Chance constrained PDE-constrained optimal design strategies under high-dimensional uncertainty

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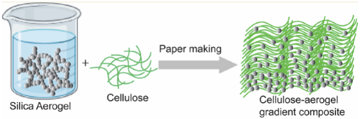
Data-Enabled Predictive Modeling, Scientific Machine Learning, and Uncertainty Quantification in Computational Mechanics

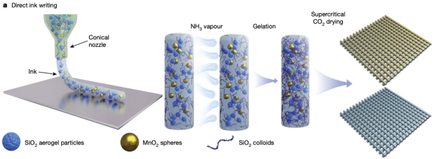
PCELab
Predictive Computational Engineering

Motivation

Silica Aerogel: High-performance materials for next-generation building insulation.

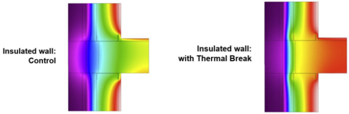


Synthesis of aerogel-cellulose composite [1]



Additive manufacturing by direct ink writing [2]

Thermal breaks: insulating components for **Net-Zero buildings**.



Effect of thermal break[3]

Design problem: finding optimal spatial distribution of materials under uncertainty

[1]Sarkar, Singh, Zhu, Faghihi, Ren, 2024, ACS Appl. Energy Mater

[2]Zhao, Siqueira, Drdova, 2020, Nature .

[3]Susorova et al., Buildings, 2016

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Outline

Forward Model

Thermomechanical continuum model:

$$\mathcal{R}(\boldsymbol{u}, \boldsymbol{\theta}, \boldsymbol{\zeta}) = 0$$

Thermal Model

$$\boxed{\begin{aligned} \rho_s \phi_s c_s \frac{\partial \theta_s}{\partial t} &= \nabla \cdot (\phi_s \kappa_s \nabla \theta_s) - h(\theta_s - \theta_f) \\ \rho_f \phi_f c_f \frac{\partial \theta_f}{\partial t} &= \nabla \cdot (\phi_f \kappa_f \nabla \theta_f) + h(\theta_s - \theta_f) \end{aligned}}$$

Mechanical Model

$$\boxed{\begin{aligned} C \frac{\partial p}{\partial t} + \frac{\partial}{\partial t}(\nabla \cdot \mathbf{u}_s) - \nabla \cdot k \nabla p &= 0 \\ \nabla \cdot \mathbf{T}_s(\mathbf{u}_s) &= 0 \\ \text{where,} \quad & \\ \mathbf{T}_s &= -\phi_s\, p\mathbf{I} + \mathbf{T}_s' \\ \mathbf{T}_s' &= 2\,\mu\,\mathbf{E}_s + \lambda\,\mathrm{tr}(\mathbf{E}_s)\mathbf{I} \end{aligned}}$$

States $\boldsymbol{u} = (\theta_s, \theta_f, \boldsymbol{u_s}, p) \rightarrow$ solid/fluid temperature, solid displacement, fluid pressure

Parameters $\boldsymbol{\theta} = (\kappa_s, \kappa_f, h, k, C, \mu, \lambda) \rightarrow$ determine from experimental data

Design variables $\boldsymbol{\zeta} = (\phi_s, \phi_f) \rightarrow$ determined to optimize component performance

Sources of uncertainty in $\boldsymbol{\zeta}$:

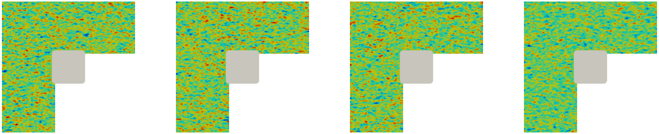
- Limited precision in manufacturing
- Layer-by-layer deposition

Design under Uncertainty

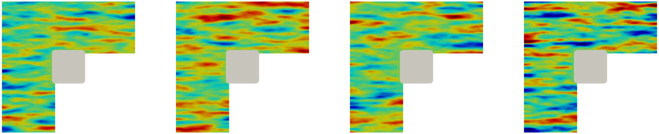
Spatially correlated uncertain parameter $m(\mathbf{x})$

- Gaussian random fields $m \sim \mathcal{N}(\bar{m}, \mathcal{C})$
- Matérn covariance kernel $\mathcal{C} = \mathcal{A}^{-2}$

$$\mathcal{A}\, m = \begin{cases} \gamma\, \nabla \cdot (\boldsymbol{\Theta}\, \nabla m) + \delta\, m & \text{in} \quad \Omega \\ (\boldsymbol{\Theta}\, \nabla m) \cdot \mathbf{n} + \dfrac{\sqrt{\delta\, \gamma}}{1.42}\, m & \text{on} \quad \Gamma \end{cases}$$



$L_c = 0.02$



$L_c = 0.25$

Design parameter $d(\mathbf{x})$

- Blue: $d = 0 \rightarrow$ porosity $\phi_f = 90\%$ weaker but more insulating aerogel
- Red: $d = 1 \rightarrow$ porosity $\phi_f = 10\%$ stronger but less insulating aerogel

Design under Uncertainty

Risk-averse optimal design statement:

$$\min_{d} \mathcal{J}(d) = \mathbb{E}[Q(m,d)] + \beta_V \, \mathbb{V}[Q(m,d)] + \beta_R \, R(d)$$

$$\text{s.t. } \mathcal{R}(\boldsymbol{u}, m, d) = 0$$

$$P(f(m,d) \geq 0) \leq \alpha_c \quad \text{in } \Omega$$

Design objectives: Thermal compliance

$$Q = -\left(\frac{1}{2}\sum_{i=s,f} \langle \phi_i \kappa_i \nabla\theta_i, \nabla\theta_i \rangle_\Omega + \sum_{i=s,f} \langle \phi_i h_{air}(\theta_i - \theta_{amb}), \theta_i \rangle \right).$$

Chance constraint: Avoid stress concentration

$$f = T_{cr} - T_{\mathsf{pn}},$$

T_{pn} is the p-norm of the Von Mises stress and T_{cr} is the limiting critical stress.

$$T_{\mathsf{pn}} = \left(\int_\Omega T_{\mathsf{VM}}^p \, d\Omega\right)^{\frac{1}{p}}$$

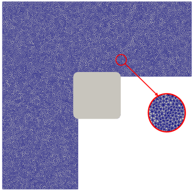
$$P(f(m,d) \geq 0) \quad = \quad \mathbb{E}[\mathbb{I}_{[0,\infty]}(f(m,d))]$$

$$\mathbb{I}_{[0,\infty]}(f(m,d)) = \begin{cases} 1 & \text{if } f(m,d) \geq 0 \\ 0 & \text{if } f(m,d) < 0 \end{cases}$$

Design under Uncertainty

Computational Challenges:

- High-Dimensional parameter space $d(\boldsymbol{x}), m(\boldsymbol{x})$



27079 elements

- Computing mean and variance of the design objective Q
  - Monte Carlo approach, for N samples, Convergence rate of $\mathcal{O}(\frac{1}{\sqrt{N}})$

$$\mathbb{E}[Q] \approx \frac{1}{N}\sum_{i=1}^{N} Q(m^{(i)}), \qquad \mathbb{V}[Q] \approx \left(\frac{1}{N}\sum_{i=1}^{N} Q^2(m^{(i)})\right) - \left(\frac{1}{N}\sum_{i=1}^{N} Q(m^{(i)})\right)^2$$

- Chance constraint
  - Non-differentiability of the discontinuous indicator function.
  - Approximation of constraint function requires large number of PDE solves.

Outline

Scalable Algorithm: Taylor approximation

Risk-averse optimal design statement:

$$\min_{d} \mathcal{J}(d) = \mathbb{E}[Q(m,d)] + \beta_V \, \mathbb{V}[Q(m,d)] + \beta_R \, R(d)$$
$$\text{s.t. } \mathcal{R}(\boldsymbol{u}, m, d) = 0$$
$$P(f(m,d) \geq 0) \leq \alpha_c \quad \text{in } \Omega$$

Mean and Variance

- Taylor approximation of Q at mean of uncertain parameter $\overline{m}$ truncated with K terms

$$T_K Q(m,d) = \sum_{k=0}^{K} \partial_m^k Q(\overline{m}, d)(m - \overline{m})^k$$

- Quadratic $K = 2$, with the objective, gradient and Hessian w.r.t. m , evaluated at mean $\bar{m}$, denoted as $\bar{Q}$, $\bar{Q}_m$ and $\bar{Q}_{mm}$, and $< \cdot, \cdot >$ denotes the inner product

$$T_2 Q(m) = \bar{Q} + < \bar{Q}_m, \, m - \bar{m} > + \frac{1}{2} < \bar{Q}_{mm}(m - \bar{m}), \, m - \bar{m} >$$

- Approximated mean and variance [4]

$$\mathbb{E}[T_2 Q] = Q(\overline{m}, d) + \frac{1}{2} \mathrm{tr}(\mathcal{C} \, \bar{Q}_{mm}), \quad \mathbb{V}[T_2 Q] = < \bar{Q}_m, \, \mathcal{C} \, \bar{Q}_m > + \frac{1}{2} \mathrm{tr}\left((\mathcal{C} \, \bar{Q}_{mm})^2 \right)$$

[4] Alexanderian, Petra, Stadler, Ghattas, 2017,SIAM Journal on Uncertainty Quantification

Scalable Algorithm: Taylor approximation

Trace estimator

- Generalize eigenvalues of $(\bar{Q}_{mm}, \mathcal{C}^{-1})$

$$< \bar{Q}_{mm}\, \psi_n,\, \phi >= \lambda_n < \mathcal{C}^{-1}\, \psi_n,\, \phi > \qquad \forall \phi \in X,\, n \geq 1$$

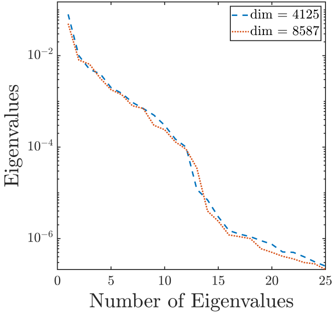
where $(\psi_n)_{n\geq 1} \in X$ are the generalized eigenfunctions, N_{eig} are number of dominant eigenvalues and N_o is the oversampling factor.

- Randomized Singular Value Decomposition (SVD) algorithm

- If eigenvalues decays rapidly, use N_{eig} dominant eigenvalues [5]

$$\mathrm{tr}\left(\mathcal{C}\, \bar{Q}_{mm}\right) \approx \sum_{n\geq 1}^{N_{eig}} \lambda_n$$

$$\mathrm{tr}\left((\mathcal{C}\, \bar{Q}_{mm})^2\right) \approx \sum_{n\geq 1}^{N_{eig}} \lambda_n^2$$



[5]Peng, Villa, Ghattas, 2019, Journal of Computational Physics

Scalable Algorithm: Control Variate

Mean correction:
The Monte Carlo correction for the mean for Scalable Solution can be written as,

$$\begin{aligned}\mathbb{E}[Q] =& \mathbb{E}[T_2 Q] + \mathbb{E}[Q - T_2 Q] \approx {\color{red}\hat{Q}} := \overline{Q} + \frac{1}{2} tr(\mathcal{C}\,\bar{Q}_{mm}) \\ &+ \frac{1}{M}\sum_{i=1}^{M}\left(Q(m_i) - \overline{Q} - < m_i - \overline{m}, \overline{Q}_m > - \frac{1}{2} < m_i - \overline{m}, \overline{Q}_{mm}(m_i - \overline{m}) > \right).\end{aligned}$$

Variance correction:
The variance can be computed as,

$$\mathbb{V}[Q] = \mathbb{E}[(T_2 Q - \overline{Q})^2] + \mathbb{E}[(Q - \overline{Q})^2 - (T_2 Q - \overline{Q})^2] - \left(\mathbb{E}[T_2 Q - \overline{Q}] + \mathbb{E}[(Q - \overline{Q}) - (T_2 Q - \overline{Q})]\right)^2$$

The above expression for variance can be approximated as,

$$\begin{aligned}{\color{red}\hat{V}} :=& < \mathcal{C}\overline{Q}_m, \overline{Q}_m > + \frac{1}{4}(tr(\mathcal{C}\,\bar{Q}_{mm}))^2 + \frac{1}{2} tr(\mathcal{C}\,\bar{Q}_{mm}{}^2) \\ &+ \frac{1}{M}\sum_{i=1}^{M}\left((Q(m_i) - \overline{Q})^2 - \left(< m_i - \overline{m}, \overline{Q}_m > + \frac{1}{2} < m_i - \overline{m}, \overline{Q}_{mm}(m_i - \overline{m} > \right)^2\right) \\ &- \left(\frac{1}{2} tr(\mathcal{H}) + \frac{1}{M}\left(Q(m_i) - < m_i - \overline{m} >, \overline{Q}_m > - \frac{1}{2} < m_i - \overline{m}, \overline{Q}_{mm}(m_i - \overline{m}) > \right)\right)^2\end{aligned}$$

Scalable Algorithm

Chance constraint

- Scalable Solution of constraint at $\overline{m}$

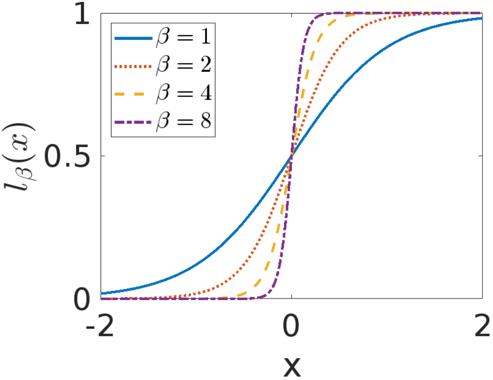
$$P(f(m,d)) \geq 0) \approx \frac{1}{M_f} \mathbb{I}_{[0,\infty)}(T_2 f(m_i, d))$$

- Smooth approximation and quadratic penalty for chance constraint function[6]

$$\mathbb{I}_{[0,\infty]}(x) \approx l_\beta(x) = \frac{1}{1+e^{-2\beta x}},$$

$$S_\gamma(x) = \frac{\gamma}{2}(max\{0,x\})^2$$

$$\min_d \mathcal{J}_d + S_\gamma(x)(\mathbb{E}[l_\beta(f)] - \alpha_c)$$



Smooth Approximation of Indicator Function

[6] Chen and Ghattas, 2021, SIAM Journal of Uncertainty Quantification

Scalable Algorithm

Lagrangian formulation

Analytical derivatives via Lagrange Formalism

The weak form can be written as,

$$r(\mathbf{u}, \mathbf{v}, m, d) = {}_{\mathcal{V}}\langle \mathbf{v}, \mathcal{R}(\mathbf{u}, m, d) \rangle_{\mathcal{V}'}$$

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

State $\mathbf{u} = \{\theta_s, \theta_f, \mathbf{u}_s, p\}$	Adjoint $\mathbf{v}$
$D_{\mathbf{v}}\mathcal{L}(\bar{m}) = 0$	State problem $\langle \tilde{\mathbf{v}}, \partial_{\mathbf{v}} \bar{r} \rangle = 0$
$D_{\mathbf{u}}\mathcal{L}(\bar{m}) = 0$	Adjoint problem $\langle \tilde{\mathbf{u}}, \partial_{\mathbf{u}} \bar{r} \rangle = -\langle \tilde{\mathbf{u}}, \partial_{\mathbf{u}} \bar{Q} \rangle$
$D_m\mathcal{L}(\bar{m}) = 0$	m-gradient $\langle \tilde{m}, \partial_m Q(\bar{m}) \rangle = \langle \tilde{m}, \partial_m \bar{r} \rangle$
$D_m f(\bar{m}) = 0$	m_f-gradient $\langle \tilde{m}, \partial_m f(\bar{m}) \rangle = \langle \tilde{m}, \partial_m \bar{r} \rangle$

Scalable Algorithm

Lagrangian formulation

Analytical derivatives via Lagrange Formalism

$$\mathcal{L}^H(\mathbf{u}, \mathbf{v}, m, d; \hat{\mathbf{u}}, \hat{\mathbf{v}}, \hat{m}) = \langle \hat{m}, \partial_m \bar{r} \rangle + \langle \hat{\mathbf{v}}, \partial_{\mathbf{v}} \bar{r} \rangle + \langle \hat{\mathbf{u}}, \partial_{\mathbf{u}} \bar{r} + \partial_{\mathbf{u}} \bar{Q} \rangle$$

State $\mathbf{u}$ Adjoint $\mathbf{v}$	Incremental State $\hat{\mathbf{u}}$ Incremental Adjoint $\hat{\mathbf{v}}$
$D_{\mathbf{v}} \mathcal{L}^H(\bar{m}) = 0$	Incremental State problem $\langle \tilde{\mathbf{v}}, \partial_{\mathbf{vu}} \bar{r}\, \hat{\mathbf{u}} \rangle = -\langle \tilde{\mathbf{v}}, \partial_{\mathbf{v}m} \bar{r}\, \hat{m} \rangle$
$D_{\mathbf{u}} \mathcal{L}^H(\bar{m}) = 0$	Incremental Adjoint problem $\langle \tilde{\mathbf{u}}, \partial_{\mathbf{uv}} \bar{r} \rangle = -\langle \tilde{\mathbf{u}}, \partial_{\mathbf{uu}} \bar{r}\, \hat{\mathbf{u}} + \partial_{\mathbf{uu}} \bar{Q}\, \hat{\mathbf{u}} + \partial_{\mathbf{u}m} \bar{r}\, \hat{m} \rangle$
$D_m \mathcal{L}^H(\bar{m}) = 0$	m-Hessian $\langle \tilde{m}, \partial_{mm} Q(\bar{m})\, \hat{m} \rangle = \langle \partial_{mm} \bar{r}\, \hat{m} \rangle$ $+\langle \tilde{m}, \partial_{m\mathbf{v}} \bar{r}\, \hat{\mathbf{v}} \rangle + \langle \partial_{m\mathbf{u}} \bar{r}\, \hat{\mathbf{u}} \rangle + \langle \partial_{mm} \bar{Q}\, \hat{m} + \partial_{m\mathbf{u}} \bar{Q}\, \hat{\mathbf{u}} \rangle$
$D_m f(\bar{m}) = 0$	m_f-Hessian $\langle \tilde{m}, \partial_{mm} f(\bar{m})\, \hat{m}^f \rangle = \langle \partial_{mm} \bar{r}\, \hat{m}^f \rangle$ $+\langle \tilde{m}, \partial_{m\mathbf{v}} \bar{r}\, \hat{\mathbf{v}}^f \rangle + \langle \partial_{m\mathbf{u}} \bar{r}\, \hat{\mathbf{u}}^f \rangle + \langle \partial_{mm} f(\bar{m})\, \hat{m} + \partial_{m\mathbf{u}} \bar{f}\, \hat{\mathbf{u}}^f \rangle$

Scalable Algorithm

Quadratically Approximated Cost Function

$$\min_{d} \mathcal{J}_{\text{quad}}(d) = \left(\bar{Q} + \frac{1}{2}\sum_{j\geq 1}^{N_{\text{eig}}} \lambda_j\right) + \beta_V \left(\langle \bar{Q}_m, \mathcal{C}\,\bar{Q}_m \rangle + \frac{1}{2}\sum_{j\geq 1}^{N_{\text{eig}}} \lambda_j^2\right) + \beta_R\, R(d)$$

$$\text{s.t.}\ \frac{1}{M_f}\sum_{i=1}^{M_f} \mathbb{I}_{[0,\infty)]}(T_2 f(m_i, d)) \leq \alpha_c \quad \text{in } \Omega$$

Quadratically Approximation as Control Variate

$$\min_{d} \mathcal{J}_{\text{quad}}^{CV}(d) = \hat{Q} + \beta_V \hat{V} + \beta_R R(d)$$

$$\text{s.t.}\ \frac{1}{M_f}\sum_{i=1}^{M_f} \mathbb{I}_{[0,\infty)]}(T_2 f(m_i, d)) \leq \alpha_c \quad \text{in } \Omega$$

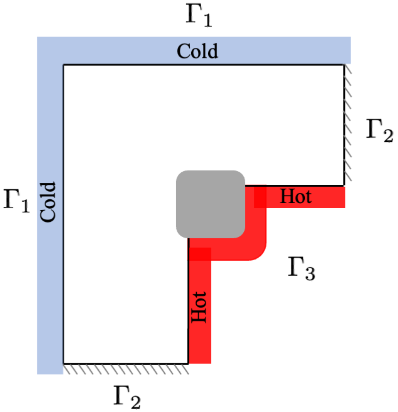
Mean: $\hat{Q} \approx \mathbb{E}[T_2 Q] + \mathbb{E}[Q - T_2 Q]$

Variance: $\hat{V} \approx \mathbb{E}[(T_2 Q - Q(\bar{m}))^2] - (\mathbb{E}[T_2 Q - Q(\bar{m})])^2$

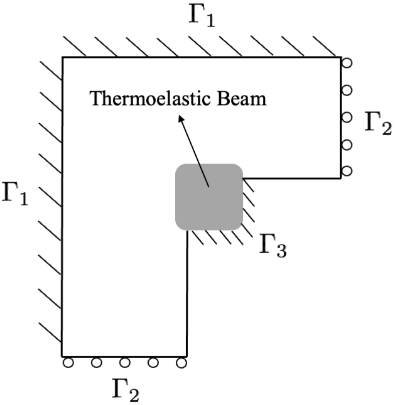
Newton Conjugate Gradient is used as optimizer through computation of design gradients.

Outline

Results: Beam-Insulator System

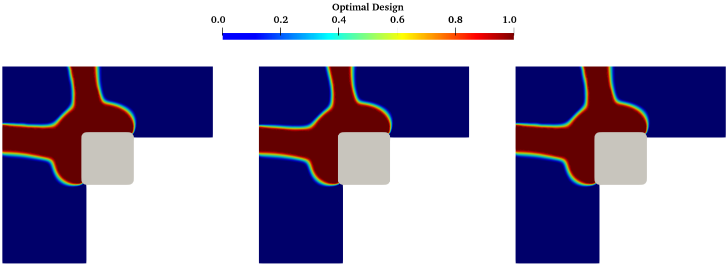


Thermal Scenario

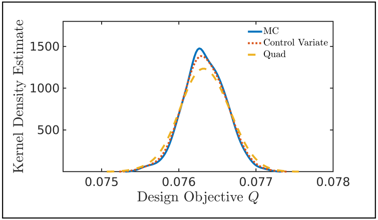


Mechanical Scenario

Results: Comparison

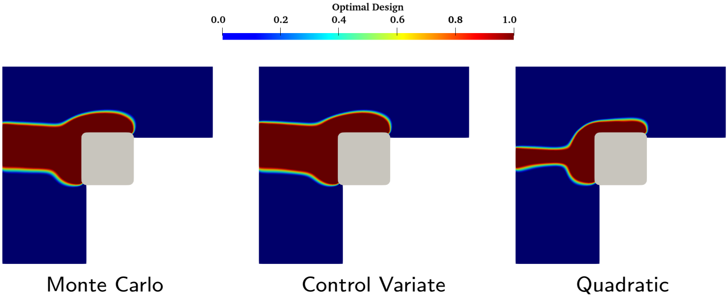


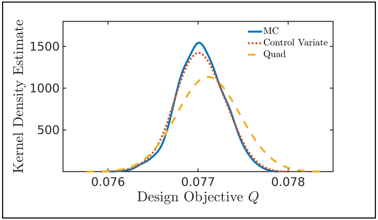
Monte Carlo Control Variate Quadratic



$$L_c = 0.25,\ \sigma = \mathbf{0.25},\ \alpha_c = 0.1,\ T_{cr} = 22.5\ \text{MPa},\ \beta_V = 1$$

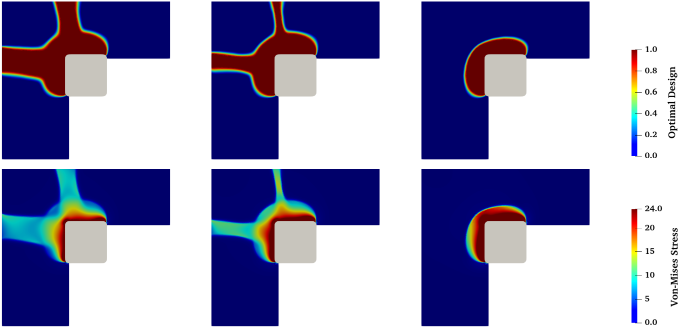
Results: Comparison



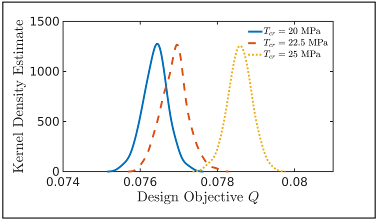


$$L_c = 0.25,\ \sigma = \mathbf{0.5},\ \alpha_c = 0.1,\ T_{cr} = 22.5\ \text{MPa},\ \beta_V = 1$$

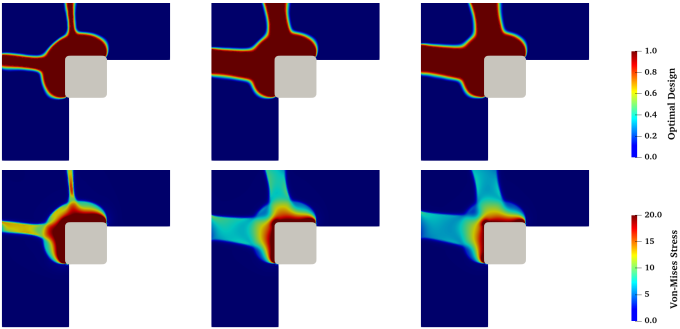
Results: Effect of critical stress



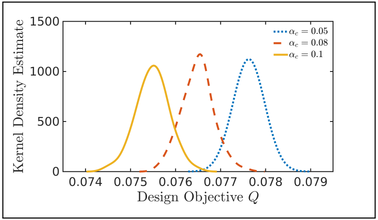
$T_{cr} = 20$ MPa $T_{cr} = 22.5$ MPa $T_{cr} = 25$ MPa



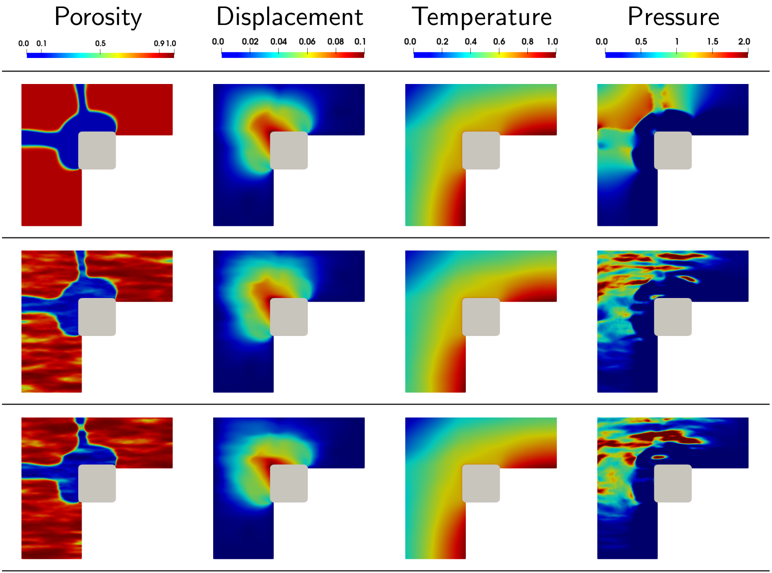
Results: Effect of critical chance



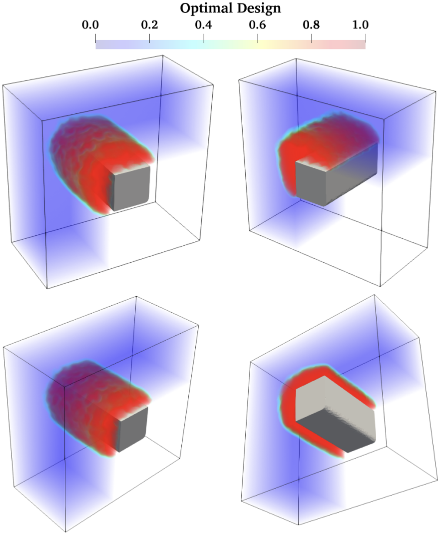
$\alpha_c = 0.05$ $\alpha_c = 0.08$ $\alpha_c = 0.1$



Results: State Plots



Results: 3D Scenario



Optimal design obtained for a dimension of 100559 design parameters

Outline

Conclusions

An efficient framework is introduced for optimal design governed by PDEs including chance constraint under high-dimensional and spatially correlated uncertainty.

- Quadratic Taylor approximation for estimating the mean and variance of the design objective with respect to uncertain parameters.
- Chance constraints are implemented using the Von-Mises criterion to avoid stress concentration within the beam-insulator system.
- Efficient trace estimation of the covariance-preconditioned Hessian using a randomized algorithm for solving generalized eigenvalue problems.
- Control variate is implemented to reduce variance under high uncertainty with the implementation of Monte-Carlo correction.

Acknowledgement:

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Thank you!