcal{C})$, Q_{quad} is non-Gaussian, but we can still express[1]

$$\mathbb{E}[Q_{\mathsf{quad}}] = Q(\bar{m}) + \frac{1}{2}\mathrm{tr}(\tilde{\mathcal{H}})$$

$$\mathrm{Var}[Q_{\mathsf{quad}}] = \langle g_m(\bar{m}), \mathcal{C} g_m(\bar{m}) \rangle + \frac{1}{2}\mathrm{tr}(\tilde{\mathcal{H}}^2)$$

  where $\tilde{\mathcal{H}} = \mathcal{C}^{1/2}\mathcal{H}_m(\bar{m})\mathcal{C}^{1/2}$ is the *covariance-preconditioned Hessian*
- Q_{quad} is corrected by using it as a control variate (cf. multifidelity methods[2]
- Need to efficiently evaluate $\mathrm{tr}(\tilde{\mathcal{H}})$ and $\mathrm{tr}(\tilde{\mathcal{H}}^2)$ and their gradients w.r.t. z

[1] A. Alexanderian, N. Petra, G. Stadler, and O. Ghattas, Mean-variance risk-averse optimal control of systems governed by PDEs with random parameter fields using quadratic approximations, *SIAM/ASA JUQ*, 2017.

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How to compute $\mathrm{tr}(\tilde{\mathcal{H}})$ efficiently?

- When the eigenvalues decay rapidly (as is common for Hessians), the trace can be approximated efficiently with small N by

$$\mathrm{tr}(\tilde{\mathcal{H}}) \approx \sum_{j=1}^{N} \lambda_j(\tilde{\mathcal{H}}) \;\text{ and }\; \mathrm{tr}(\tilde{\mathcal{H}}^2) \approx \sum_{j=1}^{N} \lambda_j^2(\tilde{\mathcal{H}})$$

  where λ_j, $j = 1, \ldots, N$, are the dominant eigenvalues of $\tilde{\mathcal{H}}$, or the dominant generalized eigenvalues of $(\mathcal{H}_m(\bar{m}), \mathcal{C}^{-1})$, i.e.,

$$\mathcal{H}_m(\bar{m})\psi_j = \lambda_j \mathcal{C}^{-1}\psi_j$$

  where ψ_j are the $\mathcal{C}^{-1}$-orthonormal eigenfunctions, i.e., $\langle \psi_i, \mathcal{C}^{-1}\psi_j \rangle = \delta_{ij}$
- Prohibitive to compute $\mathcal{H}_m$ by itself; instead can form action in a given direction at cost of pair of linearized forward/adjoint PDE solves
- $\Longrightarrow$ Need operator-free eigensolver that can capture dominant spectrum in number of operator applications that scales with effective rank

Computing the trace of $\tilde{\boldsymbol{H}}$ via randomized SVD

- Double-pass randomized SVD algorithm estimates trace at cost of $2r$ products of $\tilde{\boldsymbol{H}}$ with random vectors ($r = N + p$, N is rank of $\tilde{\boldsymbol{H}}$, p is oversampling #)
- Resulting cost is $2r$ pairs of incremental forward/adjoint solves w/same PDE operator and $4r$ Poisson solves
- Covariance operator and Hessian are often compact (Q is sensitive to limited number of modes) so composition is low-rank

Randomized SVD (double pass algorithm)

1. Generate i.i.d. Gaussian matrix $\boldsymbol{R} \in \mathbb{R}^{n\times r}$ with r = numerical rank of $\tilde{\boldsymbol{H}}$ ($r \ll n$)
2. Form $\boldsymbol{Y} = \tilde{\boldsymbol{H}}\boldsymbol{R}$
3. Compute $\boldsymbol{Q}$ = orthonormal basis for $\boldsymbol{Y}$
4. Define $\boldsymbol{B} \in \mathbb{R}^{r\times r} := \boldsymbol{Q}^T\tilde{\boldsymbol{H}}\boldsymbol{Q}$
5. Decompose $\boldsymbol{B} = \boldsymbol{Z}\boldsymbol{\Lambda}\boldsymbol{Z}^T$
6. Low-rank approximation: $\tilde{\boldsymbol{H}} \approx \boldsymbol{V}\boldsymbol{\Lambda}\boldsymbol{V}^T$, where $\boldsymbol{V} \in \mathbb{R}^{n\times r} := \boldsymbol{Q}\boldsymbol{Z}$
7. Trace estimation: $\mathrm{tr}(\tilde{\boldsymbol{H}}) \approx \mathrm{tr}(\boldsymbol{B})$

- Thus often $r \ll n$, independent of parameter dimension n, and with high probability

$$|\mathrm{tr}(\tilde{\boldsymbol{H}}) - \mathrm{tr}(\boldsymbol{B})| \leq c(p) \sum_{r<i\leq n} |\lambda_i(\tilde{\boldsymbol{H}})|$$

- Quadratic-based approximations of $\mathbb{E}[Q]$ and $\mathrm{Var}[Q]$ require $4r$ linearized PDE solves with same PDE operator (small multiple of highly nonlinear forward solve)
- See Saibaba, Alexanderian, Ipsen, *Numerische Mathematik* 2017 for analysis of trace estimate by more general randomized subspace iterations

Eigenproblem-constrained optimization

With the trace computed via randomized SVD, we obtain

$$\mathcal{J}_{\mathsf{quad}}(z) = \underbrace{Q(\bar{m}) + \frac{1}{2}\sum_{j=1}^{N}\lambda_j(\tilde{\mathcal{H}})}_{\mathbb{E}[Q]} + \underbrace{\beta\langle g_m(\bar{m}), \mathcal{C}g_m(\bar{m})\rangle + \frac{\beta}{2}\sum_{j=1}^{N}\lambda_j^2(\tilde{\mathcal{H}})}_{\beta\mathsf{Var}[Q]} + \mathcal{P}(z)$$

where $Q(\bar{m}) := \bar{Q}$ is obtained by solving the forward problem for $u \in \mathcal{U}$

$$\langle \tilde{v}, \partial_v \bar{r}(u, \tilde{v}, z)\rangle = 0, \quad \forall \tilde{v} \in \mathcal{V}$$

with $\bar{r}(u, \tilde{v}, z) = r(u, \tilde{v}, \bar{m}, z)$ for short. By defining the Lagrangian

$$\mathcal{L}(u, v, \bar{m}, z) = Q(u) + \bar{r}(u, v, z)$$

the gradient $g_m(\bar{m})$ is found from

$$\langle \tilde{m}, g_m(\bar{m})\rangle = \langle \tilde{m}, \partial_m \mathcal{L}\rangle = \langle \tilde{m}, \partial_m \bar{r}(u, v, z)\rangle, \quad \forall \tilde{m} \in \mathcal{M}$$

for which we need to compute $v \in \mathcal{V}$ by solving the adjoint problem

$$\langle \tilde{u}, \partial_u \bar{r}(u, v, z)\rangle = -\langle \tilde{u}, \partial_u \bar{Q}\rangle, \quad \forall \tilde{u} \in \mathcal{U}$$

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To compute λ_j, which satisfies for $j = 1, \ldots, N$

$$\mathcal{H}_m(\bar{m})\psi_j = \lambda_j \mathcal{C}^{-1}\psi_j, \text{ and } \langle \psi_j, \mathcal{C}^{-1}\psi_j \rangle = \delta_{ij}$$

we need Hessian action in a direction $\hat{m}$, for which we form the Lagrangian

$$\mathcal{L}^H(u, v, m, z; \hat{u}, \hat{v}, \hat{m}) = \underbrace{\langle \hat{m}, \partial_m \bar{r} \rangle}_{\text{gradient}} + \underbrace{\langle \hat{v}, \partial_v \bar{r} \rangle}_{\text{forward}} + \underbrace{\langle \hat{u}, \partial_u \bar{r} + \partial_u \bar{Q} \rangle}_{\text{adjoint}}$$

which involves the gradient, the forward problem, and the adjoint problem. The Hessian action is given by the variation of $\mathcal{L}^H$ with respect to m:

$$\langle \tilde{m}, \mathcal{H}_m(\bar{m})\,\hat{m} \rangle = \langle \tilde{m}, \partial_m \mathcal{L}^H\,\hat{m} \rangle = \langle \tilde{m}, \partial_{mv}\bar{r}\,\hat{v} + \partial_{mu}\bar{r}\,\hat{u} + \partial_{mm}\bar{r}\,\hat{m} \rangle, \quad \forall \tilde{m} \in \mathcal{M}$$

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$$\mathcal{H}_m(\bar{m})\psi_j = \lambda_j \mathcal{C}^{-1}\psi_j, \text{ and } \langle \psi_j, \mathcal{C}^{-1}\psi_j \rangle = \delta_{ij}$$

we need Hessian action in a direction $\hat{m}$, for which we form the Lagrangian

$$\mathcal{L}^H(u, v, m, z; \hat{u}, \hat{v}, \hat{m}) = \underbrace{\langle \hat{m}, \partial_m \bar{r} \rangle}_{\text{gradient}} + \underbrace{\langle \hat{v}, \partial_v \bar{r} \rangle}_{\text{forward}} + \underbrace{\langle \hat{u}, \partial_u \bar{r} + \partial_u \bar{Q} \rangle}_{\text{adjoint}}$$

which involves the gradient, the forward problem, and the adjoint problem. The Hessian action is given by the variation of $\mathcal{L}^H$ with respect to m:

$$\langle \tilde{m}, \mathcal{H}_m(\bar{m})\, \hat{m} \rangle = \langle \tilde{m}, \partial_m \mathcal{L}^H\, \hat{m} \rangle = \langle \tilde{m}, \partial_{mv}\bar{r}\, \hat{v} + \partial_{mu}\bar{r}\, \hat{u} + \partial_{mm}\bar{r}\, \hat{m} \rangle, \quad \forall \tilde{m} \in \mathcal{M}$$

where $\hat{u} \in \mathcal{U}$ is the solution of the incremental forward problem, $\partial_u \mathcal{L}^H = 0$

$$\langle \tilde{v}, \partial_{vu}\bar{r}\, \hat{u} \rangle = -\langle \tilde{v}, \partial_{vm}\bar{r}\, \hat{m} \rangle, \quad \forall \tilde{v} \in \mathcal{V}$$

and $\hat{v} \in \mathcal{V}$ is the solution of the incremental adjoint problem, $\partial_v \mathcal{L}^H = 0$

$$\langle \tilde{u}, \partial_{uv}\bar{r}\, \hat{v} \rangle = -\langle \tilde{u}, \partial_{uu}\bar{r}\, \hat{u} + \partial_{uu}\bar{Q}\, \hat{u} + \partial_{um}\bar{r}\, \hat{m} \rangle, \quad \forall \tilde{u} \in \mathcal{U}$$

OUU problem with quadratic approximation $\mathcal{J}_{\text{quad}}$

$$\min_{z \in \mathcal{Z}} \mathcal{J}_{\text{quad}}(z) := Q(\bar{m}) + \frac{1}{2}\sum_{j=1}^{N} \lambda_j(\tilde{\mathcal{H}}) + \beta \left(\langle g_m(\bar{m}), \mathcal{C} g_m(\bar{m}) \rangle + \frac{1}{2}\sum_{j=1}^{N} \lambda_j^2(\tilde{\mathcal{H}}) \right) + \mathcal{P}(z)$$

where:

forward	$\langle v^*, \partial_v \bar{r} \rangle = 0 \quad \forall v^* \in \mathcal{V}$
adjoint	$\langle u^*, \partial_u \bar{r} + \partial_u \bar{Q} \rangle = 0 \quad \forall u^* \in \mathcal{U}$
eigenvalue	$\langle \psi_j^*, (\mathcal{H}_m(\bar{m}) - \lambda_j \mathcal{C}^{-1}) \psi_j \rangle = 0 \quad \forall \psi_j^* \in \mathcal{M} \quad j = 1, \dots, N$
orthonormality	$\lambda_j^* (\langle \psi_j, \mathcal{C}^{-1} \psi_j \rangle - 1) = 0 \quad \forall \lambda_j^* \in \mathbb{R} \quad j = 1, \dots, N$
incremental forw	$\langle \hat{v}_j^*, \partial_{vu} \bar{r}\, \hat{u}_j + \partial_{vm} \bar{r}\, \psi_j \rangle = 0 \quad \forall \hat{v}_j^* \in \mathcal{V} \quad j = 1, \dots, N$
incremental adj	$\langle \hat{u}_j^*, \partial_{uv} \bar{r}\, \hat{v}_j + \partial_{uu} \bar{r}\, \hat{u}_j + \partial_{uu} \bar{Q}\, \hat{u}_j + \partial_{um} \bar{r}\, \psi_j \rangle = 0 \;\; \forall \hat{u}_j^* \in \mathcal{U} \;\; j = 1, \dots$

Lagrangian of the OUU problem

$$\mathcal{L}_{\text{quad}}\left(u, v, \{\lambda_j\}, \{\psi_j\}, \{\hat{u}_j\}, \{\hat{v}_j\}, u^*, v^*, \{\lambda_j^*\}, \{\psi_j^*\}, \{\hat{u}_j^*\}, \{\hat{v}_j^*\}, z\right) :=$$

quad obj	$= Q(\bar{m}) + \frac{1}{2}\sum_{j=1}^{N} \lambda_j(\tilde{\mathcal{H}}) + \beta\left(\langle g_m(\bar{m}), \mathcal{C} g_m(\bar{m})\rangle + \frac{1}{2}\sum_{j=1}^{N} \lambda_j^2(\tilde{\mathcal{H}})\right) + \mathcal{P}(z)$
forward	$+\ \langle v^*, \partial_v \bar{r}\rangle$
adjoint	$+\ \langle u^*, \partial_u \bar{r} + \partial_u \bar{Q}\rangle$
eigen. prob.	$+\ \sum_{j=1}^{N} \langle \psi_j^*, (\mathcal{H}_m(\bar{m}) - \lambda_j \mathcal{C}^{-1})\psi_j\rangle$
orth. cond.	$+\ \sum_{j=1}^{N} \lambda_j^* (\langle \psi_j, \mathcal{C}^{-1}\psi_j\rangle - 1)$
inc. fwd.	$+\ \sum_{j=1}^{N} \langle \hat{v}_j^*, \partial_{vu}\bar{r}\, \hat{u}_j + \partial_{vm}\bar{r}\, \psi_j\rangle$
inc. adj.	$+\ \sum_{j=1}^{N} \langle \hat{u}_j^*, \partial_{uv}\bar{r}\, \hat{v}_j + \partial_{uu}\bar{r}\, \hat{u}_j + \partial_{uu}\bar{Q}\, \hat{u}_j + \partial_{um}\bar{r}\, \psi_j\rangle$

Gradient of $\mathcal{J}_{\text{quad}}$ (assuming λ_j distinct)

- Variation of $\mathcal{L}_{\text{quad}}$ wrt λ_j vanishes:

$$\psi_j^* = \frac{1+2\beta\lambda_j}{2}\psi_j, \quad j = 1,\ldots,N$$

- Variation of $\mathcal{L}_{\text{quad}}$ wrt $\hat{v}_j$ vanishes:

$$\hat{u}_j^* = \frac{1+2\beta\lambda_j}{2}\hat{u}_j, \quad j = 1,\ldots,N$$

- Variation of $\mathcal{L}_{\text{quad}}$ wrt $\hat{u}_j$ vanishes:

$$\hat{v}_j^* = \frac{1+2\beta\lambda_j}{2}\hat{v}_j, \quad j = 1,\ldots,N$$

- Variation of $\mathcal{L}_{\text{quad}}$ wrt v vanishes: find $u^* \in \mathcal{U}$ s.t. (incr forward operator)

$$\begin{aligned}
\langle \tilde{v}, \partial_{vu}\bar{r}\, u^* \rangle &= -2\beta \langle \tilde{v}, \partial_{vm}\bar{r}\,(\mathcal{C}\partial_m \bar{r})\rangle \\
&\quad - \sum_{j=1}^{N} \langle \tilde{v}, \partial_{vmu}\bar{r}\,\hat{u}_j\,\psi_j^* + \partial_{vmm}\bar{r}\,\psi_j\,\psi_j^* \rangle \\
&\quad - \sum_{j=1}^{N} \langle \tilde{v}, \partial_{vuu}\bar{r}\,\hat{u}_j\,\hat{u}_j^* + \partial_{vum}\bar{r}\,\psi_j\,\hat{u}_j^* \rangle, \quad \forall \tilde{v} \in \mathcal{V}
\end{aligned}$$

Computing the gradient of the OUU problem

- Variation of $\mathcal{L}_{\text{quad}}$ wrt u vanishes: find $v^* \in \mathcal{V}$ s.t. (incr adjoint operator)

$$
\begin{aligned}
&\langle \tilde{u}, \partial_{uv}\bar{r}\, v^* \rangle = \\
&- \langle \tilde{u}, \partial_u \bar{Q} \rangle - 2\beta \langle \tilde{u}, \partial_{um}\bar{r}\, (\mathcal{C}\partial_m \bar{r}) \rangle \\
&- \langle \tilde{u}, \partial_{uu}\bar{r}\, u^* + \partial_{uu}\bar{Q}\, u^* \rangle \\
&- \sum_{j=1}^{N} \langle \tilde{u}, \partial_{umv}\bar{r}\, \hat{v}_j\, \psi_j^* + \partial_{umu}\bar{r}\, \hat{u}_j\, \psi_j^* + \partial_{uum}\bar{r}\, \psi_j\, \psi_j^* \rangle \\
&- \sum_{j=1}^{N} \langle \tilde{u}, \partial_{uvu}\bar{r}\, \hat{u}_j\, \hat{v}_j^* + \partial_{uvm}\bar{r}\, \psi_j\, \hat{v}_j^* \rangle \\
&- \sum_{j=1}^{N} \langle \tilde{u}, \partial_{uuv}\bar{r}\, \hat{v}_j\, \hat{u}_j^* + \partial_{uuu}\bar{r}\, \hat{u}_j\, \hat{u}_j^* + \partial_{uuu}\bar{Q}\, \hat{u}_j\, \hat{u}_j^* + \partial_{uum}\bar{r}\, \psi_j\, \hat{u}_j^* \rangle, \forall \tilde{u} \in \mathcal{U},
\end{aligned}
$$

- Finally the gradient of the cost functional can be computed as

$$
D_z \mathcal{J}_{\text{quad}}(z) = \partial_z \mathcal{L}_{\text{quad}}(\text{primal}, \text{dual}, z)
$$

- Total cost: 1 forward PDE solve, $1 + 4(N + p) + 2N + 2$ linearized PDE solves (independent of uncertain parameter or control dimensions!)

Quadratic approximation as a variance reduction

- Statistics computed by quadratic approximation may be **biased**
- Use Monte Carlo quadrature to correct quadratic approximation

$$\mathbb{E}[Q] = \mathbb{E}[Q_{\text{quad}}] + \mathbb{E}[\underbrace{Q - Q_{\text{quad}}}_{Y}] \approx \mathbb{E}[Q_{\text{quad}}] + \underbrace{\hat{Y}}_{\text{MC estimator}}$$

- Mean squared error (MSE) of MC estimate of $\mathbb{E}[Q]$ and $\mathbb{E}[Y]$

$$\text{MSE}(Q) \asymp \frac{1}{M}\text{Var}[Q] \quad \text{vs.} \quad \text{MSE}(Y) \asymp \frac{1}{M}\text{Var}[Y]$$

- A much smaller number of MC samples is required for $\mathbb{E}[Y]$ as

$$\text{Var}[Y] \ll \text{Var}[Q]$$

  provided Q_{quad} is a good approximation of (highly correlated to) Q
- Similar variance reduction can be applied for the variance $\text{Var}[Q]$.

The unbiased cost functional with variance reduction

We obtain an unbiased evaluation of the cost functional as

$$\mathcal{J}^{\mathsf{MC}}_{\mathsf{quad}}(z) = \widehat{Q}_{\mathsf{quad}} + \beta \widehat{V}^{\mathsf{quad}}_{Q} + \mathcal{P}(z)$$

where

$$\begin{aligned}\widehat{Q}_{\mathrm{quad}} &= Q(\bar{m}) + \frac{1}{2}\mathsf{tr}(\mathcal{H}) \\ &\quad + \frac{1}{M}\sum_{i=1}^{M}\Big(Q(m_i) - Q(\bar{m}) - \langle m_i - \bar{m}, g_m(\bar{m})\rangle \\ &\qquad - \frac{1}{2}\langle m_i - \bar{m}, \mathcal{H}_m(\bar{m})\,(m_i - \bar{m})\rangle\Big)\end{aligned}$$

and

$$\begin{aligned}\widehat{V}^{\mathsf{quad}}_{Q} &:= \langle \mathcal{C} g_m(\bar{m}), g_m(\bar{m})\rangle + \frac{1}{4}(\mathsf{tr}(\mathcal{H}))^2 + \frac{1}{2}\mathsf{tr}(\mathcal{H}^2) \\ &\quad + \frac{1}{M}\sum_{i=1}^{M}\Big((Q(m_i) - Q(\bar{m}))^2 \\ &\quad - \Big(\langle m_i - \bar{m}, g_m(\bar{m})\rangle + \frac{1}{2}\langle m_i - \bar{m}, \mathcal{H}_m(\bar{m})\,(m_i - \bar{m})\rangle\Big)^2\Big) \\ &\quad - \Big(\frac{1}{2}\mathsf{tr}(\mathcal{H}) + \frac{1}{M_2}\sum_{i=1}^{M_2}\Big(Q(m_i) - \langle m_i - \bar{m}, g_m(\bar{m})\rangle \\ &\qquad - \frac{1}{2}\langle m_i - \bar{m}, \mathcal{H}_m(\bar{m})\,(m_i - \bar{m})\rangle\Big)\Big)^2\end{aligned}$$

OUU Lagrangian w/variance reduction using quad approx

$$
\begin{aligned}
&\mathcal{L}^{\mathsf{MC}}_{\mathsf{quad}}\Big(u, v, \{u_i\}, \{\lambda_j\}, \{\psi_j\}, \{\hat{u}_j\}, \{\hat{v}_j\}, \{\hat{u}_i\}, \{\hat{v}_i\},\\
&\qquad u^*, v^*, \{v_i\}, \{\lambda^*_j\}, \{\psi^*_j\}, \{\hat{u}^*_j\}, \{\hat{v}^*_j\}, \{\hat{u}^*_i\}, \{\hat{v}^*_i\}, z\Big)\\
&= \mathcal{J}^{\mathsf{MC}}_{\mathsf{quad}} + \langle v^*, \partial_v \bar{r}\rangle + \langle u^*, \partial_u \bar{r} + \partial_u \bar{Q}\rangle + \sum_{i=1}^{M} r(u_i, v_i, m_i, z).\\
&+ \sum_{j=1}^{N} \langle \psi^*_j, (\mathcal{H}_m(\bar{m}) - \lambda_j \mathcal{C}^{-1})\psi_j\rangle\\
&+ \sum_{j=1}^{N} \lambda^*_j (\langle \psi_j, \mathcal{C}^{-1}\psi_j\rangle - 1)\\
&+ \sum_{j=1}^{N} \langle \hat{v}^*_j, \partial_{vu}\bar{r}\,\hat{u}_j + \partial_{vm}\bar{r}\,\psi_j\rangle\\
&+ \sum_{j=1}^{N} \langle \hat{u}^*_j, \partial_{uv}\bar{r}\,\hat{v}_j + \partial_{uu}\bar{r}\,\hat{u}_j + \partial_{uu}\bar{Q}\,\hat{u}_j + \partial_{um}\bar{r}\,\psi_j\rangle\\
&+ \sum_{i=1}^{M} \langle \hat{v}^*_i, \partial_{vu}\bar{r}\,\hat{u}_i + \partial_{vm}\bar{r}\,m_i\rangle\\
&+ \sum_{i=1}^{M} \langle \hat{u}^*_i, \partial_{uv}\bar{r}\,\hat{v}_i + \partial_{uu}\bar{r}\,\hat{u}_i + \partial_{uu}\bar{Q}\,\hat{u}_i + \partial_{um}\bar{r}\,m_i\rangle.
\end{aligned}
$$

Total: $1 + M$ forward PDE solves and $3 + 4(N + p) + 4N + 5M$ linearized PDE solves

Optimal design of acoustic metamaterial cloak: Setup

Helmholtz equation:

$$\Delta u + k^2 u = 0 \quad \text{in } D$$
$$u = u_{\text{in}} \quad \text{on } \Gamma_{\text{in}}$$
$$\lim_{r\to\infty} r(\partial_r u^s - iku^s) = 0$$

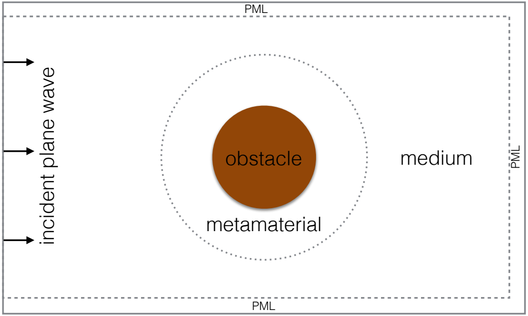
Absorbing BC on Γ_{out} via PML

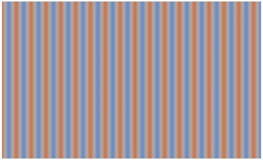
u: (complex) total field $=$ incident field $+$ scattered field

$$u = u^i + u^s$$

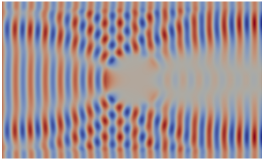
k: wavenumber ω^2/c^2, given by

$$k = \begin{cases} k_m & \text{in medium} \\ k_o & \text{in obstacle} \\ k_m e^{m+z} & \text{in metamaterial} \end{cases}$$





incident field



total field

Optimal design of acoustic cloak: Setup

- The complex field $u = u_r + iu_i$ and adjoint $v = v_r + iv_i$, are defined in the Hilbert space $(u_r, u_i), (v_r, v_i) \in V = H^1_{\Gamma_{\text{in}}} \times H^1_{\Gamma_{\text{in}}}$, where

$$H^1_{\Gamma_{\text{in}}} = \{w \in L^2(D), |\nabla w| \in L^2(D), w|_{\Gamma_{\text{in}}} = 0\}.$$

- The weak form is given by: find $(u_r, u_i) \in V$ such that

$$r(u, v, m, z) = 0 \quad \forall (v_r, v_i) \in V,$$

with $r(u, v, m, z) = r_1(u, v_r, m, z) + ir_2(u, v_i, m, z)$, where

$$r_1(u, v_r, m, z) = \int_D A_r \nabla u_r \cdot \nabla v_r + A_i \nabla u_i \cdot \nabla v_r dx - \int_D K_r u_r v_r + K_i u_i v_r dx,$$

$$r_2(u, v_i, m, z) = \int_D -A_r \nabla u_i \cdot \nabla v_i + A_i \nabla u_r \cdot \nabla v_i dx - \int_D K_r u_i v_i - K_i u_r v_i dx,$$

where A_r, A_i, K_r, K_i depend on (m, z) through the wavenumber k.

- The objective function is given by the misfit in the background medium D_{back}

$$Q(u(m, z)) = \int_{D_{\text{back}}} |u(m, z) - u_{\text{back}}|^2 dx.$$

The regularization term uses L_1-norm to promote design sparsity in metamaterial

$$\mathcal{P}(z) = \alpha \int_{D_{\text{meta}}} |z| dx.$$

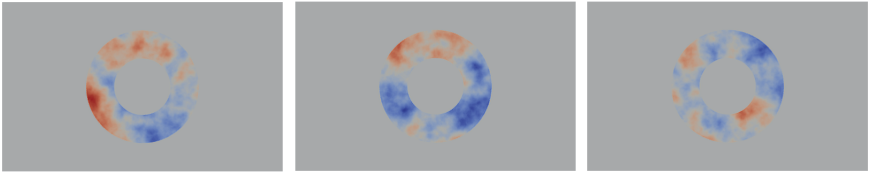
Optimal design of acoustic cloak: Samples

DOF for FE discretization of state, random, and design variables (FEniCS)

DOF	mesh1	mesh2	mesh3	mesh4	mesh5
u (P2)	40,194	159,746	636,930	2,543,618	10,166,274
m, z (P1)	940	3,336	12,487	48,288	189,736

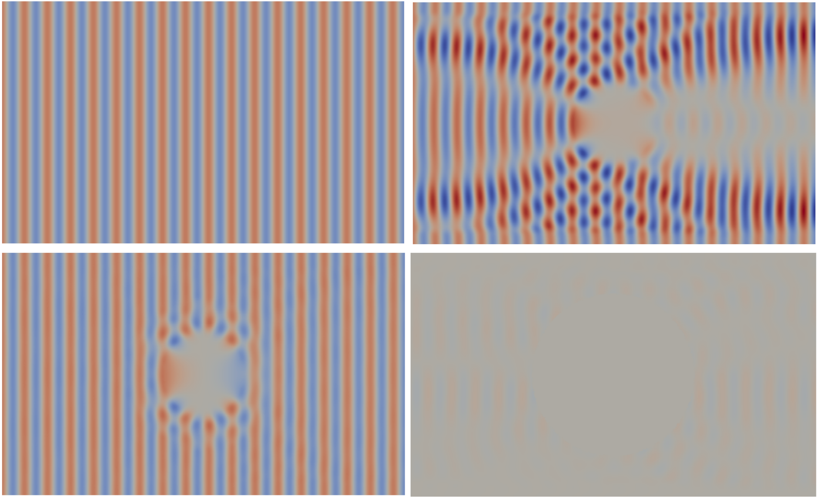
The random field $m \sim \mathcal{N}(\bar{m}, \mathcal{C})$ with mean $\bar{m} = 0$ and covariance

$$\mathcal{C} = (-\gamma\Delta + \delta I)^{-2} \quad \text{with correlation length} \sim \sqrt{\frac{\gamma}{\delta}}$$



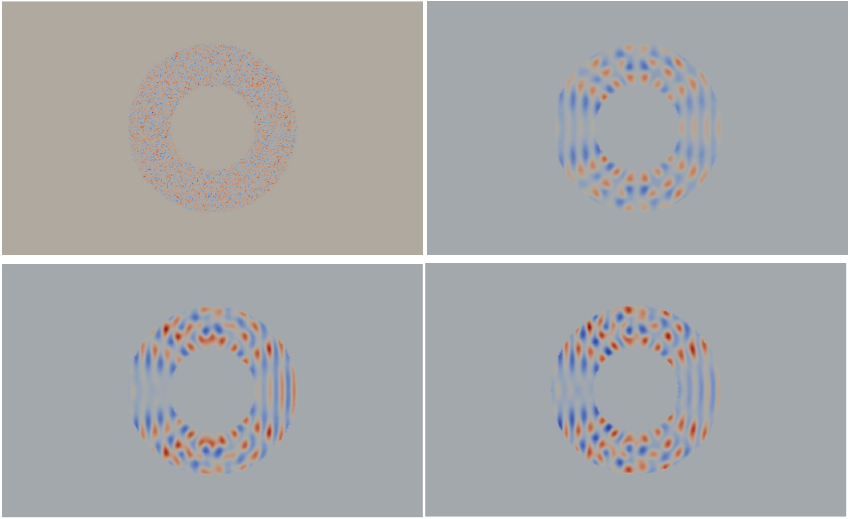
Samples of the random field m ($\gamma = \delta = 50$, corresponding to manufacturing error of $10\% \sim 15\%$ of material property)

Optimal design of acoustic cloak: Fields



Top: No cloak: Incident field and total field with obstacle
Bottom: Optimal cloak: Total field and scattered field

Optimal design of acoustic cloak: Optimal design



Optimal design (∞-dim design field z) with different approximations

Top: Random design, deterministic; Bottom: quadratic, SAA

Optimal design of cloak: Deterministic vs stochastic

Table: Estimates of $q = (Q - \bar{Q})^2$ and mean square errors with 100 samples

design	$\hat{q}$	MSE($\hat{q}$)	MSE($q - q_{\text{lin}}$)	MSE($q - q_{\text{quad}}$)
z_{random}	1.01e+01	2.97e+00	1.90e+00	1.50e-03
z_{deter}	1.13e+01	4.89e+00	4.89e+00	7.32e-02
z_{quad}	1.30e+00	4.06e-02	3.81e-02	1.07e-02
z_{saa}	1.41e+00	2.54e-02	1.54e-02	2.89e-04

Variance reduction of 100X–1000X by quadratic approximation

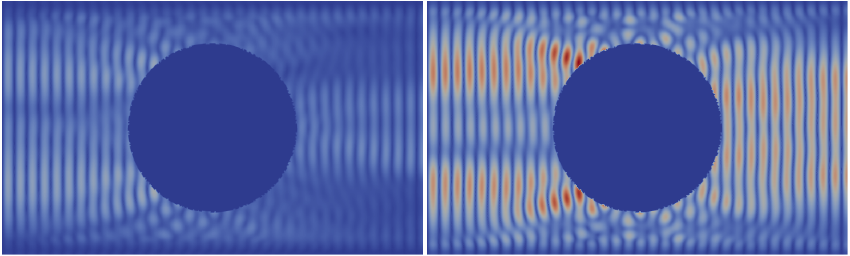


Figure: Std of the scattered field at optimal design z_{quad} (left) and z_{deter} (right)

Optimal design of acoustic cloak: Quad vs SAA

Table: Estimates of misfit Q and mean square errors with 100 samples

design	$\hat{Q}$	MSE($\hat{Q}$)	MSE($Q - Q_{\text{lin}}$)	MSE($Q - Q_{\text{quad}}$)
z_{random}	6.56e+01	9.67e-02	9.80e-03	1.63e-05
z_{deter}	2.55e+00	4.75e-02	4.75e-02	7.30e-04
z_{quad}	1.17e+00	4.85e-03	4.31e-03	6.74e-04
z_{saa}	6.46e+00	1.01e-02	1.29e-03	3.37e-05

Variance reduction of 10X–1000X by quadratic approximation

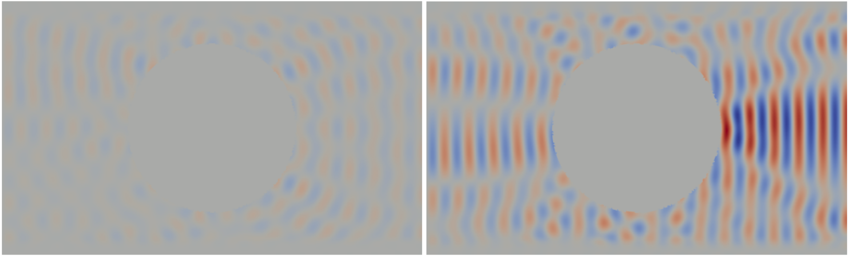
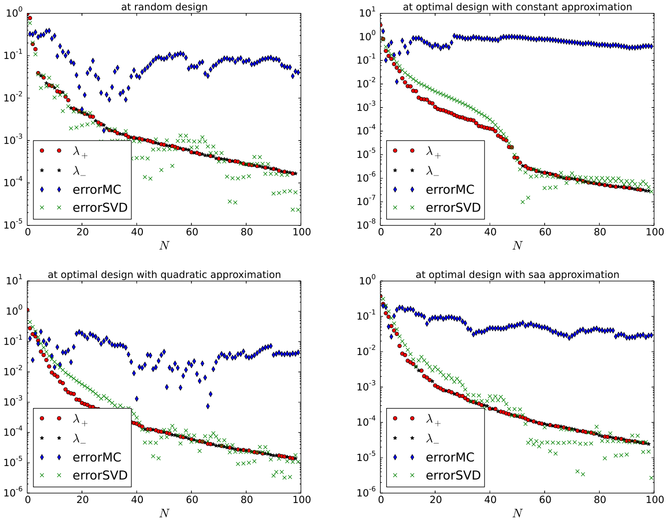


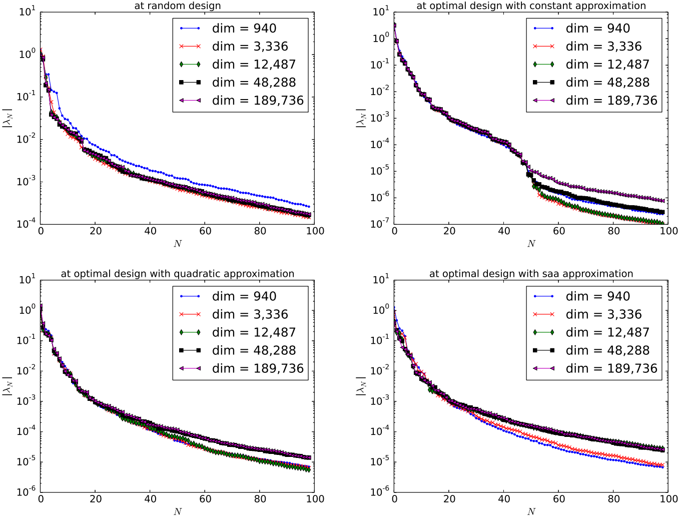
Figure: Mean of the scattered field at optimal design z_{quad} (left) and z_{saa} (right)

Optimal design of acoustic cloak: Trace estimate



Eigenvalues $\lambda_N(\mathcal{C}^{1/2}\mathcal{H}_m(\bar{m})\mathcal{C}^{1/2})$ (first 100 out of 189,736) and trace estimation errors by MC and randomized SVD

Optimal design of acoustic cloak: Scalability I



Spectrum decay of the covariance-preconditioned Hessian is scalable

Optimal design of acoustic cloak: Scalability II

Table: Estimates of misfit Q and mean square errors with 100 samples

dimension	$\hat{Q}$	MSE($\hat{Q}$)	MSE($Q - Q_{\text{lin}}$)	MSE($Q - Q_{\text{quad}}$)
940	7.33e+01	1.25e-01	7.01e-03	7.16e-05
3,336	6.87e+01	1.56e-01	9.29e-03	7.51e-05
12,487	6.56e+01	9.67e-02	9.80e-03	1.63e-05
48,288	6.94e+01	1.00e-01	1.04e-02	1.13e-04

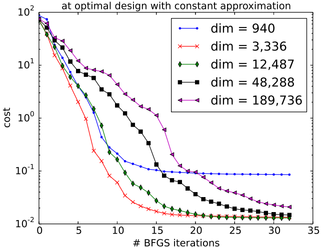
Variance reduction of 1000X (at random design) is scalable

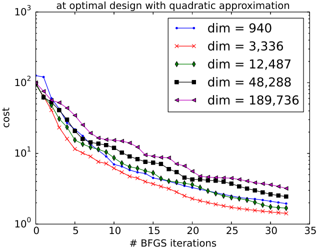
Table: Estimates of $q = (Q - Q_0)^2$ and mean square errors with 100 samples

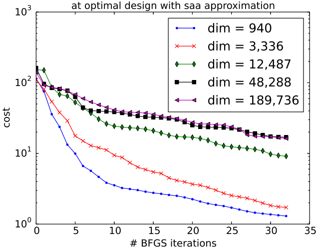
dimension	$\hat{q}$	MSE($\hat{q}$)	MSE($q - q_{\text{lin}}$)	MSE($q - q_{\text{quad}}$)
940	1.44e+01	3.19e+00	1.42e+00	7.53e-03
3,336	2.06e+01	1.13e+01	3.10e+00	1.99e-02
12,487	1.01e+01	2.97e+00	1.90e+00	1.50e-03
48,288	1.21e+01	4.82e+00	2.52e+00	4.92e-03

Variance reduction of 1000X (at random design) is scalable

Optimal design of acoustic cloak: Scalability III



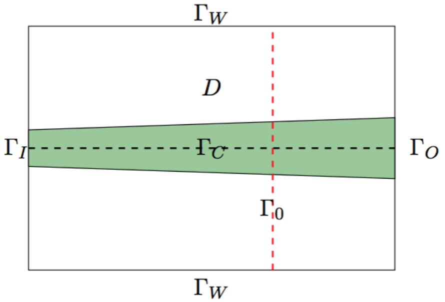




Optimization (# BFGS inter) is scalable by quadratic approximation

Optimal control for turbulent jet flow: setup

- **Control** is horizontal velocity profile at inlet boundary Γ_I
- **Objective** is to maximize jet width at Γ_0
- **Random input** is an inadequacy field for turbulent viscosity, upto 10^6 dimensions.
- **Constraint** on inlet momentum: $\int_{\Gamma_I} (\mathbf{u} \cdot \mathbf{n})^2 ds = M_I$



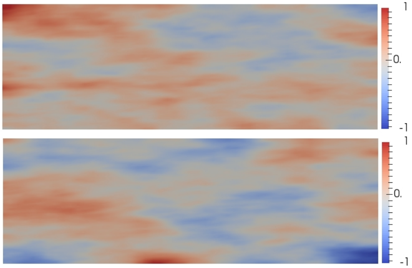


Figure: Left: sketch of the physical domain of the turbulence jet flow, with inlet boundary Γ_I, outlet boundary Γ_O, top and bottom wall Γ_W, the center axis Γ_C, and the cross-section Γ_0. The computational domain D is the top part of the physical domain. Right: two random samples drawn from the Gaussian measure $\mathcal{N}(0, \mathcal{C})$ with $\mathcal{C} = (-\nabla \cdot (\Theta \nabla) + \alpha I)^{-2}$.

Optimal control for turbulent jet flow: model

$$
\begin{aligned}
-\nabla\cdot\left((\nu+\gamma\nu_{t,0})\left(\nabla\boldsymbol{u}+\nabla\boldsymbol{u}^\top\right)\right)+(\boldsymbol{u}\cdot\nabla)\,\boldsymbol{u}+\nabla p &= 0, &&\text{in } D,\\
\nabla\cdot\boldsymbol{u} &= 0, &&\text{in } D,\\
-\nabla\cdot\left(\left(\nu+(\gamma+e^m)\,\nu_{t,0}\right)\nabla\gamma\right)+\boldsymbol{u}\cdot\nabla\gamma-\frac{1}{2}\frac{\boldsymbol{u}\cdot\boldsymbol{e}_1}{x_1+b}\gamma &= 0, &&\text{in } D,\\
\sigma_n(\boldsymbol{u})\cdot\boldsymbol{\tau}=0,\quad \boldsymbol{u}\cdot\boldsymbol{n}+\chi_W\,\phi(z) &= 0, &&\text{on } \Gamma_I,\\
\sigma_n(\boldsymbol{u})\cdot\boldsymbol{n}=0,\quad \boldsymbol{u}\cdot\boldsymbol{\tau} &= 0, &&\text{on } \Gamma_O\cup\Gamma_W,\\
\sigma_n(\boldsymbol{u})\cdot\boldsymbol{\tau}=0,\quad \boldsymbol{u}\cdot\boldsymbol{n} &= 0, &&\text{on } \Gamma_C,\\
\gamma-\gamma_0 &= 0, &&\text{on } \Gamma_I\cup\Gamma_W,\\
\sigma_n^\gamma(\gamma)\cdot\boldsymbol{n} &= 0, &&\text{on } \Gamma_O\cup\Gamma_C.
\end{aligned}
$$

$$
\begin{aligned}
\sigma_n(\boldsymbol{u}) &= (\nu+\gamma\nu_{t,0})\left(\nabla\boldsymbol{u}+\nabla\boldsymbol{u}^\top\right)\cdot\boldsymbol{n}\\
\sigma_n^\gamma(\gamma) &= (\nu+(\gamma+e^m)\nu_{t,0})\nabla\gamma\cdot\boldsymbol{n}\\
\nu_{t,0}=C\sqrt{M}(x_1+aW)^{1/2}\ \text{with}\ M &= \int_{\Gamma_I}||\boldsymbol{u}_{\mathsf{dns}}||^2 ds\\
\gamma_0=0.5-0.5\tanh\left(5\left(\frac{30-x_1}{30}\right)(x_2-1-0.5x_1)\right)&.
\end{aligned}
$$

Optimal control for turbulent jet flow: model – weak form

The weak form is defined for $u = (\boldsymbol{u}, p, \gamma), v = (\boldsymbol{v}, q, \eta) \in \mathcal{V} := (H^1(D))^2 \times L^2(D) \times H^1(D)$

$$r(u, v, m, z) = \text{Model}(u, v, m) + \text{Stablization}(u, v) + \text{Nitsche}(u, v, m, z),$$

where the first term represents the model in the weak form given by

$$\begin{aligned}
&\text{Model}(u, v, m) \\
&= \int_D (\nu + \nu_t) 2S(\boldsymbol{u}) \cdot S(\boldsymbol{v}) dx + \int_D [(\boldsymbol{u} \cdot \nabla)\boldsymbol{u}] \cdot \boldsymbol{v} dx - \int_D p \nabla \cdot \boldsymbol{v} dx \\
&+ \int_D q \nabla \boldsymbol{u} dx \\
&+ \int_D \left(\nu + (\gamma + e^m)\, \nu_{t,0}\right) \nabla\gamma \cdot \nabla\eta dx + \int_D [\boldsymbol{u} \cdot \nabla\gamma]\eta dx - \int_D \frac{1}{2} \frac{\boldsymbol{u} \cdot \boldsymbol{e}_1}{x_1 + b} \gamma\eta dx.
\end{aligned}$$

The second term represents the stabilization by Galerkin Least-Squares (GLS) method

$$\begin{aligned}
\text{Stablization}(u, v) = &\int_D \tau_1 L_1(u) \cdot D_u L_1(u)(v) dx \\
&+ \int_D \tau_2 (\nabla \cdot \boldsymbol{u})(\nabla \cdot \boldsymbol{v}) dx + \int_D \tau_3 (\boldsymbol{u} \cdot \nabla\gamma)(\boldsymbol{u} \cdot \nabla\eta) dx
\end{aligned}$$

where $L_1(u)$ represents the strong form of the momentum equation of (32), τ_1, τ_2 and τ_3 are properly chosen stabilization constants associated with the local Péclet number.

Optimal control for turbulent jet flow: model – weak form

The weak form is defined for $u = (\boldsymbol{u}, p, \gamma), v = (\boldsymbol{v}, q, \eta) \in \mathcal{V} := (H^1(D))^2 \times L^2(D) \times H^1(D)$

$$r(u, v, m, z) = \text{Model}(u, v, m) + \text{Stablization}(u, v) + \text{Nitsche}(u, v, m, z),$$

The third term represents the weak imposition of the boundary condition and the control function by Nitsche's method [Bazilevs et al., 2007], which reads

$$\begin{aligned}
\text{Nitsche}(u, v, m, z) &= C_d \int_{\Gamma_O \cup \Gamma_W} h^{-1}(\nu + \nu_t)(\boldsymbol{u} \cdot \boldsymbol{\tau})(\boldsymbol{v} \cdot \boldsymbol{\tau}) ds \\
&- \int_{\Gamma_O \cup \Gamma_W} (\sigma_n(\boldsymbol{u}) \cdot \boldsymbol{\tau})(\boldsymbol{v} \cdot \boldsymbol{\tau}) + (\sigma_n(\boldsymbol{v}) \cdot \boldsymbol{\tau})(\boldsymbol{u} \cdot \boldsymbol{\tau}) ds \\
&+ C_d \int_{\Gamma_I} h^{-1}(\nu + \nu_t)(\boldsymbol{u} \cdot \boldsymbol{n} + \chi_W \phi(z))(\boldsymbol{v} \cdot \boldsymbol{n}) ds \\
&- \int_{\Gamma_I} (\sigma_n(\boldsymbol{u}) \cdot \boldsymbol{n})(\boldsymbol{v} \cdot \boldsymbol{n}) + (\sigma_n(\boldsymbol{v}) \cdot \boldsymbol{n})(\boldsymbol{u} \cdot \boldsymbol{n} + \chi_W \phi(z)) ds,
\end{aligned}$$

where the first and the third terms enforce the boundary conditions while the second and the fourth terms represent the compatibility conditions. C_d is a constant, set as $C_d = 10^5$. h is a local length of the boundary edge along the Dirichlet boundaries.

Optimal control for turbulent jet flow: trace estimate

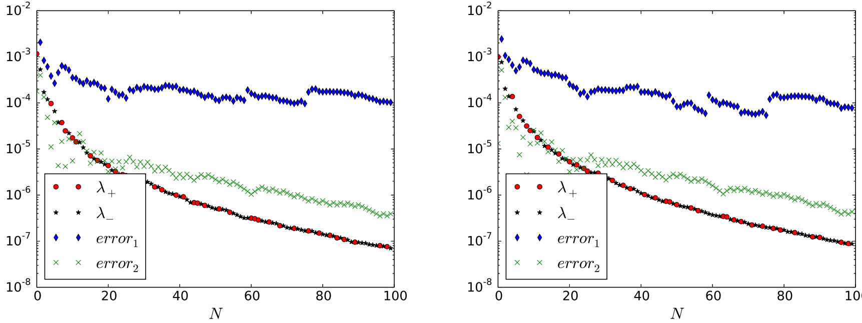


Figure: The decay of the generalized eigenvalues, λ_+ for positive eigenvalues and λ_- for negative eigenvalues, and the errors, denoted error_1 for the randomized trace estimator $\widehat{T}_1$ and error_2 for the randomized SVD-based trace estimator $\widehat{T}_2$, with respect to the number of estimate terms N. Left: $z = z_0$; right: $z = z^{\text{MC}}_{\text{quad}}$.

Optimal control for turbulent jet flow: optimal control

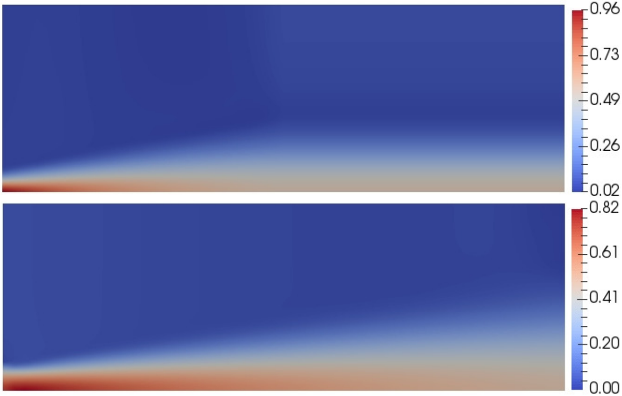


Figure: The velocity field corresponding to the initial control (top) and the optimal control with quadratic approximation and variance reduction (bottom).

Optimal control for turbulent jet flow: scalability I

- total cost = # PDE solves/iteration × # optimization iterations
- # PDE solves/iteration depends on decay of generalized eigenvalues

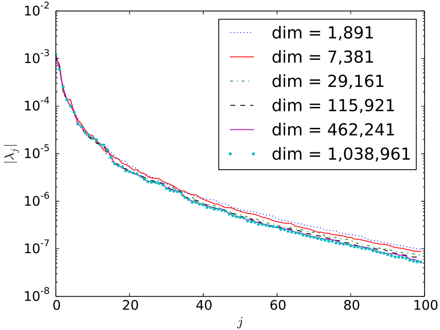


Figure: Decay of the generalized eigenvalues (in absolute value) with different parameter dimensions (dim) at optimal control. Results indicate dimension independence of per-optimization-iteration cost.

Optimal control for turbulent jet flow: scalability II

- total cost = # PDE solves/iteration × # optimization iterations
- # iterations depends how well the BFGS Hessian approximates true Hessian

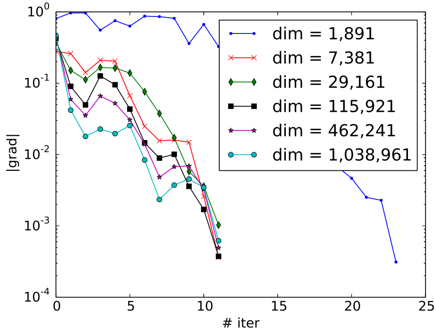


Figure: Gradient reduction with number of BFGS iterations. Simple control variable continuation employed. Results indicate dimension independence of BFGS iterations. (modulo initialization of 1M case)

Optimal control for turbulent jet flow: scalability III

How does variance reduction behave as parameter dimension increases?

Table: Mean-square-error (MSE) for $\mathbb{E}[Q]$ at optimal control.

parameter dimension	$\mathbb{E}^{\text{MC}}[-Q]$	MSE(Q)	MSE($Q - Q_{\text{lin}}$)	MSE($Q - Q_{\text{quad}}$)
1,891	-1.71e+00	7.40e-06	2.68e-08	1.81e-09
7,381	-1.59e+00	7.94e-06	1.57e-07	1.46e-08
29,161	-1.44e+00	3.82e-06	7.23e-08	1.66e-08

Table: MSE for Var$[Q]$, where $q = (Q - Q_0)^2$, $q_{\text{lin}} = (Q_{\text{lin}} - Q_0)^2$, $q_{\text{quad}} = (Q_{\text{quad}} - Q_0)^2$.

parameter dimension	$\mathbb{E}^{\text{MC}}[q]$	MSE(q)	MSE($q - q_{\text{lin}}$)	MSE($q - q_{\text{quad}}$)
1,891	8.05e-05	9.37e-10	1.76e-11	8.77e-13
7,381	8.13e-05	1.15e-09	8.87e-12	1.48e-12
29,161	5.60e-05	6.59e-10	3.39e-11	4.04e-12

100×–1000× speedup with quadratic approximation as control variate

Low-rank Hessian-based variance reduction for OUU

- Construct 2nd order Taylor approximation (wrt random parameters) of control objective, and use as a variance reduction tool for mean-variance OUU
- Hessian of parameter-to-objective map is compact, with fast decaying eigenvalues.
- Randomized SVD used to accurately and efficiently capture the low-rank
- Leads to an optimization problem constrained by a Hessian eigenvalue problem, with state and adjoint PDE constraints to define the gradient entering the objective approximation, and incremental state and adjoint PDE constraints to define the Hessian action
- Solved for sequence of OUU problems with up to 1 million random parameters, demonstrated scalability (i.e., # of PDE solves constant with increasing random parameter and control dimensions)
  - Trace estimation by randomized SVD is scalable
  - Quasi-Newton optimization iterations are scalable
  - Variance reduction is scalable
  - $\Longrightarrow$ Overall method is scalable
- Taylor approximation is local; variance reduction can deteriorate for large 3rd derivatives or large variances
- Current work: higher order Taylor and other approximations, chance constraints, alternatives to low-rank approximation, applications to deep learning of complex PDE maps

References

- P. Chen, U. Villa, and O. Ghattas. *Taylor approximation and variance reduction for PDE-constrained optimal control problems under uncertainty.* http://arxiv.org/abs/1804.04301
- A. Alexanderian, N. Petra, G. Stadler, and O. Ghattas, *Mean-variance risk-averse optimal control of systems governed by PDEs with random parameter fields using quadratic approximations*, **SIAM/ASA Journal on Uncertainty Quantification**, 5(1):1166–1192, 2017. https://doi.org/10.1137/16M106306X
- A. Alexanderian, N. Petra, G. Stadler, and O. Ghattas, *A fast and scalable method for A-optimal design of experiments for infinite-dimensional Bayesian nonlinear inverse problems*, **SIAM Journal on Scientific Computing**, 38(1):A243–A272, 2016.
- T. Bui-Thanh and O. Ghattas, *Analysis of the Hessian for inverse scattering problems. Parts I, II, III*, **Inverse Problems** 2012a, 2012b; **Inverse Problems and Imaging** 2013.
- N. Alger, V. Rao, A. Myers, T. Bui-Thanh, and O. Ghattas, *Scalable matrix-free adaptive convolution-product approximation for locally translation-invariant operators*, working paper.