Scalable methods for optimal control of systems governed by PDEs with random coefficient fields

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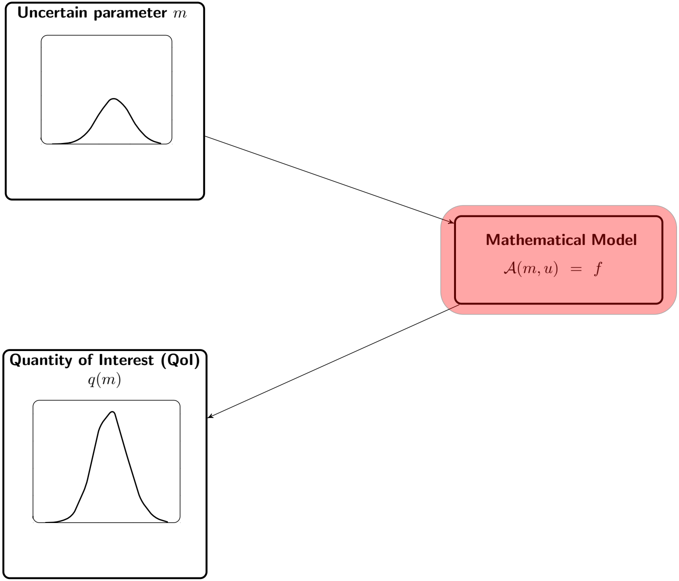
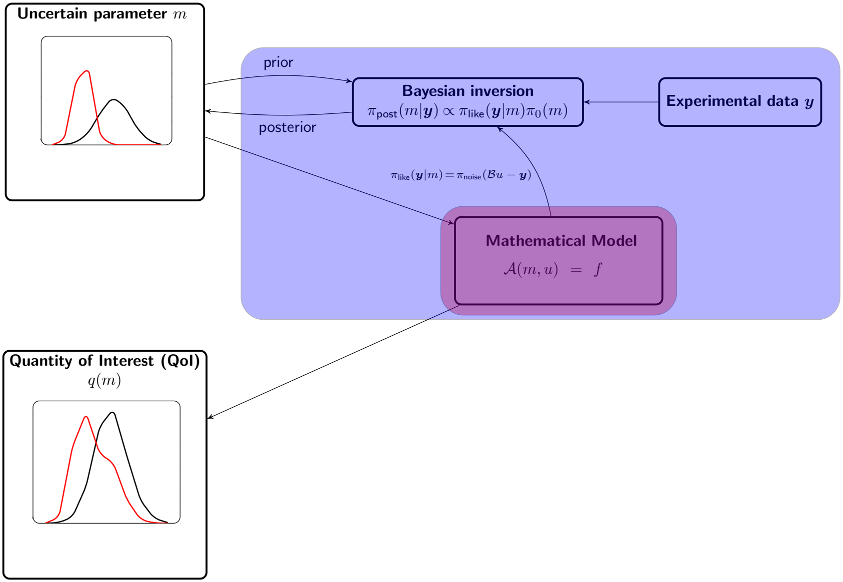
From data to decisions under uncertainty



From data to decisions under uncertainty



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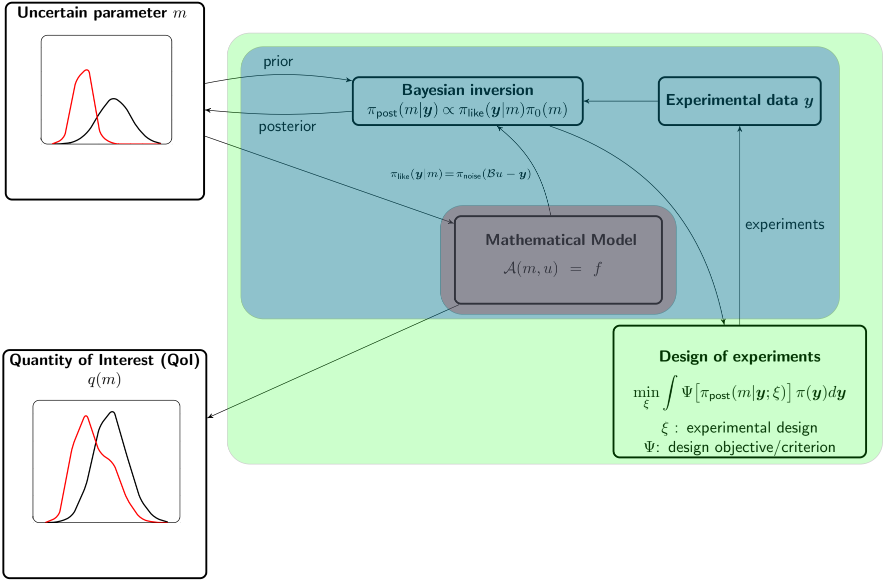

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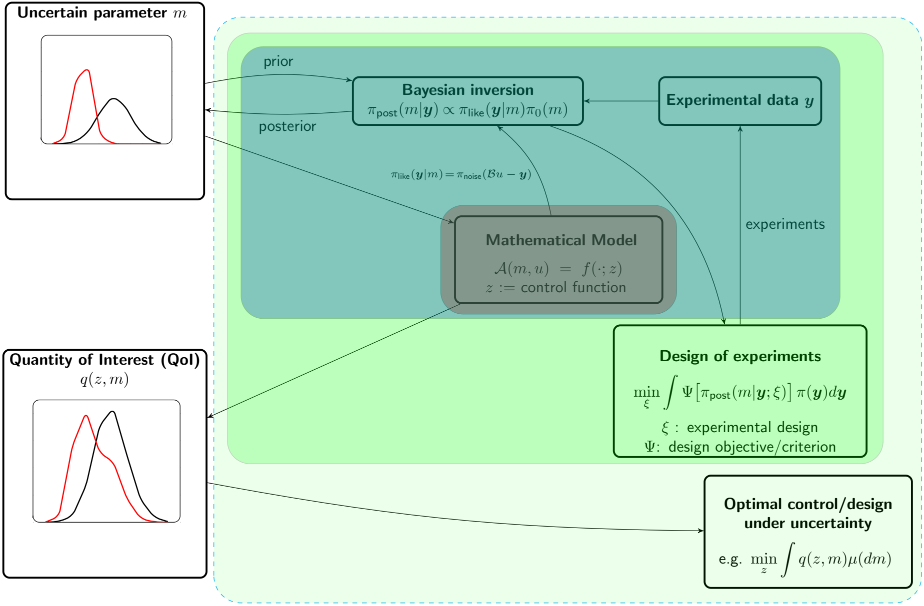
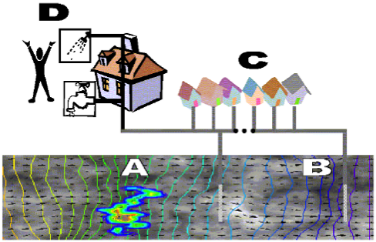
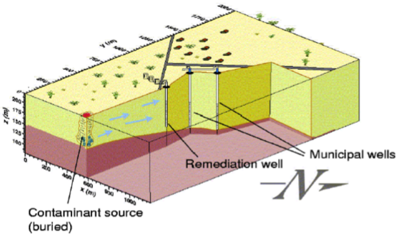
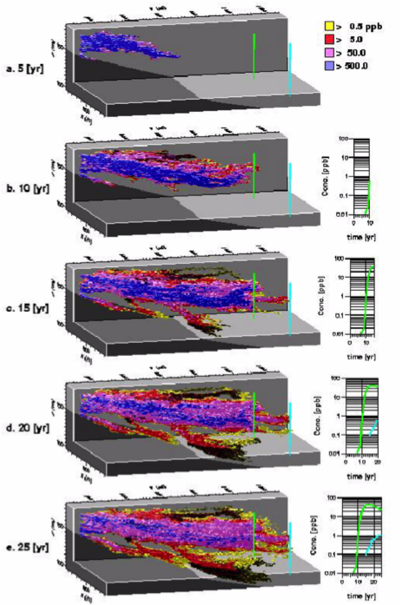


Example: Groundwater contaminant remediation





Source: Reed Maxwell, CSM



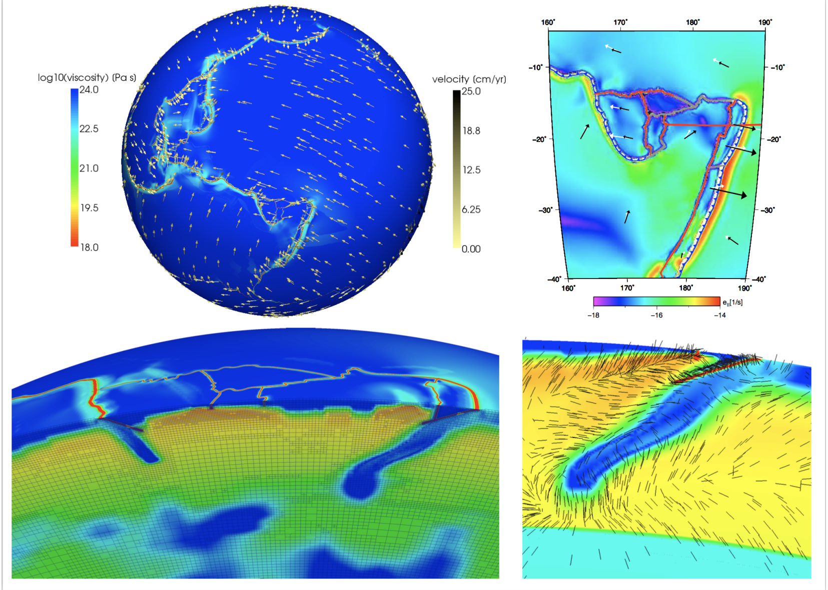
Example: Groundwater contaminant remediation

- Inverse problem
  - Infer (uncertain) soil permeability from (uncertain) measurements of pressure head at wells and from a (uncertain) model of subsurface flow and transport
- Prediction (or forward) problem
  - Predict (uncertain) evolution of contaminant concentration at municipal wells from (uncertain) permeability and (uncertain) subsurface flow/transport model
- Optimal experimental design problem
  - Where should new observation wells be placed so that permeability is inferred with the least uncertainty?
- Optimal design problem
  - Where should new remediation wells be placed so that (uncertain) contaminant concentrations at municipal wells are minimized?
- Optimal control problem
  - What should the rates of extraction/injection at remediation wells be so that (uncertain) contaminant concentrations at municipal wells are minimized?

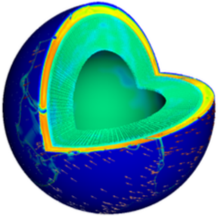
Applications of inverse problems in CCGO

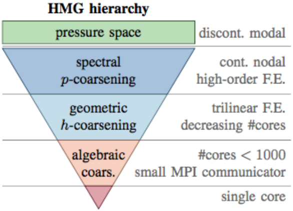
- Antarctic ice sheet flow (+ ocean dynamics)
  - Joint with Patrick Heimbach, Tom Hughes, Tobin Isaac (Georgia Tech), Tom O'Leary-Roseberry, Noemi Petra (UC-Merced), Georg Stadler (NYU), Umberto Villa, Alice Zhu
- Global and regional seismic inversion, joint seismic–EM inversion, inverse scattering
  - Joint with Hossein Aghakhani, Nick Alger, Tan Bui, Ben Crestel, David Keyes (KAUST), George Turkiyyah (KAUST), Georg Stadler (NYU), Umberto Villa
- Global mantle convection
  - Joint with Mike Gurnis (Caltech), Johann Rudi, Georg Stadler (NYU)
- Poroelastic subsurface flow inversion and management of induced seismicity
  - Joint with Amal Alghamdi, Marc Hesse, Georg Stadler (NYU), Umberto Villa, Karen Willcox (MIT)
- Turbulent combustion: inference and control
  - Joint with George Biros, Peng Chen, Matthias Heinkenschloss (Rice), Myoungkyu Lee, Bob Moser, Todd Oliver, Chris Simmons, David Sondak, Andrew Stuart (Caltech), Umberto Villa, Karen Willcox (MIT)
- Reservoir inversion
  - Joint with George Biros, Tan Bui, Clint Dawson, Sam Estes, John Lee, Umberto Villa
- Soft tissue biomechanical inversion
  - Joshua Chen, Michael Sacks, Umberto Villa

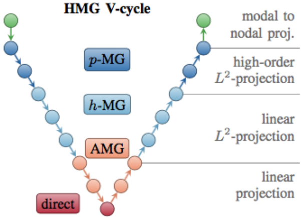
Forward and inverse global mantle convection modeling

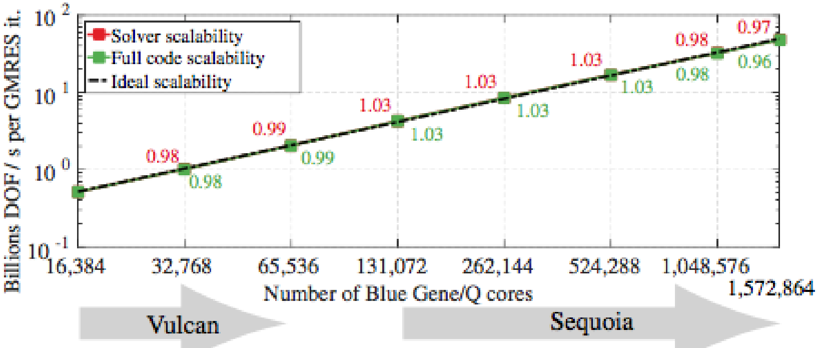


Scalable solver (2015 Gordon Bell Prize)

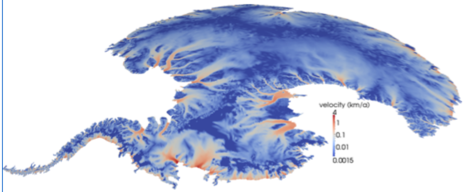




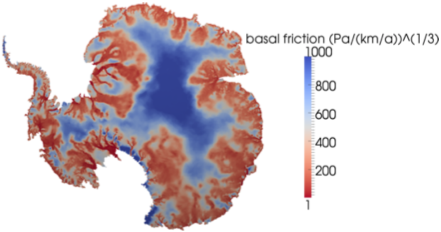




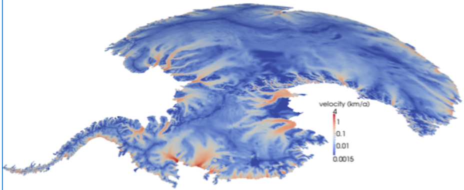
Bayesian inversion for basal friction field in Antarctica



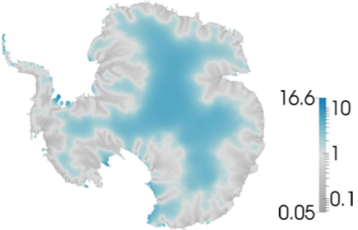
InSAR-based ice surface velocity observations



Inferred mean of basal friction field

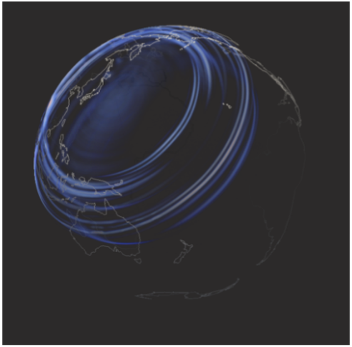


Reconstructed ice surface velocity field (based on inferred mean of basal friction field)

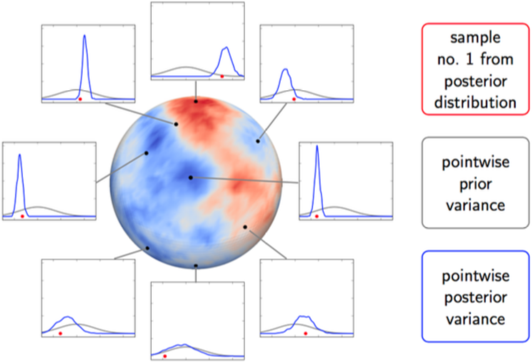


Inferred uncertainty in basal friction field (standard deviation of Gaussianized posterior of log basal friction)

Bayesian global seismic inversion



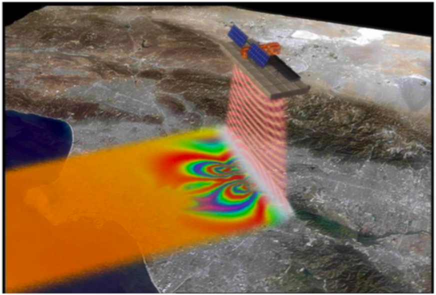
Parallel adaptive DG wave propagation

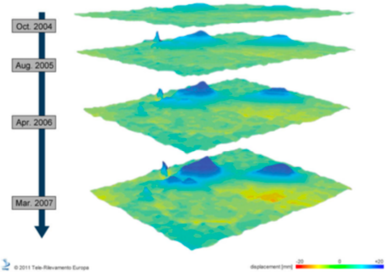


Prior and posterior seismic velocity marginals

Parallel octree AMR was finalist for 2010 Bell Prize
Bayesian Inversion was finalist for 2012 Gordon Bell Prize

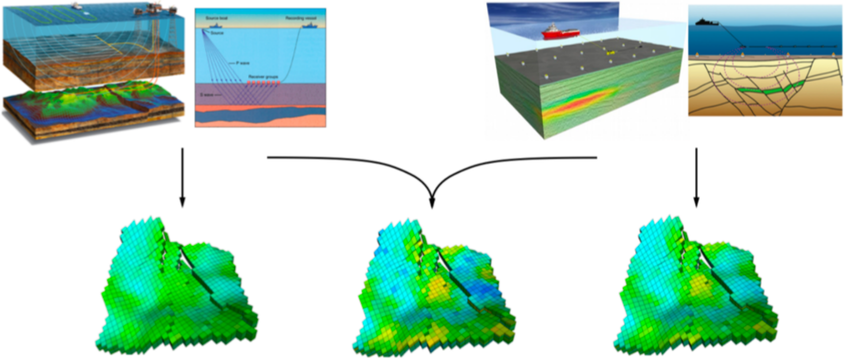
Bayesian poroelastic inversion





Use observations (InSAR, GPS) of surface deformation induced by CO2 or wastewater injection, in addition to well pressure measurements, to infer subsurface permeability and elastic properties. Forward predict and then ultimately optimize injection processes to avoid induced seismicity.

Joint seismic-electromagnetic inversion



Employ seismic (left) and electromagnetic (right) observations for joint reconstruction of subsurface properties, producing better characterization of petrophysical properties of reservoir than either one alone.

Optimal control of systems governed by PDEs with uncertain parameter fields

PDE-constrained control objective:

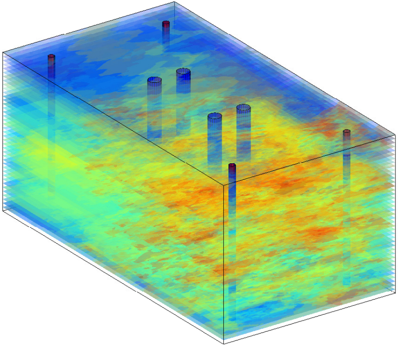
$$q = q(u(z, m), z)$$

where u depends on z and m through:

$$\mathcal{A}(u, m) = f(z)$$

- q: control objective
- $\mathcal{A}$: forward PDE operator
- u: state variable
- m: uncertain parameter field
- z: control function

Control of injection wells in porous medium flow (SPE10 permeability data)



Problem: given uncertainty model for m, find z that "optimizes" $q(u(z, m), z)$

Optimization under uncertainty (OUU)

- $\mathscr{H}$: parameter space, infinite-dimensional separable Hilbert space
- $q(z, m)$: control objective functional

  $m \in \mathscr{H}$: uncertain model parameter field, $\quad z$: control function
- Optimization under uncertainty (OUU):

$$\min_{z} \qquad q(z, m)$$

Optimization under uncertainty (OUU)

- $\mathscr{H}$: parameter space, infinite-dimensional separable Hilbert space
- $q(z, m)$: control objective functional

  $m \in \mathscr{H}$: uncertain model parameter field, z: control function
- *Risk-neutral* optimization under uncertainty (OUU):

$$\min_z \mathsf{E}_m\{q(z,m)\}$$

$$\mathsf{E}_m\{q(z,m)\} = \int_{\mathscr{H}} q(z,m)\,\mu(dm)$$

Optimization under uncertainty (OUU)

- $\mathscr{H}$: parameter space, infinite-dimensional separable Hilbert space
- $q(z, m)$: control objective functional

  $m \in \mathscr{H}$: uncertain model parameter field, z: control function
- *Risk-averse* (Mean-Var) optimization under uncertainty (OUU):

$$\min_z \mathsf{E}_m\{q(z,m)\} + \beta\,\mathsf{var}_m\{q(z,m)\}$$

$$\mathsf{E}_m\{q(z,m)\} = \int_{\mathscr{H}} q(z,m)\,\mu(dm)$$

$$\mathsf{var}_m\{q(z,m)\} = \mathsf{E}_m\{q(z,m)^2\} - \mathsf{E}_m\{q(z,m)\}^2$$

Optimization under uncertainty (OUU)

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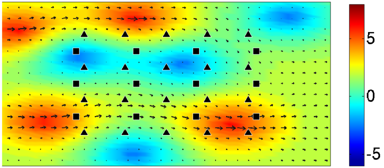
- Main challenges:
  - Integration over infinite/high-dimensional parameter space
  - Evaluation of q requires PDE solves
- Standard Monte Carlo approach (Sample Average Approximation) is prohibitive
  - Numerous (n_{mc}) samples required, each requires PDE solve
  - Resulting PDE-constrained optimization problem has n_{mc} PDE constraints

Some existing approaches for PDE-constrained OUU

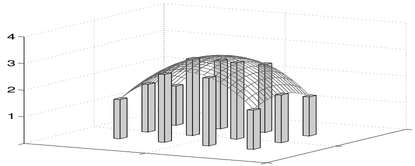
Methods based on stochastic collocation, sparse/adaptive sampling, POD, ...

- 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 reduced-order modeling*, 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.

Example: Control of injection wells in porous medium



$\bar{m}$ = mean of log permeability field



$\bar{q}$ = target pressure at production wells

- state PDE: single phase flow in a porous medium

$$-\nabla \cdot (e^m \nabla u) = \sum_{i=1}^{n_c} z_i f_i(\boldsymbol{x})$$

  with Dirichlet lateral & Neumann top/bottom BCs
- uncertain parameter: log permeability field m
- control variables: z_i, mass source at injection wells; f_i, mollified Dirac deltas
- control objective: $q(\boldsymbol{z}, m) := \frac{1}{2}\|\mathcal{Q}u(\boldsymbol{z}, m) - \bar{q}\|^2$, $\bar{q}$: target pressure
- dimensions: $n_s = n_m = 3242$, $n_c = 20$, $n_q = 12$

Porous medium with random permeability field

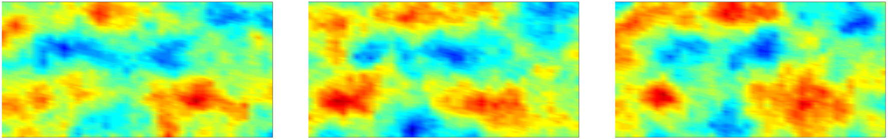
- Distribution law of m:

$$\mu = \mathcal{N}(\bar{m}, \mathcal{C}) \quad \text{(Gaussian measure on Hilbert space } \mathscr{H}\text{)}$$

- Take covariance operator as square of inverse of Poisson-like operator:

$$\mathcal{C} = (-\kappa\Delta + \alpha I)^{-2} \quad \kappa, \alpha > 0$$

- $\mathcal{C}$ is positive, self-adjoint, of trace-class; μ well-defined on $\mathscr{H}$ (Stuart '10)
- $\frac{\kappa}{\alpha} \propto$ correlation length; the larger α, the smaller the variance



Random draws for $\kappa = 2 \times 10^{-2}, \;\; \alpha = 4$

OUU with linearized parameter-to-objective map

- Mean-var risk-averse optimal control problem (including cost of controls):

$$\min_z \mathsf{E}_m\{q(z,m)\} + \beta\, \mathsf{var}_m\{q(z,m)\} + \gamma \|z\|^2$$

- **Linear approximation to parameter-to-objective map about $\bar{m}$:**

$$q_{\mathsf{lin}}(z,m) = q(z,\bar{m}) + \langle g_m(z,\bar{m}), m - \bar{m}\rangle$$

- $g_m(z,\cdot) := \dfrac{dq(z,\cdot)}{dm}$ is the gradient with respect to m

- The moments of the linearized objective:

$$\mathsf{E}_m\{q_{\mathsf{lin}}(z,\cdot)\} = q(z,\bar{m})$$

$$\mathsf{var}_m\{q_{\mathsf{lin}}(z,\cdot)\} = \langle g_m(z,\bar{m}), \mathcal{C}[g_m(z,\bar{m})]\rangle$$

$$q_{\mathsf{lin}}(z,\cdot) \sim \mathcal{N}\Big(q(z,\bar{m}), \langle g_m(z,\bar{m}), \mathcal{C}[g_m(z,\bar{m})]\rangle\Big)$$

Mean-var risk-averse optimal control problem with linearized parameter-to-objective map

State-and-adjoint-PDE constrained optimization problem (quartic in $\boldsymbol{z}$):

$$\min_{\boldsymbol{z}\in Z} \mathcal{J}(\boldsymbol{z}) := \frac{1}{2}\|\mathcal{Q}u - \bar{q}\|^2 + \frac{\beta}{2}\langle g_m(\bar{m}), \mathcal{C}[g_m(\bar{m})]\rangle + \frac{\gamma}{2}\|\boldsymbol{z}\|^2$$

with $g_m(\bar{m}) = e^{\bar{m}}\nabla u \cdot \nabla p$, where

$$-\nabla \cdot (e^{\bar{m}}\nabla u) = \sum_{i=1}^{n_c} z_i f_i \qquad \text{state equation}$$

$$-\nabla \cdot (e^{\bar{m}}\nabla p) = -\mathcal{Q}^*(\mathcal{Q}u - \bar{q}) \qquad \text{adjoint equation}$$

Lagrangian of the risk-averse optimal control problem with q_{lin}:

$$\begin{aligned}\mathscr{L}(\boldsymbol{z}, u, p, u^\star, p^\star) = {} & \frac{1}{2}\|\mathcal{Q}u - \bar{q}\|^2 + \frac{\beta}{2}\left\langle e^{\bar{m}}\nabla u \cdot \nabla p, \mathcal{C}[e^{\bar{m}}\nabla u \cdot \nabla p]\right\rangle + \frac{\gamma}{2}\|\boldsymbol{z}\|^2 \\ & + \left\langle e^{\bar{m}}\nabla u, \nabla u^\star\right\rangle - \sum_{i=1}^{n_c} z_i\langle f_i, u^\star\rangle \\ & + \left\langle e^{\bar{m}}\nabla p, \nabla p^\star\right\rangle + \langle \mathcal{Q}^*(\mathcal{Q}u - \bar{q}), p^\star\rangle\end{aligned}$$

Gradient computation for risk averse optimal control

- "State problem" for risk-averse optimal control problem with q_{lin}:

$$\left\langle e^{\bar{m}} \nabla u, \nabla \tilde{u} \right\rangle = \sum_{i=1}^{n_c} z_i \langle f_i, \tilde{u} \rangle$$

$$\left\langle e^{\bar{m}} \nabla p, \nabla \tilde{p} \right\rangle = -\langle \mathcal{Q}^* (\mathcal{Q} u - \bar{q}), \tilde{p} \rangle$$

for all test functions $\tilde{p}$ and $\tilde{u}$

- "Adjoint problem" for risk-averse optimal control problem with q_{lin}:

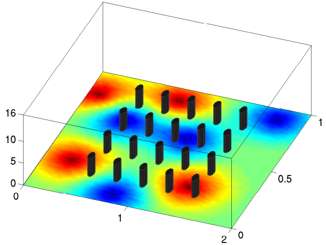
$$\left\langle e^{\bar{m}} \nabla p^\star, \nabla \tilde{p} \right\rangle = -\beta \left\langle e^{\bar{m}} \nabla u \cdot \nabla \tilde{p}, \mathcal{C}[e^{\bar{m}} \nabla u \cdot \nabla p] \right\rangle$$

$$\left\langle e^{\bar{m}} \nabla u^\star, \nabla \tilde{u} \right\rangle = -\langle \mathcal{Q}^* (\mathcal{Q} u - \bar{q}), \tilde{u} \rangle - \beta \left\langle e^{\bar{m}} \nabla \tilde{u} \cdot \nabla p, \mathcal{C}[e^{\bar{m}} \nabla u \cdot \nabla p] \right\rangle - \langle \mathcal{Q}^* \mathcal{Q} p^\star, \tilde{u} \rangle$$

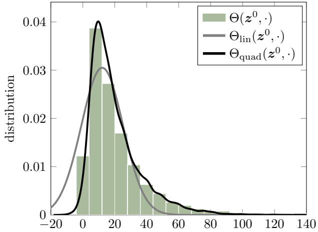
for all test functions $\tilde{p}$ and $\tilde{u}$

- Gradient: $\dfrac{\partial \mathcal{J}}{\partial z_j} = \gamma z_j - \langle f_j, u^\star \rangle, \quad j = 1, \ldots, n_c$
- Cost of objective = 2 PDE solves; cost of gradient = 2 PDE solves

Risk-averse optimal control with linearized objective

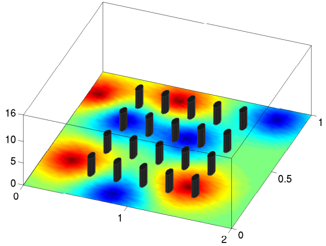


initial (suboptimal) control $\boldsymbol{z}^0$

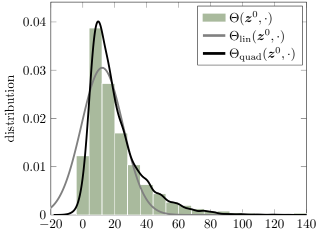


distrib. of exact & approx objectives at $\boldsymbol{z}^0$

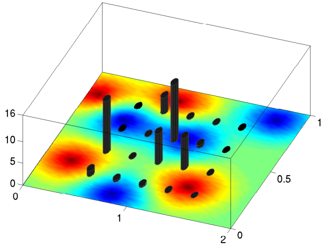
Risk-averse optimal control with linearized objective



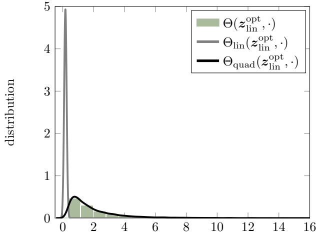
initial (suboptimal) control z^0



distrib. of exact & approx objectives at z^0



optimal control $z_{\text{lin}}^{\text{opt}}$ based on q_{lin}



distrib. of exact & approx objectives at $z_{\text{lin}}^{\text{opt}}$

Quadratic approximation to parameter-to-objective map

Quadratic approximation to the parameter-to-control-objective map:

$$q_{\mathsf{quad}}(\boldsymbol{z}, m) = q(\boldsymbol{z}, \bar{m}) + \langle g_m(\boldsymbol{z}, \bar{m}), m - \bar{m} \rangle + \frac{1}{2} \langle \mathcal{H}_m(\boldsymbol{z}, \bar{m})(m - \bar{m}), m - \bar{m} \rangle$$

- g_m: gradient of parameter-to-objective map
- $\mathcal{H}_m$: Hessian of parameter-to-objective map

Observations:

- Quadratic approximation does not lead to a Gaussian control objective
- However, can derive analytic formulas for the moments of q_{quad} in the infinite-dimensional Hilbert space setting

Analytic expressions for mean and variance with q_{quad}

- Mean:

$$\mathsf{E}_m\{q_{\text{quad}}(\boldsymbol{z},\cdot)\} = q(\boldsymbol{z},\bar{m}) + \frac{1}{2}\text{tr}\big[\tilde{\mathcal{H}}_m(\boldsymbol{z},\bar{m})\big]$$

- Variance:

$$\text{var}_m\{q_{\text{quad}}(\boldsymbol{z},\cdot)\} = \langle g_m(\boldsymbol{z},\bar{m}), \mathcal{C}[g_m(\boldsymbol{z},\bar{m})]\rangle + \frac{1}{2}\text{tr}\big[\tilde{\mathcal{H}}_m(\boldsymbol{z},\bar{m})^2\big]$$

where $\tilde{\mathcal{H}}_m = \mathcal{C}^{1/2}\mathcal{H}_m\mathcal{C}^{1/2}$ is the covariance-preconditioned Hessian

- Risk averse optimal control objective with q_{quad}:

$$J(\boldsymbol{z}) = q(\boldsymbol{z},\bar{m}) + \frac{1}{2}\text{tr}\big[\tilde{\mathcal{H}}_m(\boldsymbol{z},\bar{m})\big] + \frac{\beta}{2}\left\{\langle g_m(\boldsymbol{z},\bar{m}), \mathcal{C}[g_m(\boldsymbol{z},\bar{m})]\rangle + \frac{1}{2}\text{tr}\big[\tilde{\mathcal{H}}_m(\boldsymbol{z},\bar{m})^2\big]\right\}$$

Randomized trace estimator

- Randomized trace estimation:

$$\mathrm{tr}(\tilde{\mathcal{H}}_m) \approx \frac{1}{n_{\mathrm{tr}}} \sum_{j=1}^{n_{\mathrm{tr}}} \left\langle \tilde{\mathcal{H}}_m \xi_j, \xi_j \right\rangle = \frac{1}{n_{\mathrm{tr}}} \sum_{j=1}^{n_{\mathrm{tr}}} \langle \mathcal{H}_m \zeta_j, \zeta_j \rangle$$

$$\mathrm{tr}(\tilde{\mathcal{H}}_m^2) \approx \frac{1}{n_{\mathrm{tr}}} \sum_{j=1}^{n_{\mathrm{tr}}} \langle \mathcal{H}_m \zeta_j, \mathcal{C}[\mathcal{H}_m \zeta_j] \rangle$$

  where ξ_j are Gaussian random fields and $\zeta_j = \mathcal{C}^{1/2}\xi_j$

- In computations, we use draws $\zeta_j \sim \mathcal{N}(0, \mathcal{C}) =: \nu$

- Straightforward to show:

$$\int_{\mathscr{H}} \langle \mathcal{H}_m \zeta, \zeta \rangle \, \nu(d\zeta) = \mathrm{tr}(\tilde{\mathcal{H}}_m), \qquad \int_{\mathscr{H}} \langle \mathcal{H}_m \zeta, \mathcal{C}[\mathcal{H}_m \zeta] \rangle \, \nu(d\zeta) = \mathrm{tr}(\tilde{\mathcal{H}}_m^2)$$

- Finite dimensional algorithm: H. Avron and S. Toledo, *Randomized algorithms for estimating the trace of an implicit symmetric positive semi-definite matrix*, Journal of the ACM, 2011.

Risk-averse optimal control with quadraticized objective

$$\min_{z\in Z} \frac{1}{2}\|\mathcal{Q}u - \bar{q}\|_2^2 + \frac{1}{2n_{\text{tr}}}\sum_{j=1}^{n_{\text{tr}}} \langle \zeta_j, \eta_j \rangle + \frac{\beta}{2}\left\{\langle g_m(\bar{m}), \mathcal{C}[g_m(\bar{m})]\rangle + \frac{1}{2n_{\text{tr}}}\sum_{j=1}^{n_{\text{tr}}} \left\|\mathcal{C}^{1/2}\eta_j\right\|^2\right\}$$

with

$$g_m(\bar{m}) = e^{\bar{m}}\nabla u \cdot \nabla p$$
$$\eta_j = \underbrace{e^{\bar{m}}(\zeta_j \nabla u \cdot \nabla p + \nabla \upsilon_j \cdot \nabla p + \nabla u \cdot \nabla \rho_j)}_{\mathcal{H}_m \zeta_j} \quad j \in \{1, \ldots, n_{\text{tr}}\}$$

where

$$-\nabla \cdot (e^{\bar{m}} \nabla u) = \textstyle\sum_{i=1}^{N} z_i f_i$$
$$-\nabla \cdot (e^{\bar{m}} \nabla p) = -\mathcal{Q}^*(\mathcal{Q}u - \bar{q})$$
$$-\nabla \cdot (e^{\bar{m}} \nabla \upsilon_j) = \nabla \cdot -(\zeta_j e^{\bar{m}} \nabla u)$$
$$-\nabla \cdot (e^{\bar{m}} \nabla \rho_j) = -Q^* Q \upsilon_j + \nabla \cdot (\zeta_j e^{\bar{m}} \nabla p)$$

Risk-averse optimal control with quadraticized objective

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Risk-averse optimal control with quadraticized objective

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Risk-averse optimal control with quadraticized objective

$$\min_{z \in Z} \frac{1}{2}\|\mathcal{Q}u - \bar{q}\|_2^2 + \frac{1}{2n_{\mathsf{tr}}}\sum_{j=1}^{n_{\mathsf{tr}}} \langle \zeta_j, \eta_j \rangle + \frac{\beta}{2}\left\{ \langle g_m(\bar{m}), \mathcal{C}[g_m(\bar{m})] \rangle + \frac{1}{2n_{\mathsf{tr}}}\sum_{j=1}^{n_{\mathsf{tr}}} \left\| \mathcal{C}^{1/2}\eta_j \right\|^2 \right\}$$

with

$$g_m(\bar{m}) = e^{\bar{m}} \nabla u \cdot \nabla p$$

$$\eta_j = \underbrace{e^{\bar{m}}(\zeta_j \nabla u \cdot \nabla p + \nabla \upsilon_j \cdot \nabla p + \nabla u \cdot \nabla \rho_j)}_{\mathcal{H}_m \zeta_j} \quad j \in \{1, \ldots, n_{\mathsf{tr}}\}$$

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Risk-averse optimal control with quadraticized objective

$$\min_{z \in Z} \frac{1}{2}\|\mathcal{Q}u - \bar{q}\|_2^2 + \frac{1}{2n_{\text{tr}}}\sum_{j=1}^{n_{\text{tr}}} \langle \zeta_j, \eta_j \rangle + \frac{\beta}{2}\left\{\langle g_m(\bar{m}), \mathcal{C}[g_m(\bar{m})]\rangle + \frac{1}{2n_{\text{tr}}}\sum_{j=1}^{n_{\text{tr}}} \left\|\mathcal{C}^{1/2}\eta_j\right\|^2\right\}$$

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$$-\nabla \cdot (e^{\bar{m}} \nabla \rho_j) = -Q^* Q \upsilon_j + \nabla \cdot (\zeta_j e^{\bar{m}} \nabla p)$$

Lagrangian for risk-averse optimal control with q_{quad}

$$
\begin{aligned}
&\mathscr{L}(\boldsymbol{z}, u, p, \{\upsilon_j\}_{j=1}^{n_{\text{tr}}}, \{\rho_j\}_{j=1}^{n_{\text{tr}}}, u^\star, p^\star, \{\upsilon_j^\star\}_{j=1}^{n_{\text{tr}}}, \{\rho_j^\star\}_{j=1}^{n_{\text{tr}}}) \\
&\quad = \frac{1}{2}\left\|\mathcal{Q}u - \bar{q}\right\|_2^2 \\
&\quad + \frac{1}{2n_{\text{tr}}}\sum_{j=1}^{n_{\text{tr}}}\left\langle \zeta_j, \left[e^{\bar{m}}(\zeta_j \nabla u \cdot \nabla p + \nabla \upsilon_j \cdot \nabla p + \nabla u \cdot \nabla \rho_j)\right]\right\rangle \\
&\quad + \frac{\beta}{2}\left\langle e^{\bar{m}}\nabla u \cdot \nabla p, \mathcal{C}[e^{\bar{m}}\nabla u \cdot \nabla p]\right\rangle \\
&\quad + \frac{\beta}{4n_{\text{tr}}}\sum_{j=1}^{n_{\text{tr}}}\left\|\mathcal{C}^{1/2}\left[e^{\bar{m}}(\zeta_j \nabla u \cdot \nabla p + \nabla \upsilon_j \cdot \nabla p + \nabla u \cdot \nabla \rho_j)\right]\right\|^2 \\
&\quad + \left\langle e^{\bar{m}}\nabla u, \nabla u^\star\right\rangle - \textstyle\sum_{i=1}^{N} z_i\langle f_i, u^\star\rangle \\
&\quad + \left\langle e^{\bar{m}}\nabla p, \nabla p^\star\right\rangle + \langle \mathcal{Q}^*(\mathcal{Q}u - \bar{q}), p^\star\rangle \\
&\quad + \sum_{j=1}^{n_{\text{tr}}}\left[\left\langle e^{\bar{m}}\nabla \upsilon_j, \nabla \upsilon_j^\star\right\rangle + \left\langle \zeta_j e^{\bar{m}}\nabla u, \nabla \upsilon_j^\star\right\rangle\right] \\
&\quad + \sum_{j=1}^{n_{\text{tr}}}\left[\left\langle e^{\bar{m}}\nabla \rho_j, \nabla \rho_j^\star\right\rangle + \left\langle \mathcal{Q}^*\mathcal{Q}\upsilon_j, \rho_j^\star\right\rangle + \left\langle \zeta_j e^{\bar{m}}\nabla p, \nabla \rho_j^\star\right\rangle\right]
\end{aligned}
$$

Adjoint & gradient for risk-averse optimal control w/q_{quad}

Adjoint problem for q_{quad} approximation

$$-\nabla\cdot(e^{\bar{m}}\nabla\rho_j^\star) = b_1^{(j)} \qquad j\in\{1,\dots,n_{\text{tr}}\}$$

$$-\nabla\cdot(e^{\bar{m}}\nabla\upsilon_j^\star) + \mathcal{Q}^*\mathcal{Q}\rho_j^\star = b_2^{(j)} \qquad j\in\{1,\dots,n_{\text{tr}}\}$$

$$-\nabla\cdot(e^{\bar{m}}\nabla p^\star) - \sum_{j=1}^{n_{\text{tr}}}\nabla\cdot(\zeta_j e^{\bar{m}}\nabla\rho_j^\star) = b_3$$

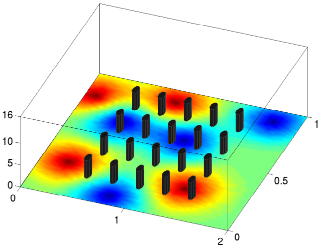
$$-\nabla\cdot(e^{\bar{m}}\nabla u^\star) + \mathcal{Q}^*\mathcal{Q}p^\star - \sum_{j=1}^{n_{\text{tr}}}\nabla\cdot(\zeta_j e^{\bar{m}}\nabla\upsilon_j^\star) = b_4$$

Gradient for q_{quad} approximation

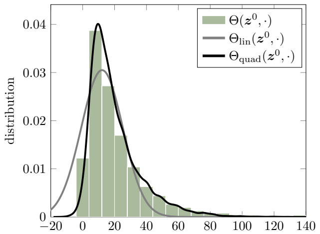
$$\frac{\partial\mathscr{L}}{\partial z_j} = \gamma z_j - \langle f_j, u^\star\rangle, \quad j=1,\dots,n_{\text{c}}$$

Cost of objective $= 2+2n_{\text{tr}}$ PDE solves; cost of gradient $= 2+2n_{\text{tr}}$ PDE solves

Risk-averse optimal control with quadraticized objective

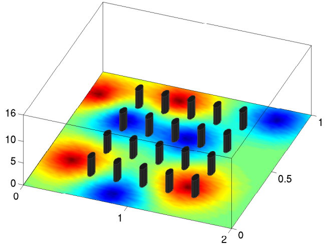


initial (suboptimal) control $\boldsymbol{z}^0$

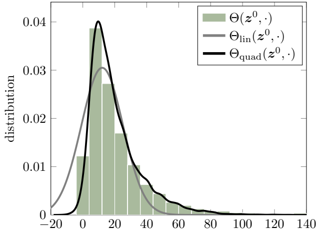


distrib. of exact & approx objectives at $\boldsymbol{z}^0$

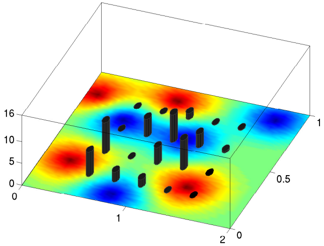
Risk-averse optimal control with quadraticized objective



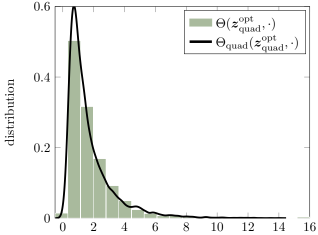
initial (suboptimal) control $\boldsymbol{z}^0$



distrib. of exact & approx objectives at $\boldsymbol{z}^0$

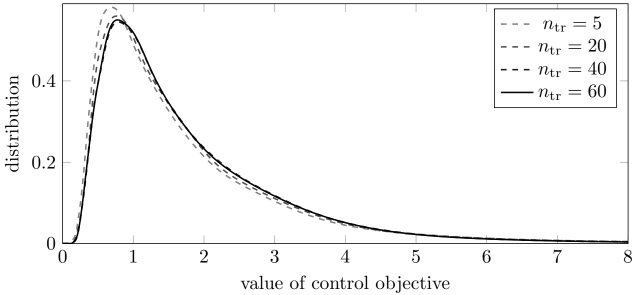


optimal control $\boldsymbol{z}_{\text{quad}}^{\text{opt}}$ based on q_{quad}



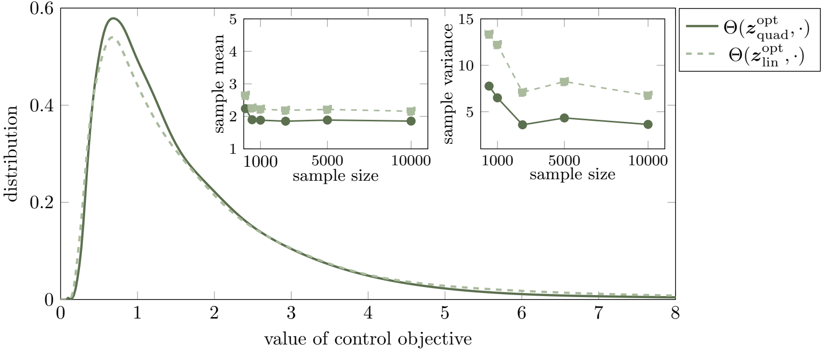
distrib. of exact & approx objectives at $\boldsymbol{z}_{\text{quad}}^{\text{opt}}$

Effect of number of trace estimator vectors on distribution of control objective evaluated at optimal controls



- Optimal controls $\boldsymbol{z}^{\mathsf{opt}}_{\mathsf{quad}}$ computed for each value of trace estimator using quadratic approximation of control objective, q_{quad}
- Each curve based on 10,000 samples of distribution of $q(\boldsymbol{z}^{\mathsf{opt}}_{\mathsf{quad}}, m)$ (control objective evaluated at optimal control)

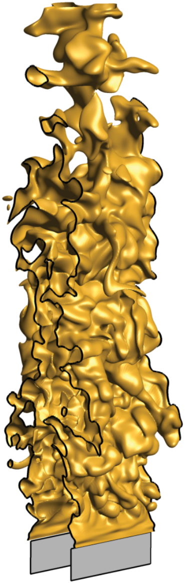
Comparison of distribution of control objective for optimal controls based on linearized and quadraticized objective



- Comparison of the distributions of $q(z^{\text{opt}}_{\text{lin}}, m)$ with $q(z^{\text{opt}}_{\text{quad}}, m)$
- $\beta = 1$, $\gamma = 10^{-5}$ and $n_{\text{tr}} = 40$ trace estimation vectors
- KDE results are based on 10,000 samples
- Inserts show Monte Carlo sample convergence for mean and variance

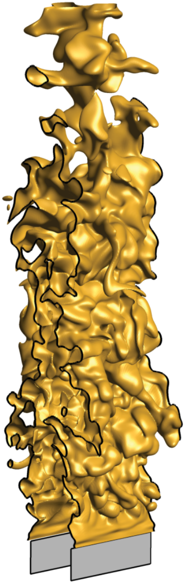
Optimal control of stochastic turbulent combustion

- Turbulent non-premixed Hydrogen-Air slot-jet flame, with co-flow
- Sources of uncertainty
  - Inputs: inlet flow conditions
  - Model parameters: turbulence models, chemical kinetics
  - Model inadequacy: chemical kinetics, flamelet model, turbulent transport
- Quantities of interest
  - Heat released over a specified distance
  - Net rate of NO_x production
- Design Problem
  - Objective: Maximize heat release with constraint on NO_x production
  - Control: Inlet profiles and optionally volumetric heat sink



UQ challenges

- Forward solves are relatively expensive
  - Naive sampling methods are cost prohibitive
- Model inadequacies are significant, complex, and deeply embedded in physical model
  - Requires physics-based approaches to inadequacy
  - Leads to high/infinite dimensional stochastic models
- Multiple QoIs, some related to rare events
  - Tail probabilities challenging to compute
  - Realistic risk measures often result in non-smooth objective functions



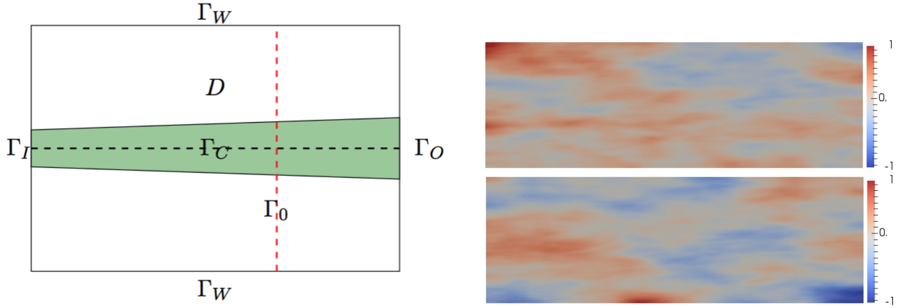
- These features are common in multiscale and multiphysics problems across scientific disciplines
- They combine to make UQ for inference, prediction, and optimization extremely challenging

Extensions (Peng Chen, Umberto Villa)

- Optimal control of turbulent jet governed by a turbulence model with embedded stochastic inadequacy model
- Randomized SVD to compute trace of $\tilde{\boldsymbol{H}}$, combined with eigenvalue sensitivities to computing gradient
- Monte Carlo corrections to quadratic approximation: Use of Taylor approximation as a control variate

Dirichlet boundary control for turbulent jet flow: problem

- **Control** is horizontal velocity profile at inlet boundary Γ_I
- **Objective** is to maximize jet width at Γ_0
- **Constraint** on inlet momentum: $\int_{\Gamma_I} (\mathbf{u} \cdot \mathbf{n})^2 ds = M_I$
- **Random input** is an inadequacy field for turbulent viscosity (5151 dimensions)



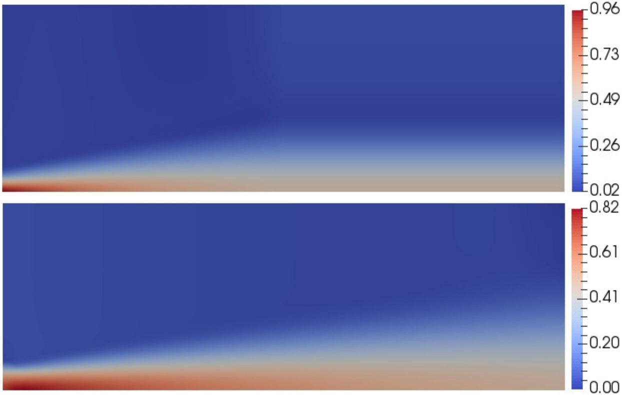
Left: sketch of the physical domain of the turbulence jet flow, with inlet boundary Γ_I, outlet boundary Γ_O, top and bottom wall Γ_W, the center axis Γ_C, and the cross-section Γ_0. The computational domain D is the top part of the physical domain. Right: two random samples drawn from the Gaussian measure $\mathcal{N}(0, \mathcal{C})$ with $\mathcal{C} = (-\alpha_1 \triangle + \alpha_2 I)^{-2}$ where $\alpha_1 = \alpha_2 = 0.5$.

Dirichlet boundary control for turbulent jet flow: model

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

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

Dirichlet boundary control for turbulent jet flow: results



The velocity field of the turbulent jet flow extracted from the DNS data (top) and obtained from the optimal control with quadratic approximation with variance reduction (bottom).

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

- Large number of randomized trace vectors might be required to compute tr$(\tilde{\boldsymbol{H}})$
- Randomized SVD estimates trace at cost of $2r$ products of $\tilde{\boldsymbol{H}}$ with random vectors (r is numerical rank of $\tilde{\boldsymbol{H}}$)
- Resulting cost is $2r$ incremental forward/adjoint solves and $4r$ Poisson solves (Steps 2 and 4)
- Covariance operator is compact and Hessian is often **low-rank** (QoI is sensitive to limited number of modes) so composition is low-rank

Randomized SVD (double pass algorithm)

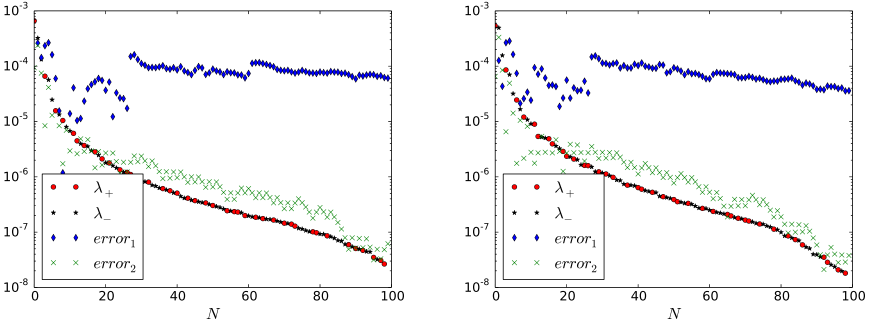
1. Generate i.i.d. Gaussian matrix $\boldsymbol{R} \in \mathbb{R}^{n \times r}$ with $r =$ numerical rank of $\tilde{\boldsymbol{H}}$ ($r \ll n$)
2. Form $\boldsymbol{Y} = \tilde{\boldsymbol{H}}\boldsymbol{R}$
3. Compute $\boldsymbol{Q} =$ orthonormal basis for $\boldsymbol{Y}$
4. Define $\boldsymbol{B} \in \mathbb{R}^{r \times r} := \boldsymbol{Q}^T \tilde{\boldsymbol{H}} \boldsymbol{Q}$
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: tr$(\tilde{\boldsymbol{H}}) \approx$ tr$(\boldsymbol{B})$

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

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

- Quadratic-based approximations of $\mathbb{E}[q]$ and var$[q]$ require $4r$ linearized forward solves (small multiple of nonlinear forward solve, for highly nonlinear forward problems)
- Computing gradient of tr$(\tilde{\boldsymbol{H}})$ wrt controls via eigenvalue sensitivity

Control of turbulent jet: Computing $\mathrm{tr}(\tilde{\boldsymbol{H}})$ via randomized SVD vs. randomized trace estimator



The decay of the generalized eigenvalues (λ_+ and λ_-) of $\tilde{\boldsymbol{H}}$ and the randomized trace estimator error (error_1) and the randomized SVD error (error_2) with the number terms N. Left: at the initial control. Right: at the optimal control.

Computation of the derivative of $\hat{T}(\tilde{\mathcal{H}}_m)$ wrt control z

- Recall the trace estimation

$$\hat{T}(\tilde{\mathcal{H}}_m) = \sum_{j=1}^{N} \lambda_j(\tilde{\mathcal{H}}_m) \text{ and } \hat{T}(\tilde{\mathcal{H}}_m^2) = \sum_{j=1}^{N} \lambda_j^2(\tilde{\mathcal{H}}_m)$$

- Eigenvalue sensitivity equation: find (λ_j', ϕ_j') s.t. $\forall \phi \in \mathcal{M}$,

$$\langle \phi, \mathcal{H}_m'(m_0)\psi_j \rangle + \langle \phi, \mathcal{H}_m(m_0)\psi_j' \rangle = \lambda_j' \langle \phi, \mathcal{C}^{-1}\psi_j \rangle + \lambda_j \langle \phi, \mathcal{C}^{-1}\psi_j' \rangle$$

  where $'$ represents the derivative w.r.t. z
- Setting $\phi = \psi_j$, and noting $\langle \psi_j, \mathcal{C}^{-1}\psi_j \rangle = 1$ as well as symmetry of $\mathcal{H}_m(m_0)$ and $\mathcal{C}^{-1}$, we obtain the expression for the eigenvalue sensitivity in terms of the Hessian derivative,

$$\lambda_j' = \langle \psi_j, \mathcal{H}_m'(m_0)\psi_j \rangle,$$

  which allows us to compute the gradient of $\text{tr}(\tilde{\mathcal{H}}_m)$ at any optimization iteration at a cost of $N + p$ pairs of linearized forward/adjoint PDE solves
- Similarly, the gradient of $\text{tr}(\tilde{\mathcal{H}}_m^2)$ can be computed with

$$(\lambda_j^2)' = 2\lambda_j\lambda_j' = 2\langle \psi_j, \mathcal{H}_m(m_0)\,\psi_j \rangle \, \langle \psi_j, \mathcal{H}_m'(m_0)\,\psi_j \rangle.$$

  where we have used the fact $\lambda_j = \langle \psi_j, \mathcal{H}_m(m_0)\,\psi_j \rangle$.

Taylor approximation as a variance reduction

- Statistics computed by Taylor approximations may be **biased**
- Use Monte Carlo quadrature to correct Taylor approximation, e.g.,

$$\mathbb{E}[Q] = \mathbb{E}[Q_{\text{lin}}] + \mathbb{E}[\underbrace{Q - Q_{\text{lin}}}_{Y}] \approx Q(m_0) + \underbrace{\hat{Y}}_{\text{MC estimator}}$$

  Similar MC correction for quadratic approximation Q_{quad}
- Mean squared error (MSE) of MC estimate of $\mathbb{E}[Q]$ and $\mathbb{E}[Y]$

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

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

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

  provided Q_{lin} is a good approximation of (i.e., highly correlated to) Q
- see Multifidelity Monte Carlo work of Karen Willcox et al.

Turbulent jet model with embedded inadequacy

Estimation of $\mathbb{E}[q]$ using Monte Carlo and variance reduction Monte Carlo where $\mathsf{E}[q_{\mathsf{lin}}] = q(\bar{m})=$ 1.04854; $\mathsf{E}[q_{\mathsf{quad}}] = q(\bar{m}) + \frac{1}{2}\mathsf{tr}\left[\tilde{\mathcal{H}}_m\right] \approx$ 1.04825.

	$\widehat{q}$	$\mathsf{E}[q_{\mathsf{lin}}] + \widehat{Y}_{\mathsf{lin}}$	$\mathsf{E}[q_{\mathsf{quad}}] + \widehat{Y}_{\mathsf{quad}}$
$\mathsf{E}[q]$	1.04800	1.04817	1.04818
MSE	1.3168E-06	5.1655E-08	1.1868E-08
N	100	100	100

Sample variance and number N of MC samples to obtain an accuracy $\tau = 10^{-4}$

	q	Y_{lin}	Y_{quad}
variance	1.3168E-04	5.1655E-06	1.1868E-06
N	13168	516	119

Variance reduction with low-rank-Hessian-based quadratic approximation of parameter-to-QoI map leads to 100X reduction in # of Monte Carlo samples for 5151-dimensional uncertain inputs.

Conclusions

- Scalable computational framework based on Taylor approximation and variance reduction for PDE-constrained optimal mean-var control
- Cost of objective/gradient evaluation measured in PDE solves is independent of parameter dimension when covariance preconditioned Hessian is a compact operator
- Randomized SVD is more efficient than randomized trace estimator; gradient computed via eigenvalue sensitivity at no additional cost in PDE solves
- Taylor approximation used as control variate leads to 100X reduction in MC samples and unbiased estimate

A. Alexanderian, N. Petra, G. Stadler, O. Ghattas, *Mean-variance risk-averse optimal control of systems governed by PDEs with random coefficient fields using local approximations*. arXiv:1602.07592, 2016.

P. Chen, U. Villa, O. Ghattas, *Taylor approximation and variance reduction for PDE-constrained optimal control under uncertainty*. Preprint, 2017.

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