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Risk-Averse Optimization of Large-Scale Multiphysics Systems

D. P. Kouri (PI, Sandia), W. Aquino (Duke), D.Ridzal (Sandia),
R. T. Rockafellar (UFlorida), A. Shapiro (Georgia Tech),
S. Uryasev (UFlorida)

DARPA EQUiPS Phase II Program Update

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Target Optimization Formulations

Goal: Develop *efficient* methods to determine *resilient* optimal controls and designs that *mitigate high-consequence rare events*.

Minimize **probability** *subject to* **risk-adjusted** *constraints:*

$$\min_{z \in Z} p_\tau(S(z)) \quad \text{subject to} \quad \mathcal{R}(J(S(z), z)) \leq c_0$$

Minimize **risk** *subject to* **probabilistic** *constraints:*

$$\min_{z \in Z} \mathcal{R}(J(S(z), z)) \quad \text{subject to} \quad p_\tau(S(z)) \leq p_0$$

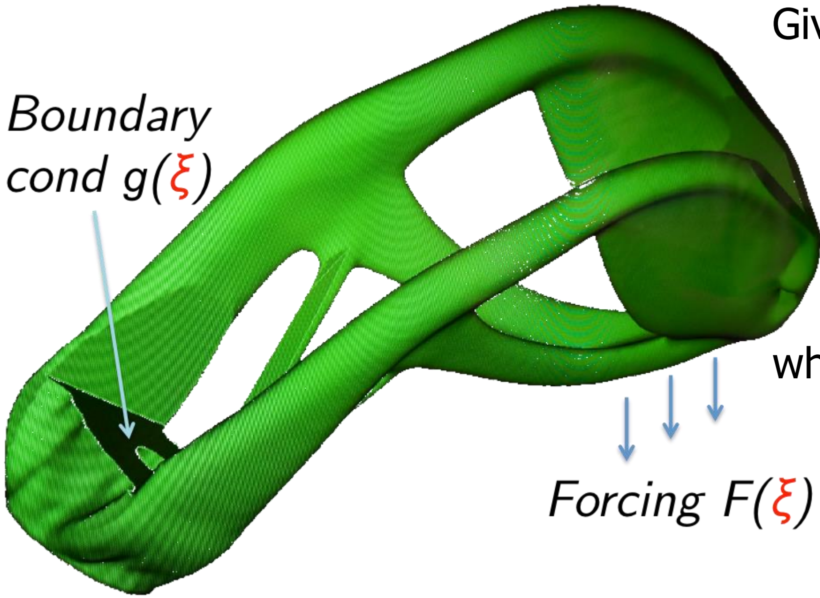
Notation: $z =$ control or design variable

$S(z) =$ solution to system of ODEs/PDEs/DAEs

Tie to EQUiPS Project: Potential to enable risk-averse design of hydrofoils and scram-jet engines

To Date: Risk-averse topology optimization, risk-averse control of chemical vapor deposition reactors

Structural Topology Optimization



Setup: The force 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 compliance tolerance τ, probability $p_0 \in (0,1)$,

$$\min_{0\le z\le 1} \int_D z\,dx =: \mathrm{vol}(z)$$

$$\text{subject to} \quad \mathrm{prob}\left(\left(\int_D F\cdot S(z)\,dx\right)\right) \le p_0$$

where $S(z) = u$ solves the **linear elasticity equations**

$$-\nabla\cdot(E(z):\varepsilon u) = F, \qquad \text{in D}$$

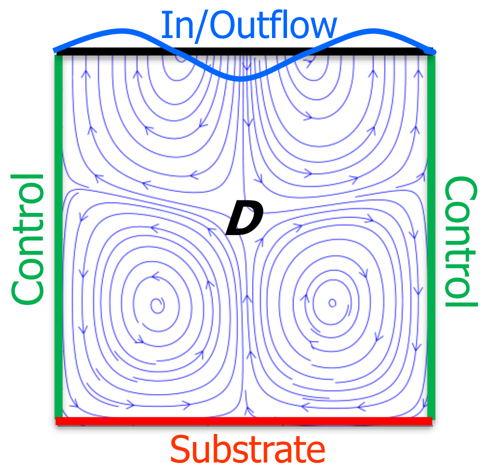
$$\varepsilon u = \tfrac{1}{2}(\nabla u + \nabla u^{\top}), \qquad \text{in } D$$

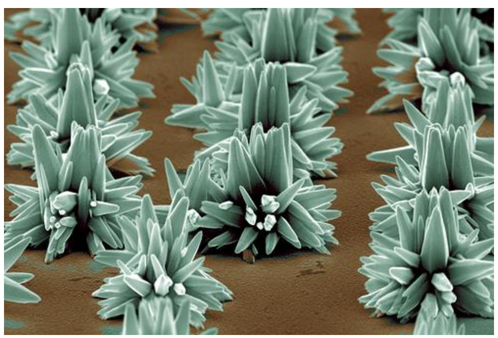
$$u = g, \qquad \text{on } \Gamma_D$$

$$\varepsilon u : n = t, \qquad \text{on } \partial D \setminus \Gamma_D$$

- Uncertain loads, materials, etc. imply displacements are uncertain.
- **Reliability formulation:** Determine light-weight design with *acceptable* probability of failure.
- **Challenge:** Constraints are nonsmooth and expensive to evaluate.

Control of Chemical Vapor Deposition Reactors





Consider the optimal control problem

$$\min_z \frac{1}{2}\mathcal{R}\left(\int_D (\nabla \times U(z))\, dx\right) + \frac{\gamma}{2}\int_{\Gamma_c} |z|^2\, dx$$

Where $S(z) = \big(U(z), P(z), T(z)\big) = (u, p, t)$ solves the **Boussinesq flow equations**

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

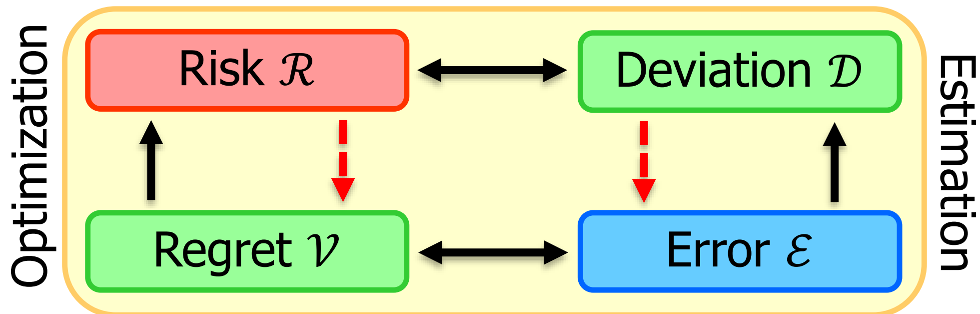
- Uncertain viscosity, thermal conductivity, substrate temperature, etc. imply flow velocity, pressure and temperature are uncertain.
- **Risk-Averse formulation:** Determine wall temperature that minimizes the average of *low-probability*, large vorticity scenarios.
- **Challenge:** Objective function is not differentiable.

Technical Overview

Risk Quadrangle: Connecting optimization and estimation

$$\mathcal{R}(X) = \mathbb{E}[X] + \mathcal{D}(X) = \min_t\{t + \mathcal{V}(X-t)\}$$

$$\mathcal{V}(X) = \mathbb{E}[X] + \mathcal{E}(X)$$

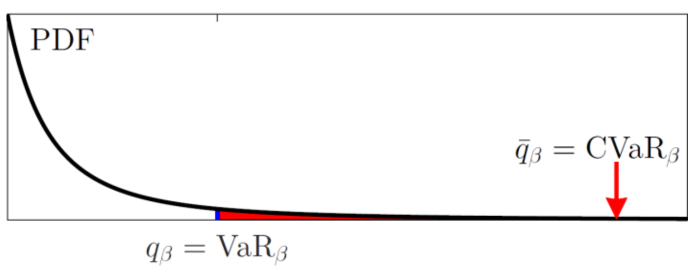


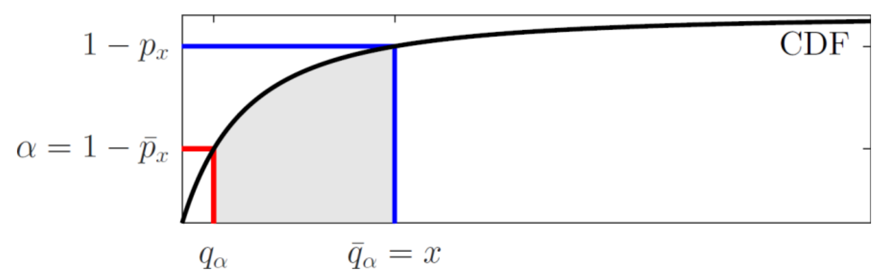
$$\mathcal{D}(X) = \mathcal{R}(X) - \mathbb{E}[X] = \min_t\{\mathcal{E}(X-t)\}$$

$$\mathcal{E}(X) = \mathcal{V}(X) - \mathbb{E}[X]$$

- $\mathcal{R}$ quantifies **hazard** --- Used in optimization as objective function or constraint
- $\mathcal{E}$ quantifies **nonzeroness** --- Used in regression analysis, e.g., polynomial chaos
- $\mathcal{V}$ quantifies **displeasure** for positive values --- Used to define risk via *disutility*
- $\mathcal{D}$ quantifies **nonconstancy** --- Used to define risk via *variability*

Buffered Probability: Conservative surrogate for probability





- $\mathrm{prob}(X > \tau)$ *counts* failures regardless of degree (i.e., magnitude) of failure
- Buffered probability adds *buffer* region to $\{X > \tau\}$ that accounts for **tail weight**

⟶ Has exceptional mathematical properties and is easy to compute

Phase I Accomplishments

1. **Solved a variety of optimization problems with PDE constraints using risk measures, buffered probability and distributionally robust optimization:**
   - Optimal control of incompressible fluid flow with uncertain viscosity and inflow;
   - Topological design of elastic structures subject to random external loads;
   - Optimal control of a counter flow heat exchanger with random conductivities;
   - Optimal contaminant mitigation subject to random sources and advection.
2. **Our research bridges stochastic programming (financial mathematics) and PDE-constrained optimization (engineering design and control):**
   - Developed application-inspired risk measures and applied to the examples above;
   - Established mathematical theory for buffered probability.
3. **Risk-averse and probabilistic optimization is computationally feasible for large-scale multiphysics applications:**
   - Demonstrated with our PDE-OPT application development kit and the risk-averse optimization capabilities in our optimization libraries (ROL and PSG);
   - Exploited high degree of concurrency in the optimization process by parallelizing over samples and linear algebra;
   - Efficiently and accurately evaluated risk of PDE solution dependent quantities of interest using adaptive reduced basis and risk-informed sampling;
   - Efficiently minimized risk using adaptive discrete density estimation, optimization-based sampling and optimization algorithms that exploit inexactness.

Challenge: Risk and BP are *Not* Differentiable

Example: Optimal control of Burger's equation using CVaR

– **Problem size is small:** 1D spatial domain, 4D stochastic domain
– PDE is nonlinear $\implies$ Objective function is not convex
– CVaR risk measure quantifies *tail weight* and is **not** differentiable

Application of an *off-the-shelf* nonsmooth opt. algorithm:

β	0.1	0.5	0.9
# iter	9,740	10,035	10,128

Required $\mathcal{O}(10^8)$ nonlinear and $\mathcal{O}(10^8)$ linearized PDE solves!

Application of smoothed $\mathcal{R}$ with globalized Newton's Method:

Required $\mathcal{O}(10^6)$ nonlinear and $\mathcal{O}(10^7)$ linearized PDE solves!

Solving real world problems is intractable without…

- Better **nonsmooth** optim. Algorithms or **differentiable** $\mathcal{R}$
- **Adaptive/variable fidelity** approx. in physical/stochastic space

Phase II Accomplishments

A risk measure $\mathcal{R}: \mathcal{X} \to \mathbb{R} \cup \{+\infty\}$ is **coherent** if for $X, X' \in \mathcal{X}$ and $t \in \mathbb{R}$

(C1) **Subadditivity:** $\mathcal{R}(X + X') \le \mathcal{R}(X) + \mathcal{R}(X')$, *i.e., diversifying decreases risk*

(C2) **Monotonicity:** $\mathcal{R}(X) \ge \mathcal{R}(X')$ when $X \ge X'$ a.e., *i.e., small value preference*

(C3) **Translation Equivariance:** $\mathcal{R}(X + t) = \mathcal{R}(X) + t$, *i.e., deterministic is riskless*

(C4) **Positive Homogeneity:** $\mathcal{R}(tX) = t\mathcal{R}(X), \forall t > 0$, *i.e., permit change of units*

$\mathcal{R}$ is **coherent** $\iff$ $\mathcal{R}(X) = \max_{\vartheta \in \mathfrak{A}} \mathbb{E}[\vartheta X]$

$\mathcal{R}(X)$ is a **worst-case** expected value $\longrightarrow$ Often **not** differentiable!

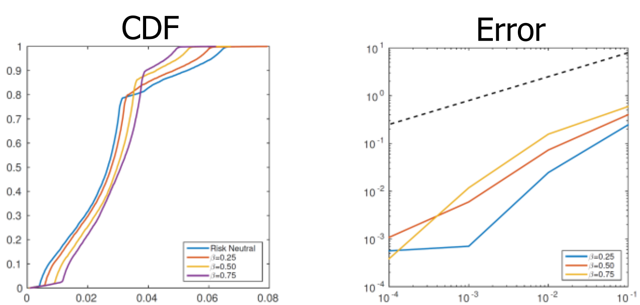
Epi-Regularized Risk Measures:

1. Smooth risk measure by regularizing the worst-case expectation

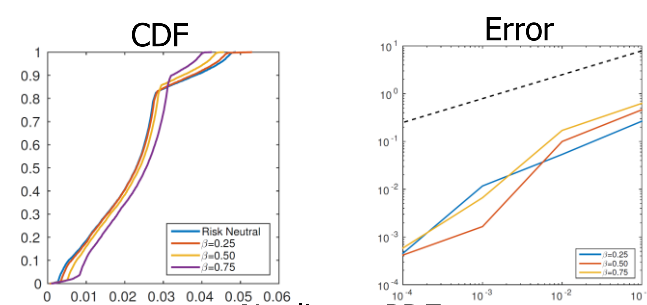
$$\mathcal{R}_\varepsilon(X) := \min_{Y \in \mathcal{X}} \{\mathcal{R}(X - Y) + \varepsilon \Phi(X/\varepsilon)\} = \max_{\vartheta \in \mathfrak{A}} \{\mathbb{E}[\vartheta X] - \varepsilon \Phi^*(\vartheta)\}, \qquad \varepsilon > 0$$

2. $\mathcal{R}_\varepsilon$ satisfies (C1), (C2), (C3), but **not** (C4), i.e., $\mathcal{R}_\varepsilon(tX) = t\mathcal{R}_{\varepsilon/t}(X)$
3. $\mathcal{R}_\varepsilon$ is differentiable $\longrightarrow$ Can minimize using derivative-based optimization

Results: Provable $\mathcal{O}(\sqrt{\varepsilon})$ error, confirmed on nonconvex application!



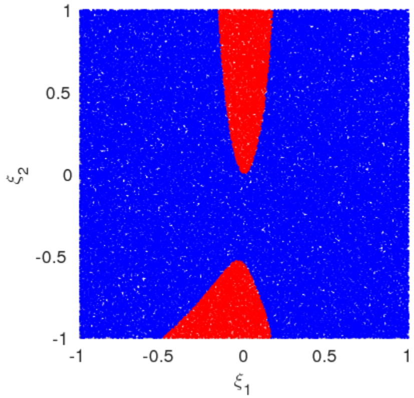
Linear PDE



Nonlinear PDE

Associated with each risk measure $\mathcal{R}$ and r.v. X is a *risk identifier*

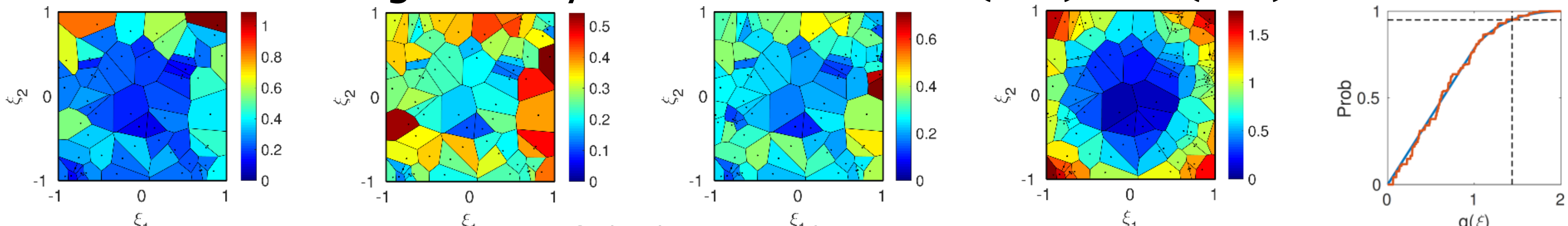
- Illuminates *risky* region in parameter space (red)
- Need accurate approximation of X in risky region
- Use risk identifier to guide adaptive sampling



Adaptive Risk-Informed Modeling:

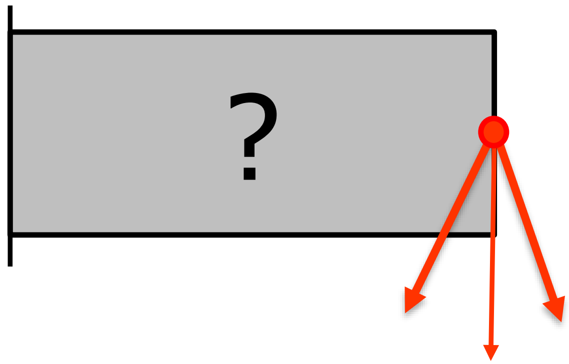
1. Construct local reduced basis models around current samples
$$\bar{u} = \sum_k \mathbb{1}_{\Xi_k} u_k, \text{ where } u_k \text{ is a reduced basis model}$$
2. Evaluate risk-informed QoI error within cell containing sample
$$\left|\mathcal{R}\left(g(u^h)\right) - \mathcal{R}(g(\bar{u}))\right| \leq K \sum_k \max_{\vartheta\in\mathfrak{A}} \mathbb{E}[\vartheta \mathbb{1}_{\Xi_k} \varepsilon_u^\alpha], \ \vartheta \in \mathfrak{A} \text{ are } \textit{risk identifiers}$$
3. Choose new samples based on largest local QoI errors
4. Combine with inexact trust-region algorithm for efficient optimization

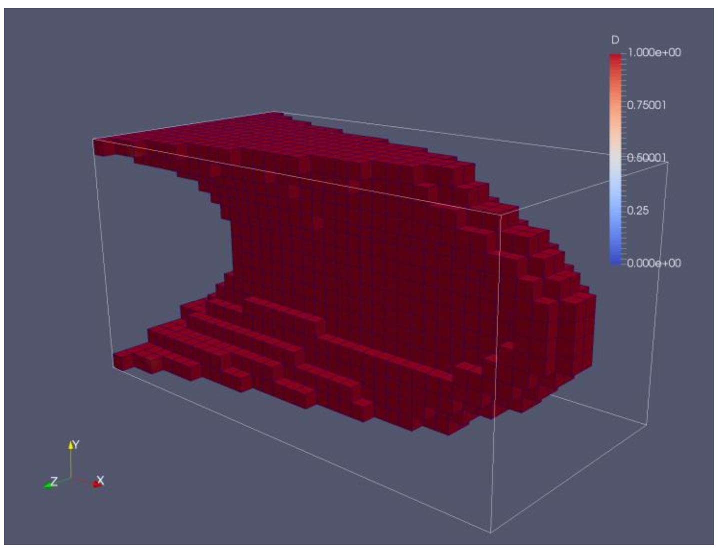
Result: Reduced high-fidelity PDE solves from $\mathcal{O}(10^6)$ to $\mathcal{O}(10^3)$!



3D Results

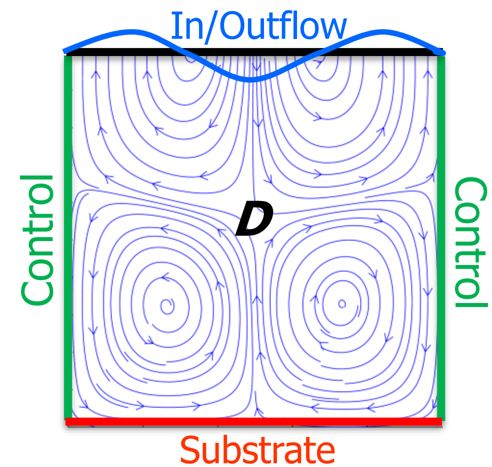
Topology Optimization

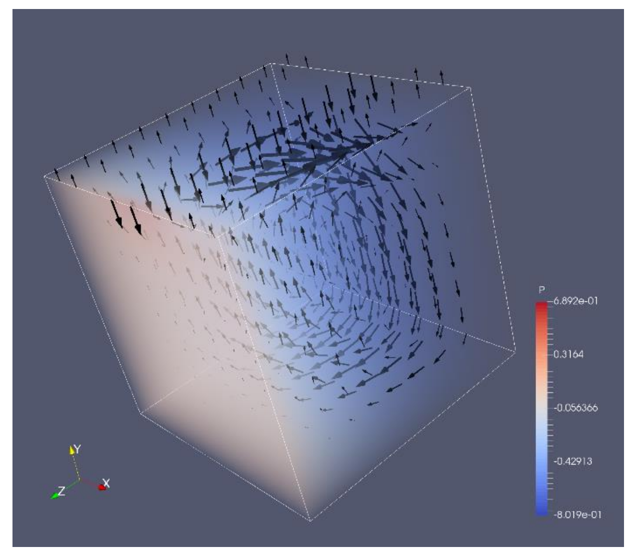




Minimal volume density that satisfies constraint on risk of compliance

Control of CVD Reactor





Controlled velocity (arrows) and pressure (color bar) using entropic risk.

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