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Scalable Algorithms and Software for PDE-Constrained Optimization Under Uncertainty

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Motivation

Optimization formulations

From expectation to risk and back

Inexact trust-region algorithms

Software

Numerical results

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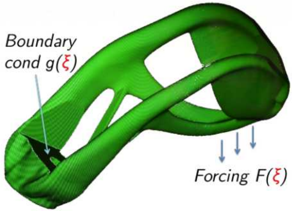
Topology Optimization for Structural Design

RISK-AVERSE DESIGN OF STRUCTURES



Setup: The forcing or load $F(\xi)$ on the right part of the bracket is uncertain. Additionally, there is an uncertain Dirichlet condition on the displacement at the bolt location, see $g(\xi)$.

Given volume fraction $V_0 \in (0,1)$, max compliance η, $\Omega \subset \mathbb{R}^3$,

$$\underset{0 \le z \le 1}{\text{Minimize}} \ \text{Prob}\left[\int_\Omega F(\xi,x)\cdot(U(z))(\xi,x)\,dx \ge \eta\right]$$

s.t. $\int_\Omega z(x)\,dx \le V_0|\Omega|$, where $U(z) = u : \Xi \to (H^1(\Omega))^3$ solves

$$-\nabla\cdot(\mathbf{E}(z) : \epsilon u(\xi)) = F(\xi), \qquad \text{in } \Omega, \text{ a.s.}$$

$$\epsilon u(\xi) = \frac{1}{2}(\nabla u(\xi) + \nabla u(\xi)^\top), \qquad \text{in } \Omega, \text{ a.s.}$$

$$u(\xi) = g(\xi), \qquad \text{on } \partial\Omega, \text{ a.s.}$$

- Uncertainty in external forces (loads) and boundary conditions.
- Reliability formulation of the compliance objective: Compute light-weight designs that reduce the probability of structural failure.

Optimal Control of Thermal Fluids

RISK-AVERSE CONTROL OF DYNAMICAL MULTIPHYSICS SYSTEMS

$$\underset{a(t) \le z(t) \le b(t)}{\text{Minimize}} \; \text{Risk}\left(\int_{\Omega_R} |\nabla \times (\mathbf{U}(z))(\xi, x, \tau^{\text{final}})|^2 dx \right)$$

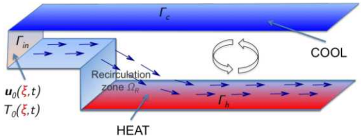
where $\mathbf{U}(z) = \mathbf{u} : \Xi \to (H^1(\Omega))^3 \times L^2([0, \tau^{\text{final}}])$ solves

$$\frac{\partial \mathbf{u}(\xi)}{\partial t} - \nu_1 \Delta \mathbf{u}(\xi) + (\mathbf{u}(\xi) \cdot \nabla)\mathbf{u}(\xi) + \nabla p(\xi) + \nu_2 T(\xi)\mathbf{g} = 0$$

$$\frac{\partial T(\xi)}{\partial t} - \nu_3 \Delta T(\xi) + \mathbf{u}(\xi) \cdot \nabla T(\xi) = 0$$

a.s., and $\nabla \cdot \mathbf{u}(\xi) = 0$, in $\Omega \times [0, \tau^{\text{final}}]$, with BCs $\mathbf{u} = \mathbf{u}_0(\xi, t)$ and $T = T_0(\xi, t)$ on $\Gamma_{\text{in}} \times [0, \tau^{\text{final}}]$, etc., and heat-flux control $z(t) = z$ satisfying

$$\frac{\partial T(\xi)}{\partial \mathbf{n}} = h(z - T(\xi)) \quad \text{on } \Gamma_h \text{ and } \Gamma_c.$$



Setup: The velocity field and temperature at the inlet Γ_{in} are time dependent and uncertain, see $\mathbf{u}_0(\xi, t)$ and $T_0(\xi, t)$. A time dependent temperature control $z(t)$ is applied on the top and bottom boundaries, Γ_c and Γ_h, to create thermal flow counteracting the vortex in the recirculation zone Ω_R.

- Uncertainty in the velocity field and temperature at the inlet.
- A thermal fluid system with time-dependent temperature control.

Challenges

- **Function-space** optimization of **PDEs with random inputs**.
- **Large-scale** numerical optimization.
- **Large-dimensional** spaces of **uncertain** parameters.
- **Risk functions**: mathematics, computational cost, usefulness.
- **Nonsmooth** objective functions and constraints.
- **Time consistency** for optimal control of dynamical systems.

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★ **Identify a computational core and discuss algorithms** ...
for nonlinear nonconvex constraints and objective functions.

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Full space and Reduced space

$$\min_{u \in U, z \in Z} \{\mathcal{R}(J_F(u, z; \xi)) + \wp(z)\}$$

subject to $c(u, z; \xi) = 0$ a.s.

$$\min_{z \in Z} \{\mathcal{R}(J_R(S(z; \xi), \xi)) + \wp(z)\}$$

a.s.:	almost surely
Probability Space:	$(\Omega, \mathcal{F}, \mathbb{P})$ where $\mathcal{F} \subseteq 2^\Omega$ and $\mathbb{P} : \mathcal{F} \to [0, 1]$
Uncertain Inputs:	$\xi : \Omega \to \Xi$ where $\Xi := \xi(\Omega) \subseteq \mathbb{R}^m$
Random Variable Space:	$\mathcal{X}$ is a space of random variables
Deterministic State Space:	U is a Hilbert space
Control Space:	Z is a Hilbert space (deterministic)
Numerical Surrogate:	$\mathcal{R} : \mathcal{X} \to \mathbb{R} \cup \{\infty\}$
Uncertain Objectives:	$J_R : U \times \Xi \to \mathcal{X}$; $J_F : U \times Z \times \Xi \to \mathcal{X}$
Random Field PDE Solution:	$S : Z \times \Xi \to U$ with $c(S(z), z; \xi) = 0$ a.s.
Control Penalty:	$\wp : Z \to \mathbb{R} \cup \{\infty\}$

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Modeling Risk

What is risk? . . .

In our optimization problems, $J_R(S(z;\xi),\xi)$ and $J_F(u,z;\xi)$ are **risks**!

We **cannot** directly minimize J_R and J_F. Range space: random variables!

We must **quantify**, i.e., **scalarize risk**.

- **Risk-Neutral Stochastic Programming:** Minimize *on average*

$$\mathcal{R}(X) = \mathbb{E}[X].$$

- **Risk-Averse Stochastic Programming:** Model *risk preference*

$$\mathcal{R}(X) = \mathbb{E}[X] + c\mathbb{E}[(X - \mathbb{E}[X])_+^p]^{1/p}.$$

- **Probabilistic Optimization:** Minimize the *probability of loss*

$$\mathcal{R}(X) = \mathbb{P}(X > \tau).$$

- **Stochastic Orders:** Model risk preference with a *benchmark Y*

$$\mathbb{P}(X \leq x) \leq \mathbb{P}(Y \leq x) \quad \forall x \in \mathbb{R}.$$

Measuring Risk

Optimized Certainty Equivalents (Ben Tal & Teboulle, 2007, Math. Fin.)

$$\mathcal{R}(X) = \inf_{t\in\mathbb{R}}\{t + \mathbb{E}[v(X-t)]\}$$

where $v : \mathbb{R} \to \mathbb{R}$ is a convex **regret** function that satisfies

$$v(0) = 0, \quad v(x) > x \quad \forall\, x \neq 0.$$

A functional $\mathcal{H} : \mathcal{X} \to \mathbb{R} \cup \{\infty\}$ is a **coherent** measure of risk if

- **Subadditivity:** $\mathcal{H}(X + X') \leq \mathcal{H}(X) + \mathcal{H}(X')$.
- **Monotonicity:** $X \geq X'$ a.e. $\implies \mathcal{H}(X) \geq \mathcal{H}(X')$.
- **Translation Equivariance:** $\mathcal{H}(X + t) = \mathcal{H}(X) + t, \quad \forall t \in \mathbb{R}$.
- **Positive Homogeneity:** $\mathcal{H}(tX) = t\mathcal{H}(X), \quad \forall t > 0$.

Properties: $\mathcal{R}$ is convex and translation equivariant.

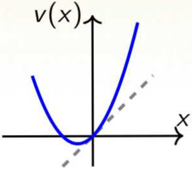
$\mathcal{R}$ is **positive homogeneous** $\iff$ v is piecewise linear with kink at 0

$\mathcal{R}$ is **monotonic** $\iff$ v is nondecreasing

Risk Measure Examples

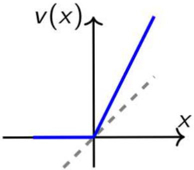
Mean-Plus-Variance: Not monotonic

$$\mathcal{R}(X) = \mathbb{E}[X] + c\mathbb{E}[|X - \mathbb{E}[X]|^2]$$
$$v(x) = x + cx^2$$



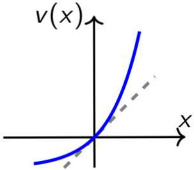
Conditional value-at-risk: Coherent, not diff'ble

$$\mathcal{R}(X) = \inf_{t \in \mathbb{R}} \left\{ t + \frac{1}{1-\beta}\mathbb{E}[(X-t)_+] \right\}$$
$$v(x) = \frac{1}{1-\beta}(x)_+$$



Entropic Risk: Not coherent, derivative not Lipschitz

$$\mathcal{R}(X) = c^{-1} \log \mathbb{E}[\exp(cX)]$$
$$v(x) = (\exp(cx) - 1)/c$$



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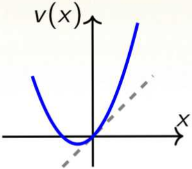

$$\mathcal{R}(X) = \mathbb{E}[X] + c\mathbb{E}[|X - \mathbb{E}[X]|^2]$$
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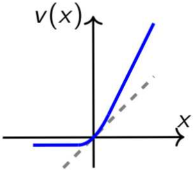
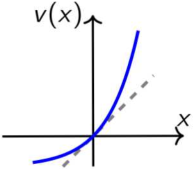
Smoothed CVaR: **Not positive homogeneous**



$$\mathcal{R}(X) = \inf_{t\in\mathbb{R}} \{t + \mathbb{E}[v(X - t)]\}$$

$$v(x) = \begin{cases} -\frac{\varepsilon}{2} & \text{if } x \le -\varepsilon \\ \frac{1}{2\varepsilon}x^2 + x & \text{if } x \in \left(-\varepsilon, \frac{\varepsilon\beta}{1-\beta}\right) \\ \frac{1}{1-\beta}\left(x - \frac{\varepsilon\beta^2}{2(1-\beta)}\right) & \text{if } x \ge \frac{\varepsilon\beta}{1-\beta} \end{cases}$$

Entropic Risk: **Not coherent, derivative not Lipschitz**



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Minimizing Expectation

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... and key for minimizing smooth approximations of nonsmooth risk measures.

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... and so for scalable computations we consider:

$$\min_{u\in U, z\in Z} \{\mathbb{E}(J_F(u,z;\xi)) + \wp(z)\}$$
$$\text{subject to } \; c(u,z;\xi) = 0 \; \text{ a.s.}$$

$$\min_{z\in Z} \{\mathbb{E}(J_R(S(z;\xi),\xi)) + \wp(z)\}$$

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... and generalize to solving smooth NLPs:

$$\min_{x \in X := \{U \times Z \times \Xi\}} J(x)$$
$$\text{subject to } c(x) = 0$$

CONSTRAINED MINIMIZATION

$$\min_{z \in Z} \mathcal{J}(z)$$

UNCONSTRAINED MINIMIZATION

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Trust Regions for Unconstrained NLPs

Given: z_0, $m_0(s) \approx \mathcal{J}(z_0 + s)$, $\mathcal{J}_0 \approx \mathcal{J}$, $\Delta_0 \geq 0$, and $\mathtt{gtol} > 0$.
While $\|\nabla m_k(s)\|_Z > \mathtt{gtol}$

1. **Model Update:** Choose a new $m_k(s) \approx \mathcal{J}(z_k + s)$. $\leftarrow$ **Adaptivity**
2. **Step Computation:** Approximate a solution, s_k, to the subproblem

$$\min_{s \in Z} \; m_k(s) \quad \text{subject to} \quad \|s\|_Z \leq \Delta_k.$$

3. **Objective Update:** Choose a new $\mathcal{J}_k(z) \approx \mathcal{J}(z)$. $\leftarrow$ **Adaptivity**
4. **Step Acceptance:** Compute

$$\rho_k = \frac{\mathcal{J}_k(z_k) - \mathcal{J}_k(z_k + s_k)}{m_k(0) - m_k(s_k)}.$$

   If $\rho_k \geq \eta \in (0,1)$, then $z_{k+1} = z_k + s_k$ else $z_{k+1} = z_k$.

5. **Trust Region Update:** Choose a new trust region radius, Δ_{k+1}.

EndWhile

Inexact Gradients and Objective Functions

Kouri, Heinkenschloss, Ridzal, van Bloemen Waanders, 2014, SISC

Inexact Gradients

There exists $c > 0$ independent of k such that

$$\|\nabla m_k(0) - \nabla \mathcal{J}(z_k)\|_Z \leq c \min\{\|\nabla m_k(0)\|_Z, \Delta_k\}$$

(Carter 1989, Heinkenschloss and Vicente 2001).

Inexact Objective Functions

There exists $K > 0$, $\omega \in (0,1)$, and $\theta_r(z,s) \to 0$ as $r \to 0$ such that

$$|(\mathcal{J}(z_k) - \mathcal{J}(z_k + s_k)) - (\mathcal{J}_k(z_k) - \mathcal{J}_k(z_k + s_k))| \leq K\theta_{r_k}(z_k, s_k)$$

$$\theta_{r_k}(z_k, s_k)^{\omega} \leq \eta \min\{(m_k(0) - m_k(s_k)), r_k\}.$$

Here, $\eta > 0$ is tied to algorithmic parameters and $\lim_{k\to\infty} r_k = 0$.
(Carter 1989, Ziems and Ulbrich 2013).

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- **Cannot** compute $\mathcal{J}(z_k)$ and $\nabla \mathcal{J}(z_k)$.

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$$\theta_{r_k}(z_k, s_k)^\omega \leq \eta \min\{(m_k(0) - m_k(s_k)), r_k\}.$$

Here, $\eta > 0$ is tied to algorithmic parameters and $\lim_{k\to\infty} r_k = 0$.
(Carter 1989, Ziems and Ulbrich 2013).

- **Cannot** compute $\mathcal{J}(z_k)$ and $\nabla \mathcal{J}(z_k)$.
- Control errors using **dimension-adaptive sparse grids**, by estimating them on a forward neighborhood of a current index set.

Adaptive sparse grids for the gradient

- Admissible index set $\mathcal{I}_k^{\mathrm{g}} \subset \mathbb{N}^m$ and quadrature approximation of $\mathcal{J}(z) = \mathbb{E}[\, J_R(z;\xi)\,]$, i.e., $\mathcal{J}_{\mathcal{I}_k^{\mathrm{g}}}(z) = \sum_{\mathbf{i}\in\mathcal{I}_k^{\mathrm{g}}} (\delta_1^{i_1} \otimes \cdots \otimes \delta_m^{i_m})[\, J_R(z;\xi)\,]$.
- $\left\| \sum_{\mathbf{i}\notin\mathcal{I}_k^{\mathrm{g}}} (\delta_1^{i_1} \otimes \cdots \otimes \delta_M^{i_M})[\nabla J_R(z;\xi)] \right\|_Z \leq c \min\left\{ \|\nabla \mathcal{J}_{\mathcal{I}_k^{\mathrm{g}}}(z_k)\|_Z, \Delta_k \right\}$

Initialization: Set $\mathbf{i} = (1,\dots,1)$, $\mathcal{A} = \{\mathbf{i}\}$, $\mathcal{O} = \emptyset$, $g_{\mathbf{i}} = (\delta_1^{i_1} \otimes \cdots \otimes \delta_M^{i_M})[\nabla J_R(z_k;\xi)]$ and $\beta = \beta_{\mathbf{i}} = \|g_{\mathbf{i}}\|_{\mathcal{Z}}$, $g = g_{\mathbf{i}}$, and $\mathtt{TOL} = c \min\{\|g\|_Z, \Delta_k\}$.

While $\beta > \mathtt{TOL}$

1. Select $\mathbf{i} \in \mathcal{A}$ corresponding to the largest $\beta_{\mathbf{i}}$
2. Set $\mathcal{A} \leftarrow \mathcal{A} \setminus \{\mathbf{i}\}$ and $\mathcal{O} \leftarrow \mathcal{O} \cup \{\mathbf{i}\}$
3. Update the error indicator $\beta \leftarrow \beta - \beta_{\mathbf{i}}$
4. **For** $\ell = 1,\dots,m$
   1. Set $\mathbf{j} = \mathbf{i} + \mathbf{e}_\ell$
   2. **If** $\mathcal{O} \cup \{\mathbf{j}\}$ is admissible
      1. Set $\mathcal{A} \leftarrow \mathcal{A} \cup \{\mathbf{j}\}$
      2. Set $g_{\mathbf{j}} = (\delta_1^{j_1} \otimes \cdots \otimes \delta_m^{j_m})[\nabla J_R(z_k;\xi)]$
      3. Set $\beta_{\mathbf{j}} = \|g_{\mathbf{j}}\|_{\mathcal{Z}}$
      4. Update the gradient approximation $g \leftarrow g + g_{\mathbf{j}}$
      5. Update the error indicator $\beta \leftarrow \beta + \beta_{\mathbf{j}}$
      6. Update the stopping tolerance $\mathtt{TOL} = c \min\{\|g\|_Z, \Delta_k\}$
   3. **EndIf**
5. **EndFor**

EndWhile

Set $\mathcal{I}_k^{\mathrm{g}} = \mathcal{A} \cup \mathcal{O}$ and $\nabla m_k(0) = g$.

Adaptive sparse grids for the objective

- $\left|\sum_{\mathbf{i}\notin\mathcal{I}_k^{\circ}}(\delta_1^{i_1}\otimes\cdots\otimes\delta_m^{i_m})[J_R(z_k+s_k;\xi)-J_R(z_k;\xi)]\right| = \theta_k$

Intialization: Set $\mathbf{i}=(1,\ldots,1)$, $\mathcal{A}=\{\mathbf{i}\}$, $\mathcal{O}=\emptyset$, $\mathtt{TOL}=(\eta\min\{\mathrm{pred}_k, r_k\})^{1/\omega}$, $\tilde{\theta}_k=\vartheta_{\mathbf{i}}=(\delta_1^{i_1}\otimes\cdots\otimes\delta_M^{i_M})[J_R(z_k+s_k;\xi)-J_R(z_k;\xi)]$ and $cred_k=\vartheta_{\mathbf{i}}$.

While $|\tilde{\theta}_k|>\mathtt{TOL}$

1. Select $\mathbf{i}\in\mathcal{A}$ corresponding to the largest $|\vartheta_{\mathbf{i}}|$
2. Set $\mathcal{A}\leftarrow\mathcal{A}\setminus\{\mathbf{i}\}$ and $\mathcal{O}\leftarrow\mathcal{O}\cup\{\mathbf{i}\}$
3. Update the error indicator $\tilde{\theta}_k\leftarrow\tilde{\theta}_k-\vartheta_{\mathbf{i}}$
4. **For** $\ell=1,\ldots,m$
    1. Set $\mathbf{j}=\mathbf{i}+\mathbf{e}_\ell$
    2. **If** $\mathcal{O}\cup\{\mathbf{j}\}$ is admissible
        1. Set $\mathcal{A}\leftarrow\mathcal{A}\cup\{\mathbf{j}\}$
        2. Set $\vartheta_{\mathbf{j}}=(\delta_1^{j_1}\otimes\cdots\otimes\delta_m^{j_m})[J_R(z_k+s_k;\xi)-J_R(z_k;\xi)]$
        3. Update the computed reduction $cred_k\leftarrow cred_k+\vartheta_{\mathbf{j}}$
        4. Update the error indicator $\tilde{\theta}_k\leftarrow\tilde{\theta}_k+\vartheta_{\mathbf{j}}$
    3. **EndIf**
5. **EndFor**

EndWhile

Return $\mathcal{I}_k^{\circ}=\mathcal{A}\cup\mathcal{O}$ and $cred_k$.

Trust Regions for Constrained NLPs

Solve equality-constrained optimization problem:

$$\min_{x \in X} \; J(x) \qquad \text{subject to} \qquad c(x) = 0$$

Define Lagrangian functional $L : X \times C \to \mathbb{R}$:

$$L(x, \lambda) = J(x) + \langle \lambda, c(x) \rangle_C$$

If *regular* point x_* is a local solution of the NLP, then there exists a $\lambda_* \in C$ satisfying the *first-order necessary optimality conditions*:

$$\begin{aligned} \nabla_x J(x_*) + c_x(x_*)^* \lambda_* &= 0 \\ c(x_*) &= 0 \end{aligned}$$

Solve a sequence of *nonconvex* quadratic trust-region subproblems:

$$\begin{aligned} \min_{s \in X} \quad & \frac{1}{2} \langle \nabla_{xx} L(x_k, \lambda_k) s, s \rangle_X + \langle \nabla_x L(x_k, \lambda_k), s \rangle_X + L(x_k, \lambda_k) \\ \text{s.t.} \quad & c_x(x_k) s + c(x_k) = 0 \,, \quad \|s\|_X \le \Delta_k \end{aligned}$$

Possible incompatibility of constraints: composite-step approach.

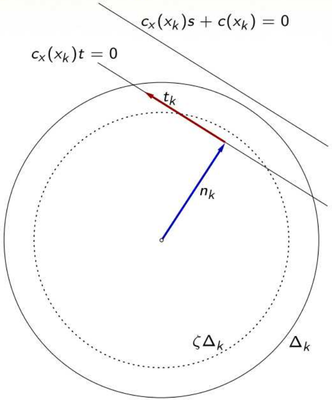
Composite-step Approach for the Solution of the Trust-region Subproblem

- **Trust-region step**:
  $s_k = n_k + t_k$

- **Quasi-normal step** n_k:
  reduces linear infeasibility

$$\min_{n\in X} \quad \|c_x(x_k)n + c(x_k)\|_C^2$$
$$\text{s.t.} \quad \|n\|_X \le \zeta\Delta_k$$

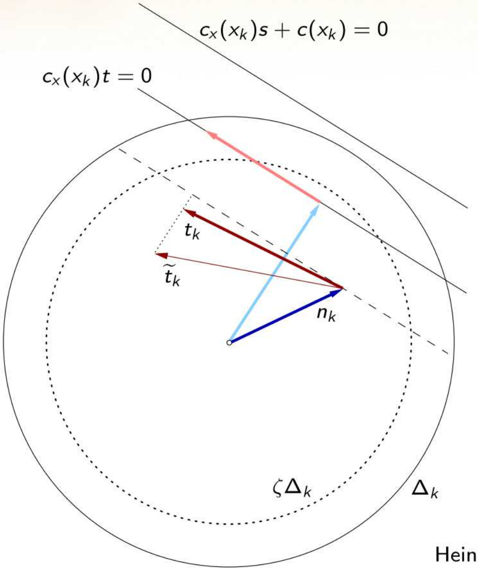
- **Tangential step** t_k:
  improves optimality while staying in the null space of the linearized constraints



$$\min_{t\in X} \quad \frac{1}{2}\langle \nabla_{xx}L(x_k,\lambda_k)(t+n_k), t+n_k\rangle_X + \langle \nabla_x L(x_k,\lambda_k), t+n_k\rangle_X + L(x_k,\lambda_k)$$
$$\text{s.t.} \quad c_x(x_k)t = 0, \quad \|t+n_k\|_X \le \Delta_k$$

Omojokun (1989), Byrd, Hribar, Nocedal (1997), Dennis, El-Alem, Maciel (1997)

Matrix-free Composite-step Algorithm

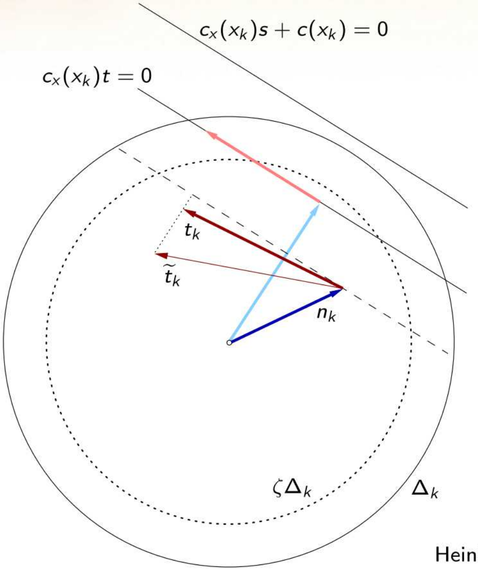


Composite step: $s_k = n_k + t_k$

1. Compute quasi-normal step n_k using **Powell's dogleg method**, satisfying inexactness conditions.
2. Solve tangential subproblem for $\widetilde{t}_k$ with **projected Steihaug-Toint CG**, satisfying inexactness conditions.
3. Restore linearized feasibility, yielding tangential step t_k.
4. Update Lagrange multipliers λ_{k+1}.
5. Evaluate progress.

Heinkenschloss, Ridzal, *SIAM J. Opt. (2014)*

Matrix-free Composite-step Algorithm



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Inexactness is interpreted in the context of linear systems, and their iterative solution.

Heinkenschloss, Ridzal, *SIAM J. Opt. (2014)*

Linear Systems

... are all augmented constraint systems

$$\begin{pmatrix} I & c_x(x_k)^* \\ c_x(x_k) & 0 \end{pmatrix} \begin{pmatrix} y^1 \\ y^2 \end{pmatrix} = \begin{pmatrix} b^1 \\ b^2 \end{pmatrix} + \begin{pmatrix} e^1 \\ e^2 \end{pmatrix}$$

- The size of $(e^1 \; e^2)$ is governed by various model reduction conditions, i.e., the progress of the optimization algorithm:

$$\|e^1\|_X + \|e^2\|_C \leq \text{func}\left(\|b^1\|_X, \|b^2\|_C, \|y^1\|_X, \Delta_k, \xi\right)$$

- **Preconditioning** for $X = U \times Z$ with $c_x(x_k) = C_x = [C_u \;\; C_z]$:

$$\begin{pmatrix} I_U & 0 & C_u^* \\ 0 & I_Z & C_z^* \\ C_u & C_z & 0 \end{pmatrix} \longrightarrow \mathcal{P} = \begin{pmatrix} I_U & 0 & 0 \\ 0 & I_Z & 0 \\ 0 & 0 & C_u^{-*} C_u^{-1} \end{pmatrix}$$

Semi-discretization for the Expected Value

- We approximate $\mathbb{E}[X] = \int_\Xi \rho(\xi) X(\xi) \mathrm{d}\xi$ with the quadrature $\mathbb{E}_Q$,

$$\mathbb{E}_Q[X] = \sum_{k=1}^{Q} w_k X(\xi_k), \text{ with points } \{\xi_1, ..., \xi_Q\}, \text{ weights } \{w_1, ..., w_Q\}.$$

- Our semi-discrete optimization problem is

$$\underset{u_1,\dots,u_Q \in U,\, z \in Z}{\text{minimize}} \sum_{k=1}^{Q} w_k J_F(u_k, z) \quad \text{subject to} \quad c(u_k, z; \xi_k) = 0,\ k = 1, ..., Q$$

- Family of possible Lagrangians $L_Q : U^Q \times Z \times U^Q \to \mathbb{R} \cup \{\infty\}$,

$$L(u_1, ..., u_Q, z, \lambda_1, ..., \lambda_Q) = \sum_{k=1}^{Q} w_k J_F(u_k, z) + \sum_{k=1}^{Q} v_k \langle \lambda_k, c(u_k, z; \xi_k) \rangle_C,$$

governed by the choice of weights $\{v_k\}_{k=1}^{Q}$. Two choices are:

— $v_k = 1$, $k = 1, ..., Q$, for a "finite-dimensional" view; and

— $v_k = w_k$, $k = 1, ..., Q$, for an "infinite-dimensional" view.

Augmented System for Minimizing Expectation

$$\begin{pmatrix}
I_U & 0 & \dots & 0 & 0 & v_1(C_u^1)^* & 0 & \dots & 0 \\
0 & I_U & \dots & 0 & 0 & 0 & v_2(C_u^2)^* & \dots & 0 \\
\vdots & \vdots & \ddots & 0 & \vdots & \vdots & \vdots & \ddots & 0 \\
0 & 0 & \dots & I_U & 0 & 0 & 0 & \dots & v_Q(C_u^Q)^* \\
0 & 0 & \dots & 0 & I_Z & v_1(C_z^1)^* & v_2(C_z^2)^* & \dots & v_Q(C_z^Q)^* \\
v_1 C_u^1 & 0 & \dots & 0 & v_1 C_z^1 & 0 & 0 & \dots & 0 \\
0 & v_2 C_u^2 & \dots & 0 & v_2 C_z^2 & 0 & 0 & \dots & 0 \\
\vdots & \vdots & \ddots & 0 & \vdots & \vdots & \vdots & \ddots & 0 \\
0 & 0 & \dots & v_Q C_u^Q & v_Q C_z^Q & 0 & 0 & \dots & 0
\end{pmatrix}$$

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I_U & 0 & \dots & 0 & 0 & v_1(C_u^1)^* & 0 & \dots & 0 \\
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0 & 0 & \dots & 0 & I_Z & v_1(C_z^1)^* & v_2(C_z^2)^* & \dots & v_Q(C_z^Q)^* \\
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0 & v_2 C_u^2 & \dots & 0 & v_2 C_z^2 & 0 & 0 & \dots & 0 \\
\vdots & \vdots & \ddots & 0 & \vdots & \vdots & \vdots & \ddots & 0 \\
0 & 0 & \dots & v_Q C_u^Q & v_Q C_z^Q & 0 & 0 & \dots & 0
\end{pmatrix}
$$

- **Applying the preconditioner $\mathcal{P}$ to this system is scalable, due to the parallelization in block-diagonal operators C_u and $(C_u)^*$.**
- **Inverses of each C_u^i and $(C_u^i)^*$ are applied *very* inexactly.**

Motivation

Optimization formulations

From expectation to risk and back

Inexact trust-region algorithms

Software

Numerical results

Rapid Optimization Library

- Trilinos package for **matrix-free nonlinear optimization**: unconstrained, equality-constrained, inequality-constrained, line searches, trust regions, ...

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ROL

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  - **Risk modeling** based on various concepts: risk neutrality, risk aversion, buffered probability, stochastic orders.
  - Utilities for **statistical estimation**; concept of **risk quadrangle**.
  - **Bring-your-own sampler**, in addition to the default Monte Carlo.
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  - Interface to **Dakota** for sparse grids.
- **If you have a (parametrized) deterministic optimization ready, turning it into stochastic optimization amounts to flipping a few switches in the ROL options file.**

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Optimizing CVD Reactors under Uncertainty

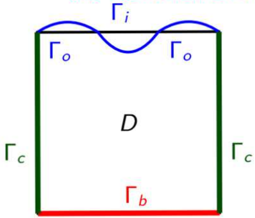
$$\min_{z\in Z} \frac{1}{2}\mathbb{E}\left[\int_D (\nabla \times u(z))\,\mathrm{d}x\right] + \frac{\gamma}{2}\int_{\Gamma_c} |z|^2\,\mathrm{d}x$$

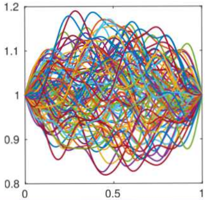
where $S(z) = (u(z), p(z), T(z))$ solves the Boussinesq flow equations,

$$\begin{aligned}
-\nu(\xi)\nabla^2 u + (u\cdot\nabla)u + \nabla p + \eta(\xi)Tg &= 0, && && \text{in } D, \text{ a.s.},\\
\nabla\cdot u &= 0, && && \text{in } D, \text{ a.s.},\\
-\kappa(\xi)\Delta T + u\cdot\nabla T &= 0, && && \text{in } D, \text{ a.s.},\\
u - u_i &= 0, && T = 0, && \text{on } \Gamma_i, \text{ a.s.},\\
u - u_o &= 0, && \kappa(\xi)\tfrac{\partial T}{\partial n} = 0, && \text{on } \Gamma_o, \text{ a.s.},\\
u &= 0, && T = T_b(\xi), && \text{on } \Gamma_b, \text{ a.s.},\\
u &= 0, && \kappa(\xi)\tfrac{\partial T}{\partial n} + h(\xi)(z - T) = 0, && \text{on } \Gamma_c, \text{ a.s.},
\end{aligned}$$

where $\Gamma_i = [1/3, 2/3]\times\{1\}$, $\Gamma_o = ([0,1/3]\cup[2/3,1])\times\{1\}$, $\Gamma_b = [0,1]\times\{0\}$ and $\Gamma_c = \{0,1\}\times[0,1]$. The inflow and outflow velocities, u_i and u_o are deterministic while the coefficients ν, η, κ, h and T_b are uncertain.

Comput. domain D.





Scenarios of T_b (Brownian bridge-like).

Optimizing CVD Reactors under Uncertainty

- **Uncertain variables:**

$$\nu = \frac{1}{\mathrm{Re}} = \frac{100}{1+0.01\xi_{N+1}}, \quad \eta = \frac{\mathrm{Gr}}{\mathrm{Re}^2} = 0.72\frac{1+0.01\xi_{N+1}}{1+0.01\xi_{N+2}},$$
$$\text{and} \quad \kappa = \frac{1}{\mathrm{Re}\,\mathrm{Pr}} = 10^5\frac{1+0.01\xi_{N+3}}{(1+0.01\xi_{N+1})^2}$$

  where Re is the Reynolds number, Gr is the Grashof number and Pr is the Prandtl number.

- The offset N is the total number of random variables associated with T_b and h. The uncertainty in T_b is modeled by the expansion

$$T_b(x,\xi) = 1 + 0.025\sum_{k=1}^{n_b}\xi_k\frac{\sqrt{2}\sin(\pi kx)}{\pi k}.$$

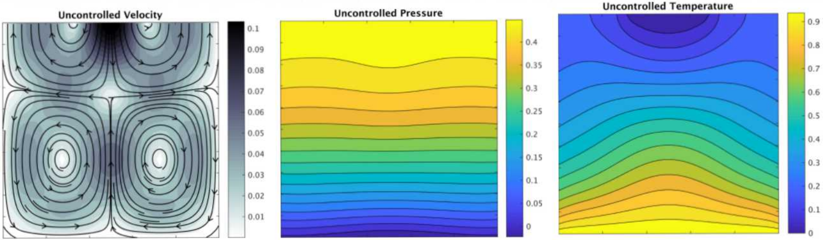
  The coefficient h has a similar expansion for $x=0$ and for $x=1$ with n_ℓ and n_r terms respectively. **All ξ_k are uniformly distributed on $[-1,1]$.**

- The curves on the top of the computational domain schematic are the inflow and outflow profiles of the velocity, given by

$$u(x) = \begin{cases} 2\left(\frac{1}{3}-x\right)x & \text{if } 0 \le x \le \frac{1}{3} \\ -4\left(x-\frac{1}{3}\right)\left(\frac{2}{3}-x\right) & \text{if } \frac{1}{3} < x < \frac{2}{3} \\ 2\left(x-\frac{2}{3}\right)(1-x) & \text{if } \frac{2}{3} \le x \le 1 \end{cases}.$$

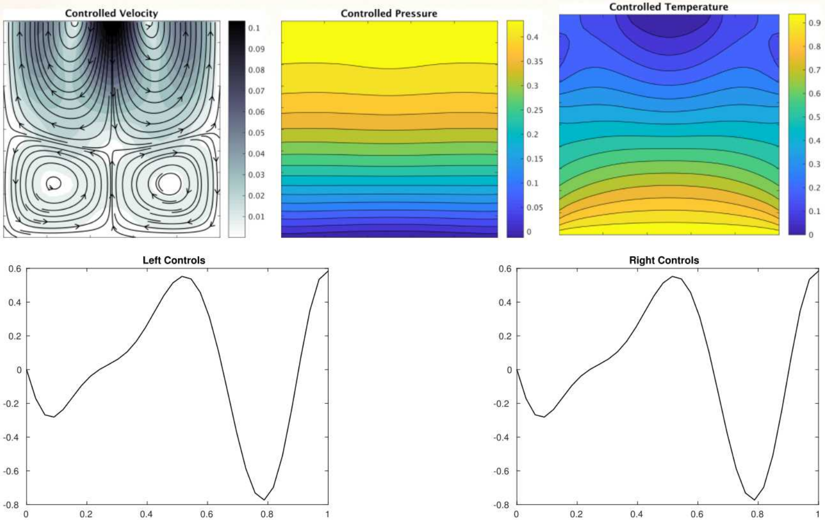
Uncontrolled State

Expected values of the uncontrolled velocity field (left), pressure (middle) and temperature (right):



- Finite elements on a uniform mesh of 33×33 quadrilaterals.
- For the velocity and pressure, Q2-Q1 Taylor-Hood finite element pair; for the temperature, Q2 finite element.
- Sparse grids built on one-dimensional Clenshaw-Curtis quadrature.
- Maximum sparse grid: level-3 isotropic Clenshaw-Curtis, $Q = 2245$ points.
- Implemented in ROL, PDE-OPT Application Development Kit.

Reduced Space: Sparse-grid Adaptivity



Optimal controls along the left vertical side wall (left image) and the right vertical side wall (right image) of the problem domain D.

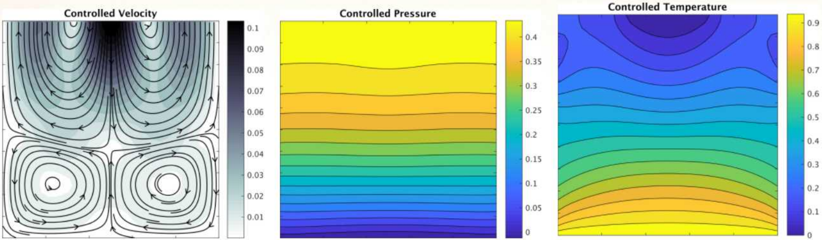
Reduced Space: Sparse-grid Adaptivity

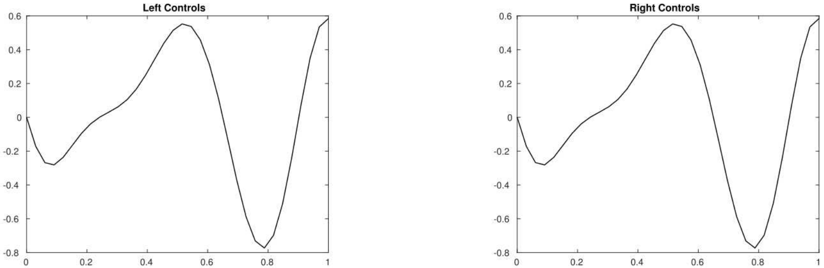
iter	$\mathcal{J}_k(z_k)$	$\lVert\nabla m_k(0)\rVert_Z$	$\lVert s_k\rVert_Z$	Δ_k	cg	accept	obj	grad
0	0.07457916	5.063×10^{-2}	—	10.000	—	—	1	3
1	0.07469930	5.063×10^{-2}	10.000	1.445	1	0	3	3
2	0.07469930	5.063×10^{-2}	1.445	0.361	1	0	3	3
3	0.05636707	4.875×10^{-2}	0.361	0.903	1	1	3	3
4	0.05636707	4.875×10^{-2}	0.903	0.226	1	0	3	3
5	0.04757099	2.059×10^{-2}	0.226	0.226	1	1	3	3
6	0.04680338	1.143×10^{-2}	0.226	0.226	2	1	103	117
7	0.04611002	3.468×10^{-3}	0.226	0.564	2	1	139	195
8	0.04511802	3.255×10^{-3}	0.564	1.411	2	1	117	233
9	0.04494516	1.085×10^{-3}	1.411	3.527	3	1	229	579
10	0.04499733	2.331×10^{-4}	2.838	8.818	6	1	579	949
11	0.04499338	6.211×10^{-5}	0.967	22.045	7	1	2245	1219
12	0.04499329	1.002×10^{-6}	0.127	55.113	8	1	2245	2245
13	0.04499327	7.034×10^{-9}	0.072	137.784	11	1	2245	2245

Iteration history for reduced-space adaptive sparse-grid approach.

- Sequential solution, direct linear solver, single computational core.

Reduced Space: Sparse-grid Adaptivity





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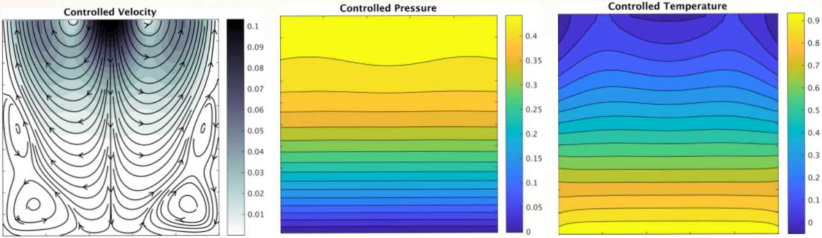
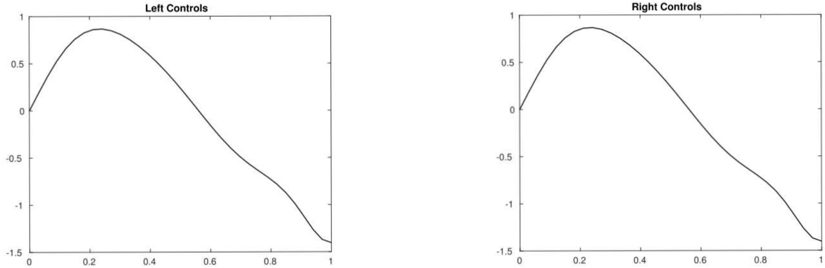
Full Space: Inexact Linear Solvers





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Full Space: Inexact Linear Solvers

- F-GMRES used to solve augmented systems; `tol` $= 10^{-6}$.
- F-GMRES used to solve "inner" linearized forward and adjoint solves, C_u^{-1} and C_u^{-*} in the $\mathcal{P}$ preconditioner; `tol` $= 10^{-4}$.
- Non-overlapping additive Schwarz domain decomposition used to precondition inner solves: 4 subdomains, horizontal strips.
- Infinite-dimensional view of Lagrangian, $v_k = w_k$.
- Full fixed level-3 Clenshaw-Curtis sparse grid.

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- Serrano cluster at Sandia Labs; 80 dual-socket nodes, used 36 cores per core, i.e., 2880 cores total.
- Cores partitioned into 720 groups, for quadrature, with 4 cores each dedicated to iterative linear solver.
- **Hierarchical parallelism enabled through ROL.**

Full Space: Inexact Linear Solvers

iter	$J(x_k)$	$\|c(x_k)\|_C$	$\|\nabla L(x_k, \lambda_k)\|_X$	Δ_k	pcg	accept	ls calls	ls iters
0	0.07484675	7.820623×10^{-15}	8.377793×10^{-3}	1.00×10^{4}	—	—	—	—
1	0.05533699	1.661657×10^{-2}	3.641571×10^{-4}	1.00×10^{4}	11	1	16	597
2	0.03588474	3.052458×10^{-3}	9.338262×10^{-5}	1.00×10^{4}	13	1	33	1292
3	0.03515891	1.017679×10^{-4}	7.117806×10^{-5}	1.00×10^{4}	20	1	56	2303
4	0.03480817	1.444319×10^{-4}	2.439603×10^{-5}	1.00×10^{4}	15	1	75	3108
5	0.03480817	1.444319×10^{-4}	2.439321×10^{-5}	4.08×10^{0}	20	0	98	4157
6	0.03465050	2.237452×10^{-6}	4.364539×10^{-6}	3.03×10^{1}	2	1	104	4438
7	0.03464773	2.716452×10^{-7}	1.042585×10^{-7}	3.03×10^{1}	8	1	116	4989

Iteration history for full-space approach with iterative augmented system solves.

- About 43 F-GMRES iterations per solve; encouraging, considering that the size of the state space is more than 30 million, and that a fairly tight tolerance was used (10^{-6}).
- Many improvements are possible.

Conclusions

- **Expectation minimization** is an important **computational core** for optimization under uncertainty with a variety of risk models.
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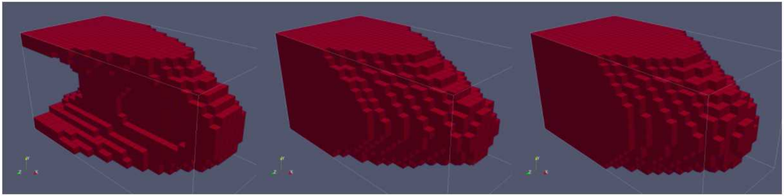
- Working on deploying these algorithms in structural optimization:

Mean Value **Risk Neutral** **Buffered Prob.**



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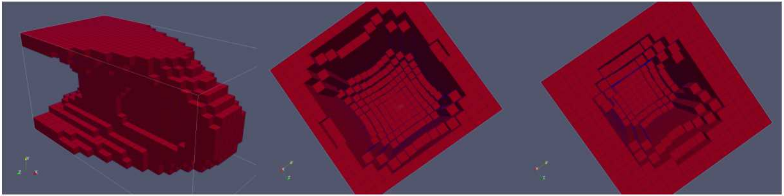

Topology changes from beam to thin shell to thick shell!

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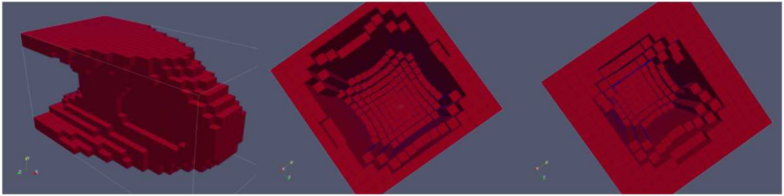

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- For a deep dive, see Drew Kouri's Minitutorial MT8, **Thursday, April 19, 2:30pm-4:30pm, Grand Ballroom G**.