Robust Optimization Approaches for PDE-Constrained Problems under Uncertainty

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SIMUROM

Nonlinear Optimization

Optimization and Inversion under Uncertainty, RICAM, Linz, November 13, 2019

Outline

- Robust formulation of PDE-constrained optimization with uncertain data
- (First and) second order approximation of the robust counterpart
- Equivalent reformulations for second order approximation using optimality or duality theory
- Nonsmooth reduced formulation
- Update strategy for the expansion point
- Invoking reduced order models with error estimation
- Application to shape optimization of synchronous motors and for the elastodynamic wave equation
- Conclusion and outlook

PDE-Constrained Optimization under Uncertainty

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Uncertain PDE-Constrained Optimization Problem

$$\begin{aligned} \min_{y \in Y,\ x \in X} \quad & h_0(y, x; p) \\ \text{s.t.} \quad & h_i(y, x; p) \leq 0, \quad i \in I, \\ & C(y, x; p) = 0. \end{aligned} \tag{P}$$

- Typically nonconvex, design variables x, state y, uncertain parameters p
- h_0, $h_i : Y \times X \times \mathbb{R}^{n_p} \to \mathbb{R}$, $C : Y \times X \times \mathbb{R}^{n_p} \to Z$ sufficiently smooth
- $C(y, x; p) = 0$ has a unique solution $y = y(x; p)$ for all relevant x, p
- $\partial_y C \in \mathcal{L}(Y, Z)$ is invertible

PDE-Constrained Optimization under Uncertainty

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Uncertainty to be considered:

- Parameter p is uncertain with $p \in \mathcal{U}_p = \{p \in \mathbb{R}^{n_p} : \|p - \bar{p}\|_{B_p} \le 1\}$
  $\|v\|_B := (v^T B v)^{1/2}$ for a symmetric positive definite matrix B
- p can also be coefficients in an expansion, e.g. Karhunen-Loéve expansion
- Constraint-wise uncertainties also possible
- Also possible: Design x uncertain, $x \in \mathcal{U}_x = \{x \in X = \mathbb{R}^{n_x} : \|x - \bar{x}\|_{B_x} \le 1\}$

Robust Optimization - Basic Idea

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Uncertain Optimization Problem

$$\begin{aligned} \min_x \quad & \hat{h}_0(x;p) \\ \text{s.t.} \quad & \hat{h}_i(x;p) \le 0, \quad i \in I. \end{aligned} \tag{Pr}$$

Assumption: Parameter p is uncertain. We only know that $p \in \mathcal{U}_p$.

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Assumption: Parameter p is uncertain. We only know that $p \in \mathcal{U}_p$.

Consider the **"Robust Counterpart"** of (Pr):

$$\min_x \quad \max_{p \in \mathcal{U}_p} \hat{h}_0(x;p)$$
$$\text{s.t.} \quad \hat{h}_i(x;p) \le 0 \quad \forall p \in \mathcal{U}_p, \ i \in I.$$

[e.g. Ben-Tal, Bertsimas, El Ghaoui, Nemirovski, Nesterov, Zowe,. . .]

Robust Optimization - Basic Idea

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$$\iff$$

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Relation to Probabilistic Constraints

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$$\min_x \quad \max_{p \in \mathcal{U}_p} \hat{h}_0(x;p)$$
$$\text{s.t.} \quad \max_{p \in \mathcal{U}_p} \hat{h}_i(x;p) \le 0, \quad i \in I.$$

If $\mathcal{U}_p$ is confidence region for the random variable p of probability α then the solution x satisfies the constraints with probability $\ge \alpha$.

Alternative approach:

Probabilistic constraints, e.g. [Prékopa 95, Henrion, Römisch 10, Van Ackooij, Henrion 14, Chen, Ghattas et al. 18].

PDE-Constrained Optimization under Uncertainty

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- Also possible: Design x uncertain, $x \in \mathcal{U}_x = \{x \in X = \mathbb{R}^{n_x} : \|x - \bar{x}\|_{B_x} \le 1\}$

Robust Formulation of (P)

Worst-case values of objective function and inequality constraints:

$$h_i^{\mathrm{wc}}(x) := \max_{y \in Y,\, s \in \mathbb{R}^{n_p}} h_i(y, x; \bar{p} + s) \quad \text{s.t.} \quad C(y, x; \bar{p} + s) = 0, \ \ \|s\|_{B_p} \leq 1.$$

Reduced formulation:

$$h_i^{\mathrm{wc}}(x) := \max_{s \in \mathbb{R}^{n_p}} \hat{h}_i(x; \bar{p} + s) := h_i(y(x; \bar{p} + s), x; \bar{p} + s) \ \ \text{s.t.} \ \ \|s\|_{B_p} \leq 1,$$

where $C(y(x; \bar{p} + s), x; \bar{p} + s) = 0$.

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where $C(y(x; \bar{p} + s), x; \bar{p} + s) = 0$.

Robust Counterpart of (P)

$$\min_{x \in X} \; h_0^{\mathrm{wc}}(x) \quad \text{s.t.} \quad h_i^{\mathrm{wc}}(x) \leq 0, \quad i \in I. \tag{R}$$

Robust Formulation of (P)

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In the nonconvex case (R) is in general computationally intractable!

Approximation of Robust Formulation of (P)

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Robust Counterpart of (P)

$$\min_{x \in X} \quad h_0^{wc}(x) := \max_{p \in \mathcal{U}_p} \hat{h}_0(x;p)$$
$$\text{s.t.} \quad h_i^{wc}(x) := \max_{p \in \mathcal{U}_p} \hat{h}_i(x;p) \leq 0, \quad i \in I. \tag{R}$$

In the nonconvex case (R) is in general computationally intractable!

Possible approaches:

Approximate h^{wc} by $\tilde{h}^{wc}$ such that $\tilde{h}^{wc}$ and $\nabla \tilde{h}^{wc}$ can be computed efficiently or $\tilde{h}^{wc}$ can be characterized conveniently by differentiable constraints.

- Linearize $\hat{h}_i(x;p)$ w.r.t. p [Diehl, Bock, Kostina 06; Zhang 07]
- **In this talk:** Approximate $\hat{h}_i(x;p)$ by second order Taylor expansion w.r.t. p [Sichau 13; Lass, SU 17; Alla, Hinze, Lass, Kolvenbach, SU 19; Kolvenbach, Lass, SU 18; cf. also Houska, Diehl 12; Alexanderian, Petra, Stadler, Ghattas 16; Chen, Villa, Ghattas 18; Milz, Ulbrich 19]

Approximation of Robust Formulation of (P)

Approximated Robust Counterpart of (P)

$$
\begin{aligned}
\min_{x \in X} \quad & \tilde{h}_0^{wc}(x) := \max_{p \in \mathcal{U}_p} \ \hat{h}_0^{appr}(x;p) \\
\text{s.t.} \quad & \tilde{h}_i^{wc}(x) := \max_{p \in \mathcal{U}_p} \ \hat{h}_i^{appr}(x;p) \le 0, \quad i \in I.
\end{aligned}
\qquad \text{(RA)}
$$

In the nonconvex case (R) is in general computationally intractable!

Possible approaches:

Approximate h^{wc} by $\tilde{h}^{wc}$ such that $\tilde{h}^{wc}$ and $\nabla \tilde{h}^{wc}$ can be computed efficiently or $\tilde{h}^{wc}$ can be characterized conveniently by differentiable constraints.

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First Order Approximation

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Approximated worst-case value:

$$\tilde{h}_i^{\mathrm{wc},1}(x;\bar{p}) := \max_{s\in\mathbb{R}^{n_p}} \hat{h}_i(x;\bar{p}) \;+\; \partial_p \hat{h}_i(x;\bar{p})s \quad \text{s.t.} \quad \|s\|_{B_p} \le 1.$$
$$= \hat{h}_i(x;\bar{p}) \;+\; \left\|\partial_p \hat{h}_i(x;\bar{p})\right\|_{B_p^{-1}}$$

Sensitivity approach:

$$\tilde{h}_i^{\mathrm{wc},1}(x;\bar{p}) = h_i(\bar{y},x;\bar{p}) \;+\; \left\|(\partial_p h_i + \partial_y h_i D)(\bar{y},x;\bar{p})\right\|_{B_p^{-1}}$$
$$C(\bar{y},x;\bar{p}) = 0, \quad \partial_y C(\bar{y},x;\bar{p})D + \partial_p C(\bar{y},x;\bar{p}) = 0$$

Adjoint approach:

$$\tilde{h}_i^{\mathrm{wc},1}(x;\bar{p}) = h_i(\bar{y},x;\bar{p}) \;+\; \left\|(\partial_p h_i + \mu_i \partial_p C)(\bar{y},x;\bar{p})\right\|_{B_p^{-1}}$$
$$C(\bar{y},x;\bar{p}) = 0, \quad \partial_y C(\bar{y},x;\bar{p})^* \mu_i + \partial_y h_i(\bar{y},x;\bar{p}) = 0$$

See e.g. [Diehl, Bock, Kostina 06; Zhang 07]

First Order Approximation
Adjoint-based Formulation of (RA1)

$$\min_{\bar{y}\in Y, x\in X, \mu_i\in Z^*} \quad h_0(\bar{y},x;\bar{p}) + \left\|(\partial_p h_0 + \mu_0 \partial_p C)(\bar{y},x;\bar{p})\right\|_{B_p^{-1}}$$

$$\text{s.t.} \quad h_i(\bar{y},x;\bar{p}) + \left\|(\partial_p h_i + \mu_i \partial_p C)(\bar{y},x;\bar{p})\right\|_{B_p^{-1}} \le 0, \ i \in I, \qquad \text{(RA1a)}$$

$$C(\bar{y},x;\bar{p}) = 0,$$

$$\partial_y C(\bar{y},x;\bar{p})^* \mu_i + \partial_y h_i(\bar{y},x;\bar{p}) = 0, \ i \in I_0.$$

$I_0 := I \cup \{0\}$.

Remarks:

- $(\bar{y}, (\mu_i)_{i\in I_0})$ is the extended state
- If $|I_0| \le n_p$ is moderate: Efficiently solvable by PDE-constrained optimization techniques in connection with appropriate handling of second order cone constraints.
- If $n_p \le |I_0|$ is moderate: Use sensitivity approach instead.

First Order Approximation
Sensitivity-based Formulation of (RA1)

$$
\begin{aligned}
\min_{\bar{y}\in Y, x\in X, D\in Y^{n_p}} \quad & h_0(\bar{y}, x; \bar{p}) + \left\| (\partial_p h_0 + \partial_y h_0 D)(\bar{y}, x; \bar{p}) \right\|_{B_p^{-1}} \\
\text{s.t.} \quad & h_i(\bar{y}, x; \bar{p}) + \left\| (\partial_p h_i + \partial_y h_i D)(\bar{y}, x; \bar{p}) \right\|_{B_p^{-1}} \leq 0, \;\; i \in I, \\
& C(\bar{y}, x; \bar{p}) = 0, \\
& \partial_y C(\bar{y}, x; \bar{p}) D + \partial_p C(\bar{y}, x; \bar{p}) = 0.
\end{aligned} \tag{RA1s}
$$

Remark:

- $(\bar{y}, D)$ is the extended state

Second Order Approximation
Motivation and Basic Approach

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Motivation:

- For large uncertainty sets the linear approximation (RA1) is not accurate enough.
- A quadratic approximation is often much more accurate.

Approximated worst-case value (quadratic approximation):

$$\tilde{h}_i^{\mathrm{wc},2}(x;\bar{p}) := \max_{s\in\mathbb{R}^{n_p}} \hat{h}_i(x;\bar{p}) + \partial_p \hat{h}_i(x;\bar{p})s + \frac{1}{2}s^T \partial_{pp}\hat{h}_i(x;\bar{p})\, s \quad \text{s.t. } \|s\|_{B_p} \leq 1.$$

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This is a Trust-Region Problem:

$$\begin{aligned}\tilde{h}_i^{\mathrm{wc},2}(x) = \max_{s\in\mathbb{R}^{n_p}} \; & \hat{h}_i(x;\bar{p}) + g_i(x;\bar{p})^T s + \frac{1}{2}s^T H_i(x;\bar{p})s \\ \text{s.t.} \quad & \|s\|_{B_p} \leq 1.\end{aligned}$$

Second Order Approximation
Computation of $\mathbf{H_i}(\mathbf{x};\bar{\mathbf{p}}) = \partial_{\mathbf{pp}}\hat{\mathbf{h}}_{\mathbf{i}}(\mathbf{x};\bar{\mathbf{p}})$

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Approximated worst-case value (quadratic approximation):

$$\tilde{h}_i^{\mathrm{wc},2}(x;\bar{p}) := \max_{s\in\mathbb{R}^{n_p}} \hat{h}_i(x;\bar{p}) + \partial_p\hat{h}_i(x;\bar{p})s + \frac{1}{2}s^T\,\partial_{pp}\hat{h}_i(x;\bar{p})\,s \quad \text{s.t. } \|s\|_{B_p} \leq 1.$$

Computation of $\partial_{\mathbf{pp}}\hat{\mathbf{h}}_{\mathbf{i}}(\mathbf{x};\bar{\mathbf{p}})$:

With the auxiliary Langrangian

$$L_i(y,x,\mu_i;p) = h_i(y,x;p) + \mu_i C(y,x;p)$$

the well-known formula holds

$$\partial_{pp}\hat{h}_i(x;\bar{p}) = \begin{pmatrix} D \\ I \end{pmatrix}^* \begin{pmatrix} \partial_{yy}L_i & \partial_{yp}L_i \\ \partial_{py}L_i & \partial_{pp}L_i \end{pmatrix}(\bar{y},x,\mu_i;\bar{p}) \begin{pmatrix} D \\ I \end{pmatrix}$$

with the state $\bar{y}$, the sensitivities D and the adjoint state μ_i as above, i.e.,

$$C(\bar{y},x;\bar{p}) = 0, \quad \partial_y C(\bar{y},x;\bar{p})D + \partial_p C(\bar{y},x;\bar{p}) = 0, \quad \partial_y C(\bar{y},x;\bar{p})^*\mu_i + \partial_y h_i(\bar{y},x;\bar{p}) = 0.$$

Calculation of $\tilde{\mathbf{h}}_{\mathbf{i}}^{\mathbf{wc,2}}(\mathbf{x};\bar{\mathbf{p}})$ for Second Order Approximation by Trust-Region Problem

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Approximated worst-case value (quadratic approximation):

$$\tilde{h}_i^{\mathrm{wc},2}(x;\bar{p}) := \max_{s\in\mathbb{R}^{n_p}} \hat{h}_i(x;\bar{p}) + g_i(x)^T s + \frac{1}{2} s^T H_i(x)\, s \quad \text{s.t.} \quad \|s\|_{B_p} \leq 1. \tag{TR}$$

where $\quad g_i(x) := \partial_p \hat{h}_i(x;\bar{p})^T, \quad H_i(x) := \partial_{pp}\hat{h}_i(x;\bar{p}).$

Calculation of $\tilde{\mathbf{h}}_{\mathbf{i}}^{\mathbf{wc,2}}(\mathbf{x};\bar{\mathbf{p}})$: [Moré, Sorensen 83]

s_i solves the trust-region problem (TR) if and only if with a multiplier λ_i holds

(1) $\left(-H_i(x) + \lambda_i B_p\right) s_i = g_i(x)$,

(2) $\left(-H_i(x) + \lambda_i B_p\right)$ is positive semidefinite,

(3) $\lambda_i \geq 0, \quad \|s_i\|_{B_p} \leq 1, \quad \lambda_i(\|s_i\|_{B_p} - 1) = 0.$

Then: $\quad \tilde{h}_i^{\mathrm{wc},2}(x;\bar{p}) = \hat{h}_i(x;\bar{p}) + g_i(x)^T s_i + \frac{1}{2} s_i^T H_i(x)\, s_i.$

Difficulty: Points x might exist where $\tilde{h}_i^{\mathrm{wc},2}(x;\bar{p})$ is nondifferentiable.

Calculation of $\tilde{\mathbf{h}}_i^{\mathrm{wc},2}(\mathbf{x};\bar{\mathbf{p}})$ for Second Order Approximation by Trust-Region Problem

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Approximated worst-case value (quadratic approximation):

$$\tilde{h}_i^{\mathrm{wc},2}(x;\bar{p}) := \max_{s\in\mathbb{R}^{n_p}} q_i(s;x) := \hat{h}_i(x;\bar{p}) + g_i(x)^T s + \frac{1}{2} s^T H_i(x)\, s \quad \text{s.t.} \quad \|s\|_{B_p} \le 1,$$

where $\quad g_i(x) := \partial_p \hat{h}_i(x;\bar{p}), \quad H_i(x) := \partial_{pp}\hat{h}_i(x;\bar{p}).$

Difficulty: Points x might exist where $\tilde{h}_i^{\mathrm{wc},2}(x;\bar{p})$ is nondifferentiable.

- Can occur if $\det\left(-H_i(x) + \bar{\lambda}_i B_p\right) = 0$ (hard case)
- However: $x \mapsto \tilde{h}_i^{\mathrm{wc},2}(x;\bar{p})$ is locally Lipschitz-continuous [Fiacco, Ishizuka 90, Bonnans, Shapiro 00]

Possible solutions:

- Apply nonsmooth optimization methods
- Use a smooth reformulation of (RA2) by optimality or duality theory
- Use S-procedure to characterize $\tilde{h}_i^{\mathrm{wc},2}(x;\bar{p})$ by an SDP-constraint [Boyd, Vandenberghe 04, Pólik, Terlaky 07; cf. also Fortin, Wolkowicz 04]

Approach 1: Reformulation as MPEC (Reduced Form)

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Using the reduced objective function and reduced constraints

$$\hat{h}_i(x;p) = h_i(y(x;p), x; p)$$

we obtain with

$$g_i(x) := \partial_p \hat{h}_i(x;\bar{p})^T, \quad H_i(x) := \partial_{pp} \hat{h}_i(x;\bar{p}),$$

$$\begin{aligned}
\min_{s_0, s_i, \lambda_0, \lambda_i, x} \quad & \hat{h}_0(x;\bar{p}) + g_0(x)^T s_0 + \tfrac{1}{2} s_0^T H_0(x) s_0 \\
\text{s.t.} \quad & \hat{h}_i(x;\bar{p}) + g_i(x)^T s_i + \tfrac{1}{2} s_i^T H_i(x) s_i \le 0, \; i \in I, \\
& \begin{pmatrix} \left(-H_i(x) + \lambda_i B_p\right) s_i - g_i(x) \\ \lambda_i \cdot \left(\|s_i\|_{B_p}^2 - 1\right) \end{pmatrix} = 0, \; i \in I_0, \qquad (\mathrm{RA2_{MPEC}}) \\
& \lambda_i \ge 0, \quad \|s_i\|_{B_p}^2 - 1 \le 0, \; i \in I_0, \\
& \left(-H_i(x) + \lambda_i B_p\right) \succeq 0, \; i \in I_0,
\end{aligned}$$

Reformulation as MPEC

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- ($RA2_{MPEC}$) can be solved by NLP methods [Scholtes 01; Anitescu 05; Fletcher, Leyffer, Ralph, Scholtes 05; Steffensen, M. Ulbrich 10;...]
- Our approach: SQP method with NCP-reformulation of complementarity condition [Leyffer 06].
- Usually $H_i \not\preceq 0$, then one has strict complementarity $\|s_i\|_B = 1$, $\lambda_i > 0$. Hence, B-stationarity and strong stationarity likely holds at local solutions.

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- Usually $H_i \not\preceq 0$, then one has strict complementarity $\|s_i\|_B = 1$, $\lambda_i > 0$. Hence, B-stationarity and strong stationarity likely holds at local solutions.

- It is possible to take a hybrid approach: apply quadratic approximation only for selected uncertain parameters and use linearization for the remaining
- Quadratic model could also be based on Quasi-Newton approximations of H_i, approximate trust region solvers, interpolation models or on reduced order models [Lass, SU SISC 17; Alla, Hinze, Kolvenbach, Lass, SU ACOM 19]

Approach 2: SDP-Formulation by Using the S-Procedure

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One can show [Boyd, Vandenberghe 04]:

$$t_i \geq \tilde{h}_i^{\mathrm{wc},2}(x;\bar{p}) := \max_{s\in\mathbb{R}^{n_p}} q_i(s;x) := \hat{h}_i(x;\bar{p}) + g_i(x)^T s + \frac{1}{2} s^T H_i(x)\, s \quad \text{s.t. } \|s\|_{B_p} \leq 1.$$

if and only if there exists $\lambda_i \geq 0$ such that

$$\lambda_i \begin{pmatrix} B_p & 0 \\ 0 & -1 \end{pmatrix} - \begin{pmatrix} H_i(x) & g_i(x) \\ g_i(x)^T & 2(\hat{h}_i(x;\bar{p}) - t_i) \end{pmatrix} \succeq 0.$$

Resulting Reformulation of ($\mathrm{RA2_{MPEC}}$):

$$\begin{aligned} \min_{\lambda_i, t_i, x} \quad & t_0 \\ \text{s.t.} \quad & \lambda_i \begin{pmatrix} B_p & 0 \\ 0 & -1 \end{pmatrix} - \begin{pmatrix} H_i(x) & g_i(x) \\ g_i(x)^T & 2(\hat{h}_i(x;\bar{p}) - t_i) \end{pmatrix} \succeq 0, \ i \in I_0, \\ & t_i = 0, \ i \in I, \\ & \lambda_i \geq 0, \ i \in I_0. \end{aligned} \qquad (\mathrm{RA2_{SDP}})$$

Approach 3: Formulation by Duality Theory

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Trust region problems satisfy strong duality [Stern, Wolkowicz 95]:

$$
\begin{aligned}
\tilde{h}_i^{\mathrm{wc},2}(x;\bar{p}) &:= \max_{s\in\mathbb{R}^{n_p}} \; q_i(s;x) := \hat{h}_i(x;\bar{p}) + g_i(x)^T s + \frac{1}{2} s^T H_i(x)\, s \quad \text{s.t.} \quad \|s\|_{B_p} \le 1, \\
&= \min_{\lambda_i \ge 0} \sup_{s\in\mathbb{R}^{n_p}} \; q_i(s;x) + \frac{\lambda_i}{2}(1 - s^T B_p s) \\
&= \min_{\lambda_i \ge 0} \; \hat{h}_i(x;\bar{p}) + g_i(x)^T s + \frac{1}{2} s^T (H_i(x) - \lambda_i B_p)\, s + \frac{\lambda_i}{2} \\
&\quad \text{s.t.} \quad (-H_i(x) + \lambda_i B_p) \succeq 0, \quad (-H_i(x) + \lambda_i B_p) s = g_i(x), \\
&= \min_{\lambda_i \ge 0} \; \hat{h}_i(x) + \frac{1}{2} g_i(x)^T s + \frac{\lambda_i}{2} \\
&\quad \text{s.t.} \quad (-H_i(x) + \lambda_i B_p) \succeq 0, \quad (-H_i(x) + \lambda_i B_p) s = g_i(x).
\end{aligned}
$$

Similar approach by [Milz, Ulbrich 19], Michael's talk on Monday.

Approach 3: Formulation by Duality Theory (2)

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Resulting Reformulation of $(\text{RA2}_{\text{MPEC}})$:

$$\begin{aligned} \min_{s_0, s_i, \lambda_0, \lambda_i, x} \quad & \hat{h}_0(x;\bar{p}) + \tfrac{1}{2} g_0(x)^T s_0 + \tfrac{1}{2}\lambda_0 \\ \text{s.t.} \quad & \hat{h}_i(x;\bar{p}) + \tfrac{1}{2} g_i(x)^T s_i + \tfrac{1}{2}\lambda_i \le 0, \ i \in I, \\ & (-H_i(x) + \lambda_i B_p) s_i - g_i(x) = 0, \ i \in I_0, \\ & \lambda_i \ge 0, \ i \in I_0, \\ & \big(-H_i(x) + \lambda_i B_p\big) \succeq 0, \ i \in I_0, \end{aligned} \qquad (\text{RA2}_{\text{DUAL}})$$

Approach 4: Nonsmooth Reduced Approach

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Approximated Robust Counterpart of (P)

$$\min_{x \in X} \quad \tilde{h}_0^{\mathrm{wc},2}(x) \qquad \text{s.t.} \quad \tilde{h}_i^{\mathrm{wc},2}(x) \le 0, \quad i \in I. \tag{RA2}$$

$$\tilde{h}_i^{\mathrm{wc},2}(x;\bar{p}) := \max_{s \in \mathbb{R}^{n_p}} q_i(s;x) := \hat{h}_i(x;\bar{p}) + g_i(x)^\top s + \tfrac{1}{2} s^\top H_i(x) s \ \text{ s.t. } \ \|s\|_{B_p} \le 1. \quad \text{(TR)}$$

- $x \mapsto \tilde{h}_i^{\mathrm{wc},2}(x;\bar{p})$ is locally Lipschitz-continuous [Fiacco, Ishizuka 90]
- Clarke's subdifferential is given by

  $$\partial_x^{cl} \tilde{h}_i^{\mathrm{wc},2}(x;\bar{p}) = \mathrm{conv}\left\{ \nabla_x q_i(\bar{s};x) : \bar{s} \text{ solves (TR)} \right\}$$

  Hence, a subgradient can be computed efficiently by adjoint method.
- Methods for nonsmooth opt. with nonsmooth constraints applicable to (RA2).
- Allows to use iterative trust-region solvers, e.g. LSTRS [Rojas, Santos, Sorensen 00; Kolvenbach, Lass, SU OPTE 18].

Possible Extensions

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The following will be explained and used for the application examples:

- Use reduced order models with error estimation to compute $\tilde{h}_i^{wc,2}(x; \bar{p})$ to sufficient accuracy [Lass, SU SISC 17; Alla, Hinze, Kolvenbach, Lass, SU ACOM 19]
- Update iteratively the parameters p where the quadratic model $q_i(s; x)$ for the computation of $\tilde{h}_i^{wc,2}(x; p)$ is built (instead of using $p = \bar{p}$) [Lass, SU SISC 17; Alla, Hinze, Kolvenbach, Lass, SU ACOM 19]
- For high-dimensional uncertain parameters p: Use reduced approach with matrix-free trust-region solver [Kolvenbach, Lass, SU OPTE 18], e.g.
  - Rojas, Santos, Sorensen: *A new matrix-free algorithm for the large-scale trust-region subproblem* (2000) – *LSTRS*

Moving the Expansion Point $\bar{p}$ in the Quadratic Model

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Motivation: Update the expansion point $\bar{p}$ in the quadratic model $\tilde{h}_i^{\mathrm{wc},2}(x;\bar{p})$ to predict the worst case value $h_i^{\mathrm{wc}}(x)$ more accurately.

Expansion point update strategy [Alla, Hinze, Kolvenbach, Lass, SU ACOM 19]

- Let $\bar{p}_i^{k-1}$ be the current expansion point (we start with $\bar{p}_i^0 = \bar{p}$)
- Apply one or several steps of a globally convergent optimization method (e.g., projected gradient method) with starting point $\bar{p}_i^{k-1}$ to obtain

$$\bar{p}_i^k \approx \operatorname*{argmax}_{\|p-\bar{p}\|_{B_p}\le 1} \hat{h}_i(x^k;p)$$

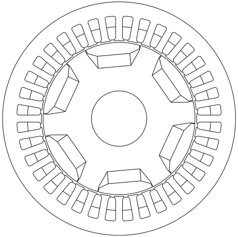
- Compute x^{k+1} by using

$$\tilde{h}_i^{\mathrm{wc},2}(x;\bar{p}_i^k) := \max_{\left\|s+\bar{p}_i^k-\bar{p}\right\|_{B_p}\le 1} \hat{h}_i(x;\bar{p}_i^k) + \partial_p\hat{h}_i(x;\bar{p}_i^k)^T s + \frac{1}{2}s^T\,\partial_{pp}\hat{h}_i(x;\bar{p}_i^k)\,s.$$

Result: If (x^k) is bounded and $\sum_k \|\bar{p}_i^{k+1}-\bar{p}_i^k\| < \infty$ then $\bar{p}_i^k \to \bar{p}_i$ with $\bar{p}_i$ stationary and (x^k) has convergence properties as for fixed expansion point.

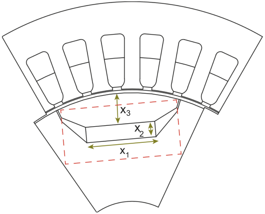
Example: Robust Geometry Optimization of Permanent Magnets in a Synchronous Motor [Lass, SU SISC 17]

- 3-phase 6-pole Permanent Magnet Synchronous Machine (PMSM)
- 1 buried permanent magnet per pole
- Operated at 50Hz



Design parameters:

- x_1, x_2 width and height of permanent magnet
- x_3 distance from rotor surface



Uncertainties:

- field angle p_i of all 6 magnets i
- design x of the magnets

Triangulate (blue) subregion of the geometry that can be transformed (red lines).

Example: Robust Geometry Optimization of Permanent Magnets in a Synchronous Motor [Lass, SU SISC 17]

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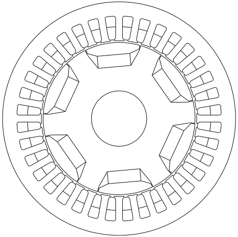

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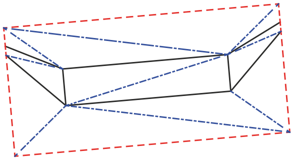

Triangulate (blue) subregion of the geometry that can be transformed (red lines).

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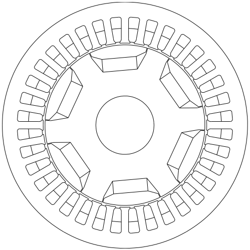

The magnetic vector potential is obtained by the magnetostatic approximation of Maxwell's equations with transient rotor movement

$$\nabla \times (\nu \nabla \times A) = J_{\mathrm{src}}(\vartheta) - \nabla \times H_{\mathrm{pm}} \quad \text{on} \quad \Omega(\vartheta), \quad \vartheta \in [0, 2\pi]$$

with adequate boundary conditions.

Magnetostatic Approximation of Maxwell's Equations

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In the 2D planar case the magnetostatic approximation of Maxwell's equations for the magnetic vector potential can be rewritten as the elliptic equation

$$-\nabla \cdot (\nu \nabla y(\vartheta)) = J_{\mathrm{src}}(\vartheta) + J_{\mathrm{pm}} \quad \text{on} \quad \Omega(\vartheta)$$

Using the finite element method we get the discrete systems

$$\mathbf{K}_\nu(\vartheta)\mathbf{y}(\vartheta) = \mathbf{j}_{\mathrm{src}}(\vartheta) + \mathbf{j}_{\mathrm{pm}}$$

- The rotation is realized using a domain decomposition method with two domains (stator, rotor) and locked step method [Shi et al.]

$$\begin{pmatrix} \mathbf{K}_{ss} & 0 & \mathbf{K}_{sl} \\ 0 & \mathbf{K}_{rr} & \mathbf{K}_{rl}(\vartheta^k) \\ \mathbf{K}_{sl}^\top & \mathbf{K}_{rl}^\top(\vartheta^k) & \mathbf{K}_{ll}(\vartheta^k) \end{pmatrix} \begin{pmatrix} \mathbf{y}_{s,k} \\ \mathbf{y}_{r,k} \\ \mathbf{y}_{l,k} \end{pmatrix} = \begin{pmatrix} \mathbf{f}_s \\ \mathbf{f}_r \\ \mathbf{f}_l(\vartheta^k) \end{pmatrix}, \; \vartheta^k = k\Delta\vartheta, \; 0 \le k \le 899.$$

- The mechanical power (torque) is computed by the power balance method.
- We use **affine decomposition** to compute $\mathbf{K}_\nu(\vartheta), \mathbf{f}_l(\vartheta)$ and its derivatives efficiently [Patera et al., Rozza et al.].

Optimization Problem

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Uncertain Optimization Problem

$$\min_{\Omega} \quad \hat{h}_0(\Omega) := V_{pm}(\Omega)$$

$$\text{subject to} \quad -\nabla \cdot (\nu \nabla y) - J_{src}(\vartheta) - J_{pm} = 0 \quad \text{on } \Omega(\vartheta),\ \vartheta \in [0, 2\pi]$$

$$M^d - M(y) \leq 0,$$

$$D(\Omega) \leq 0.$$

with

Ω	...	Geometry
$V_{pm}(\Omega)$	...	Volume of the permanent magnet
$M(y)$	...	Mechanical power (Torque)
M^d	...	Desired Torque
$D(\Omega)$	...	Constraints on the design

Geometry Description

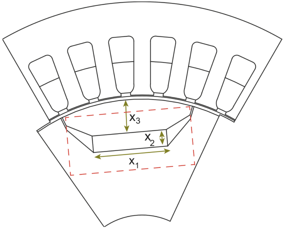
We describe the size and location of the permanent magnet using parameters.

Design parameters:

- x_1, x_2 width and height of permanent magnet
- x_3 distance from rotor surface

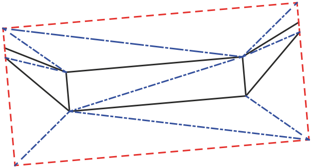
Uncertainties:

- field angle p_i of all 6 magnets i
- design x of the magnets



Define subregion of the geometry that can be transformed (red lines).

By partitioning the geometry into L triangular subdomains, the transformation can be computed explicitly (blue lines).



Geometry Preconditioning

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Domain transformation in each triangle:

$$\mathbf{z} \mapsto T^i(\mathbf{z}, x) = C^i(x) + G^i(x)\mathbf{z}, \quad i = 1, \dots, L$$

Transformation to reference domain: $\Omega(\vartheta, x) \to \Omega_0(\vartheta)$

$$-\nabla \cdot (\nu(x)\nabla y) = J_{\mathrm{src}}(\vartheta, x) + J_{\mathrm{pm}}(x, p) \quad \text{on } \Omega_0(\vartheta) \text{ (reference domain)}$$

Discrete setting: We get $\quad \mathbf{K}_\nu(\vartheta, x)y = \mathbf{f}(\vartheta, x, p)$

$$\mathbf{K}_\nu(\vartheta, x) = \sum_{i=1}^{L} \theta^i_{\mathbf{K}}(x)\mathbf{K}^{0,i}_\nu(\vartheta) \quad \text{and} \quad \mathbf{f}(\vartheta, x, p) = \sum_{i=1}^{L} \theta^i_{\mathbf{f}}(x, p)\mathbf{f}^{0,i}(\vartheta)$$

In our case only $\mathbf{K}_{rr}(\vartheta)$ and $\mathbf{f}_r(\vartheta)$ are affected. [Patera et al., Rozza et al.]

Hence, derivatives with respect to x, p are given by the derivatives of the scalar functions $\theta^i_{\mathbf{K}}$ and $\theta^i_{\mathbf{f}}$.

Optimization Problem (discretized version)

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Uncertain Design Optimization Problem for the Motor

$$\min_{x,y} \quad \hat{h}_0(x, \mathbf{y}) := V_{\mathrm{pm}}(x) = x_1 x_2$$

$$s.t. \quad \mathbf{K}_\nu(\vartheta_k, x)\mathbf{y_k} = \mathbf{f}(\vartheta_k, x, p), \quad \vartheta_k = k\Delta\vartheta, k = 0, \dots, K,$$

$$D(x) \leq 0, \quad M^d - M(\mathbf{y}) \leq 0.$$

with

$V_{\mathrm{pm}}(x)$	...	Volume of the permanent magnet
$M(\mathbf{y})$	...	Mechanical power (Torque)
M^d	...	Desired Torque
$D(x)$	...	Constraints on the design

Optimization Problem (discretized version)

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$$\min_{x,y} \quad \hat{h}_0(x, \mathbf{y}) := V_{\mathrm{pm}}(x) = x_1 x_2$$

$$s.t. \quad \mathbf{K}_\nu(\vartheta_k, x)\mathbf{y_k} = \mathbf{f}(\vartheta_k, x, p), \quad \vartheta_k = k\Delta\vartheta, k = 0, \ldots, K,$$

$$D(x) \leq 0, \quad M^d - M(\mathbf{y}) \leq 0.$$

Since the solution to the PDEs are unique, this is of our general form

Uncertain PDE-Constrained Optimization Problem

$$\begin{aligned} \min_{y \in Y,\ x \in X} \quad & h_0(y, x; p) \\ \text{s.t.} \quad & h_i(y, x; p) \leq 0, \quad i \in I, \\ & C(y, x; p) = 0, \end{aligned} \tag{P}$$

where now p and x are uncertain.

Reduced Order Model (ROM) by using POD

Strategy to reduce computational complexity: [Lass, SU SISC 17]

- We replace

$$\mathbf{K}_\nu(\vartheta_k, x)\mathbf{y_k} = \mathbf{f}(\vartheta_k, x, p), \quad \vartheta_k = k\Delta\vartheta, k = 0, \dots, K = 899,$$

  by a reduced order model with error control.
- By an adaptive greedy strategy we pick a subset $(\vartheta_k)_{k\in M} \subset (\vartheta_k)_{0\le k\le K}$ of rotation angles and compute corresponding FE-solutions $\mathbf{y_k}$ (snapshots)
- Compute by POD a reduced basis $\Psi = \{\psi^1, \dots, \psi^\ell\}$ that approximates $\mathrm{span}(\mathbf{y_k})_{k\in M})$ with a given accuracy.
- Form the reduced system

$$\Psi^\top \mathbf{K}_\nu(\vartheta, p)\Psi\, \hat{\mathbf{y}}^\ell = \Psi^\top \mathbf{f}(\vartheta, p)$$

- Evaluate error estimators for $\hat{\mathbf{y}}^\ell(\vartheta_k)$ and its sensitivities for $0 \le k \le K$.
- If error is too large add further angles ϑ_k, compute snapshots and update reduced basis Ψ.

Proper Orthogonal Decomposition
Decay of Eigenvalues

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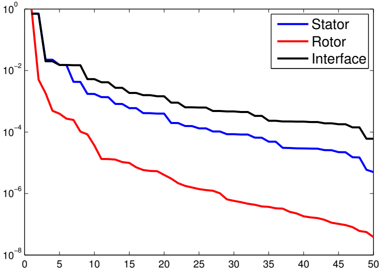
Choice of ℓ (energy represented by reduced basis):

$$\varepsilon(\ell) = \frac{\sum_{i=1}^{\ell} \lambda^i}{\sum_{i=1}^{d} \lambda^i}$$

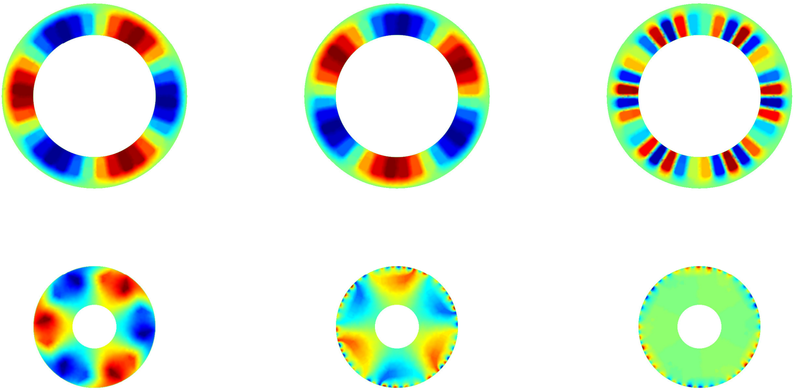
We consider independent models for the stator and rotor. The interface is not being reduced.



Reduced order model: The model is of size $\ell_s + \ell_r + N_I$

$$\begin{pmatrix} \Psi_s^\top \mathbf{K}_{ss} \Psi_s & 0 & \Psi_s^\top \mathbf{K}_{sI} \\ 0 & \Psi_r^\top \mathbf{K}_{rr}(p) \Psi_r & \Psi_r^\top \mathbf{K}_{rI}(\vartheta^k) \\ \mathbf{K}_{sI}^\top \Psi_s & \mathbf{K}_{rI}^\top(\vartheta) \Psi_r & \mathbf{K}_{II}(\vartheta^k) \end{pmatrix} \begin{pmatrix} \hat{\mathbf{y}}_s^\ell \\ \hat{\mathbf{y}}_r^\ell \\ \hat{\mathbf{y}}_I^\ell \end{pmatrix} = \begin{pmatrix} \Psi_s^\top \mathbf{f}_s \\ \Psi_r^\top \mathbf{f}_r(x) \\ \mathbf{f}_I(\vartheta^k) \end{pmatrix}$$

Proper Orthogonal Decomposition
POD Basis Vectors



First three POD basis vectors for the stator (top) and rotor (bottom)

Sensitivities and Error Estimator for ROM

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Fast and accurate computation of derivatives required during the robust optimization. The n-**th order sensitivity equation** is given by ($p \in \mathbb{R}$)

$$\mathbf{K}(\vartheta, x)\mathbf{y}^n = \mathbf{f}^{(n)}(\vartheta, x) - \sum_{k=1}^{n} \binom{n}{k} \mathbf{K}^{(k)}(\vartheta, x)\mathbf{y}^{(n-k)}$$

The derivatives $\mathbf{K}^{(k)}$ and $\mathbf{f}^{(n)}$ are given by the derivatives of $\theta_{\mathbf{K}}^{(i)}$ and $\theta_{\mathbf{f}}^{(i)}$.

Sensitivities and Error Estimator for ROM

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$$\mathbf{K}(\vartheta, x)\mathbf{y}^n = \mathbf{f}^{(n)}(\vartheta, x) - \sum_{k=1}^{n} \binom{n}{k} \mathbf{K}^{(k)}(\vartheta, x)\mathbf{y}^{(n-k)}$$

The derivatives $\mathbf{K}^{(k)}$ and $\mathbf{f}^{(n)}$ are given by the derivatives of $\theta_{\mathbf{K}}^{(i)}$ and $\theta_{\mathbf{f}}^{(i)}$.

A posteriori error estimator: Check the accuracy of the ROM by using cf. [Patera, Rozza 2006; Rozza, Huynh, Patera 2008]

$$\|\mathbf{y}^n(\vartheta, x) - \hat{\mathbf{y}}^{\ell,n}(\vartheta, x)\|_Y \leq \Delta\mathbf{y}^n := \frac{\|r^n(\hat{\mathbf{y}}^{\ell,n}, \vartheta, x)\|_{Y^*}}{\alpha(\vartheta, x)} + \sum_{k=1}^{n} \binom{n}{k} \frac{\gamma^k(\vartheta, p)}{\alpha(\vartheta, p)} \Delta\mathbf{y}^{n-k}$$

$\alpha(\vartheta, x)$ coercivity constant, $\gamma^k(\vartheta, x)$ continuity constant.

Remark: Similar for derivatives w.r.t. p, usually nonlinear influence over the right hand side, i.e., $\mathbf{f}(\vartheta, x, p) = n(p)\mathbf{f}(\vartheta, x)$.

Numerical Results

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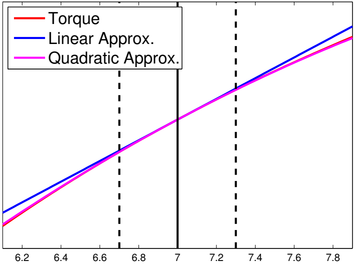
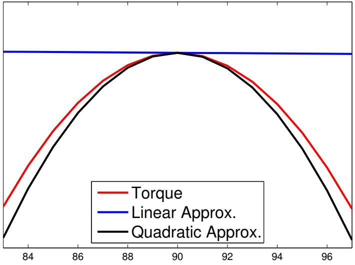
Setting:

- FEM Discretization: 42061 nodes, 900 nodes on the Interface
- ROM Settings: Tolerance for error indicator is 10^{-2}
- OPT Settings: Stopping at relative error of 10^{-4}
- Linear approximation for uncertainty in optimization variable (± 0.3 mm)
- Quadratic approximation for uncertainty in magnetic field angle ($\pm 5^\circ$)





Numerical Results

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Results:

		V_{pm}	p	M	M^{worst}	%
	Initial	133.00	(19.00, 7.00, 7.00)	4.0622	3.9406	100
F	Nominal	62.62	(21.08, 2.97, 6.63)	4.0622	3.8780	47
E	Robust	88.90	(20.81, 4.27, 6.96)	4.2117	4.0601	67
M	Robust-Adapt	90.93	(20.82, 4.37, 6.97)	4.2246	4.0622	68
R	Nominal	62.62	(21.08, 2.97, 6.62)	4.0622	3.8786	47
O	Robust	88.83	(20.81, 4.27, 6.96)	4.2112	4.0601	67
M	Robust-Adapt	91.37	(20.82, 4.39, 6.97)	4.2273	4.0637	68

Performance:

	FEM		ROM		
	iter.	CPU time	iter.	CPU time	Factor
Nominal	14	41928	13	2508	16.72
Robust	9	300820	7	15385	19.55
Robust-Adapt	9	304875	7	14885	20.48

Numerical Results

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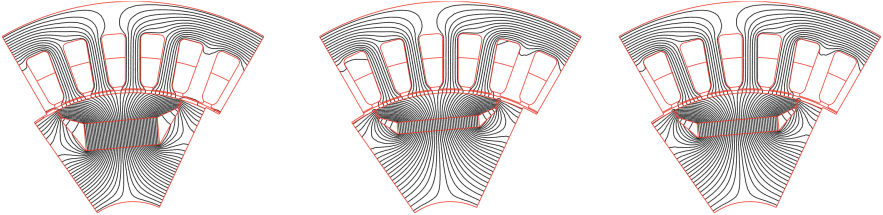

(a) (b) (c)

a) initial geometry b) nominal optimum c) robust optimum

[Lass, SU SISC 17], [Ion, Bontinck, Loukrezis, Römer, Lass, SU, Schöps, De Gersem Electr. Eng. 18]

Example: Shape Optimization under Uncertainty for Elastodynamic Wave Equations [Kolvenbach, Lass, SU OPTE 18]

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Shape optimization of load-carrying structures under uncertainty

- State equation $C(y, x; p) = 0$ given by elastodynamic wave equation
- Uncertainty $p = f_S$

State equation: Find y as weak solution of

$$\begin{aligned} \rho \ddot{y} - \nabla \cdot \sigma(y) &= f_V && \text{on } \Omega(x) \times (0, T), \\ y &= y_D && \text{on } \Gamma_D \times (0, T), \\ \sigma(y) n &= f_S && \text{on } \Gamma_N \times (0, T), \\ y(0) = 0, \quad \dot{y}(0) &= 0 && \text{on } \Omega(x). \end{aligned}$$

C_{el}	elasticity tensor
f_V	volume force
f_S	surface force
x	design variable
y	displacement

with Cauchy stress tensor $\sigma(y) = C_{el} \cdot (\nabla y + \nabla y^T)$.

Objective function:

- $h_0(y, x) := \dfrac{\|y\|^2_{L^2(0,T;L^2(\Omega(x)))}}{\text{vol}(\Omega(x))}$ (normalized L^2-displacement)

Numerical Example: Initial Geometry

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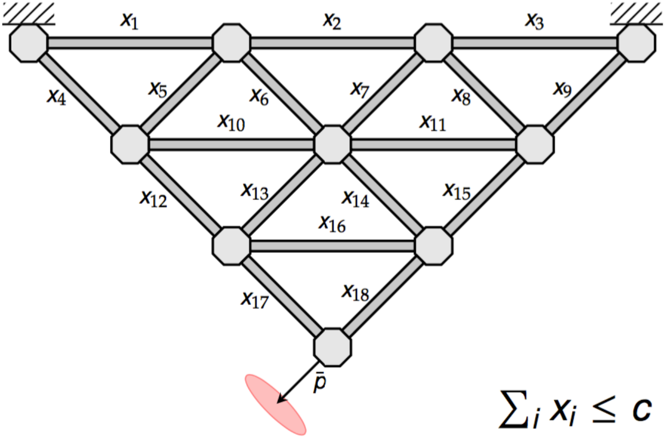

$$\sum_i x_i \leq c$$

$$a \leq x_i \leq b$$

Numerical Example

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Shape optimization of a 2D-truss under uncertain loading

- Inequality constraints only contain restrictions on the design (volume constraint, bounds on bar thickness)
- Uncertain dynamic loading on the lowermost node, Newmark time-marching
- Globalized BFGS-SQP method (GRANSO) for reduced formulation (RA2)

Considered uncertain shape optimization problem

$$\min_{y \in Y,\ x \in X} \ h_0(y, x; f_S) \quad \text{s.t.} \quad h_i(x) \leq 0,\ i \in I, \quad C(y, x; f_S) = 0$$

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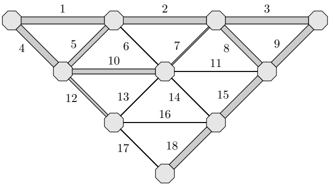
Robust optimization approach:

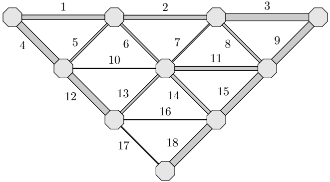
- Robust optimization with linear (RA1) or quadratic (RA2) approximation
- Uncertainty set for parameter $p = f_S$ (20%):

$$\mathcal{U}_{f_S} := \left\{ f_S : [0, T] \to \mathbb{R}^2 : \left\| f_S - \bar{f}_S \right\|_{L^2(0,T;L^2(\Omega))} \leq 0.2 \left\| \bar{f}_S \right\|_{L^2(0,T;L^2(\Omega))} \right\}, \ \bar{f}_S := \begin{pmatrix} -1 \\ -1 \end{pmatrix}.$$

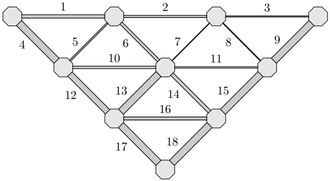
Results for 500 Time Steps



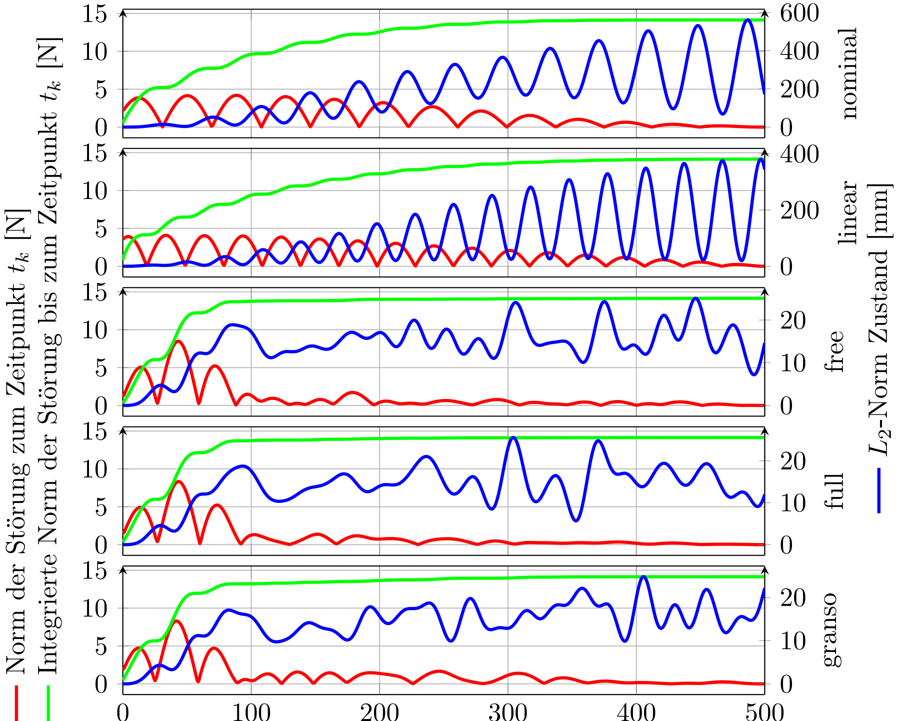
(a) Non-robust optimal solution



(b) Robust optimum, Linear approximation



(c) Robust optimum, Quadratic approximation



Norm der Störung zum Zeitpunkt t_k [N]
Integrierte Norm der Störung bis zum Zeitpunkt t_k [N]
L_2-Norm Zustand [mm]
nominal
linear
free
full
granso

Results for 500 Time Steps

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#	Formulation / Method	$\tilde{h}_0^{wc}(x)$	$h_0^{wc}(x)$	it.	PDEs
1	Reference	–	26.6344	–	–
2	Non-robust	–	99.2707	163	344
3	Linearized	1.2058	56.3082	123	506
4	Quadr. red. matrix free	7.4775	7.4775	69	14810
5	Quadr. red.	7.3219	7.3219	102	132834

$\tilde{h}_0^{wc}(x)$ Approximated worst case objective used

$h_0^{wc}(x)$ Exact worst case objective

it. Iterations

PDEs Number PDE solutions incl. linearized and adjoint solves

Video

Conclusion and Outlook

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Summary:

Second order approximation for robust counterpart of uncertain PDE-constrained optimization problems

- Worst-case values $\tilde{h}^{wc,2}(x;\bar{p})$ given by trust-region problems
- Reformulation of approximated robust counterpart using optimality conditions or duality theory
- Alternatively nonsmooth reduced formulation
- Update of expansion point
- Model order reduction with error control
- Application examples

Current work:

- Extension to topology optimization (with A. Matei)
- Time dependent unsteady motor model based on quasilinear magnetostatic approximation with reduced order models (with B. Polenz)