Surrogate Modeling in PDE Constrained Optimization

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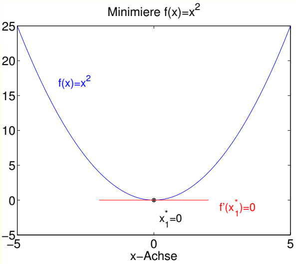
Projection Based Model Reduction:
RB Methods, POD, and Low Rank Tensor Approximations, November 23-29, 2014

Universität Konstanz

Minimization with Inequality Constraints

- **"Problem"**: min $\{f(x) = x^2 \,:\, -\infty < x < \infty\}$
- **Optimality condition**: $f'(x_1^*) \overset{!}{=} 0$ with $f'(x) = 2x$
- **Solution**: $x_1^* = 0$



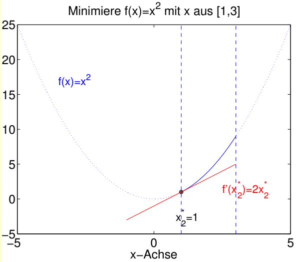
- **Problem**: min $\{f(x) = x^2 \,:\, 1 \le x \le 3\}$
- **Lagrange functional**:

$$L(x, \mu_a, \mu_b) = f(x) + \mu_a(1 - x) + \mu_b(x - 3)$$

- **Optimality condition**:

$$\begin{pmatrix} f'(x_2^*) - \mu_a^* + \mu_b^* \\ \mu_a^*(1 - x_2^*) \\ \mu_b^*(x_2^* - 3) \end{pmatrix} \overset{!}{=} \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \Leftrightarrow \underbrace{f'(x_2^*)(x - x_2^*)}_{2(x-1)} \ge 0 \;\forall x \in [1,3]$$

- **Solution**: $x_2^* = 1$, $\mu_a^* = 2$, $\mu_b^* = 0$



Outline of Lecture 2

- **Quadratic Programming (QP) Problems**
- **Extensions to Nonlinear PDE Constrained Optimization**

Quadratic Programming (QP) Problems

Topics:

- Linear-quadratic optimal control problems
- POD-Galerkin schemes for first-order optimality system
- A-priori and a-posteriori error analysis
- Basis updates
- Regularized state constraints

Linear-Quadratic, Time-Variant Optimal Control Problem

- **Quadratic programming (QP) problem**:

$$\min_{x=(y,u)} J(x) = \frac{1}{2}\|y(t_f)-y_d\|_H^2 + \frac{\kappa}{2}\int_{t_\circ}^{t_f}\|u(t)\|_U^2\,\mathrm{d}t$$

subject to the linear evolution problem

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle y(t),\varphi\rangle_H + a(t;y(t),\varphi) = \langle (f+\mathscr{B}u)(t),\varphi\rangle_{V',V} \quad \forall\varphi\in V \text{ a.e. in } (t_\circ,t_f]$$

with $y(t_\circ)=y_\circ$ in H and to bilateral control constraints

$$u\in\mathscr{U}_{ad} = \{\tilde u\in\mathscr{U}\,|\,u_a(t)\le\tilde u(t)\le u_b(t)\text{ a.e. in }[t_\circ,t_f]\}$$

- **State**: $y(t)\in V\hookrightarrow H$ with Hilbert spaces V, H
- **Control (Hilbert) space**: $\mathscr{U}=L^2(t_\circ,t_f;U)$ with $U=\mathbb{R}^{N_u}$, $U=L^2(\Omega)$ or $U=L^2(\Gamma)$
- **Input/control**: $u\in\mathscr{U}_{ad}$ (boundary or distributed control)
- **Bilinear form**: $a(t;\cdot,\cdot)$ continuous and $a(t;\varphi,\varphi)\ge\gamma_1\|\varphi\|_V^2-\gamma_2\|\varphi\|_H^2$
- **Control operator**: $\mathscr{B}:\mathscr{U}\to L^2(t_\circ,t_f;V')$ linear, bounded
- Applicable also for **elliptic control problems** (Kahlbacher/V.'12, Tonn/Urban/V.'11, Tröltzsch/V.'09)

First-Order Necessary and Sufficient Optimality Conditions

- **Quadratic programming (QP) problem**:

$$\min_{x=(y,u)} J(x) = \frac{1}{2}\,\|y(t_f)-y_d\|_H^2 + \frac{\kappa}{2}\int_{t_\circ}^{t_f} \|u(t)\|_U^2\,\mathrm{d}t$$

$$\text{s.t. } \frac{\mathrm{d}}{\mathrm{d}t}\langle y(t),\varphi\rangle_H + a(t;y(t),\varphi) = \langle (f+\mathscr{B}u)(t),\varphi\rangle_{V',V}\ \forall\varphi\in V \text{ a.e. in } (t_\circ,t_f]$$

$$y(t_\circ) = y_\circ \text{ in } H \quad \text{and} \quad u_a(t)\le u(t)\le u_b(t),\ t\in[t_\circ,t_f]$$

- Optimal state $\bar{y}$, optimal control $\bar{u}\in\mathscr{U}_{ad} = \{u\,|\,u_a\le u\le u_b \text{ in } [t_\circ,t_f]\}$
- **Adjoint/dual equation**:

$$-\frac{\mathrm{d}}{\mathrm{d}t}\langle \bar{p}(t),\varphi\rangle_H + a(t;\varphi,\bar{p}(t)) = 0\ \forall\varphi\in V \text{ a.e. in } [t_\circ,t_f), \quad \bar{p}(t_f) = \bar{y}(t_f)-y_d$$

- **Variational inequality**:

$$\int_{t_\circ}^{t_f} \big\langle \kappa\bar{u}(t) - (\mathscr{B}^\star\bar{p})(t), u(t)-\bar{u}(t)\big\rangle_U\,\mathrm{d}t \ge 0 \quad \forall u\in\mathscr{U}_{ad} \qquad \textbf{(VI)}$$

- **Reduced cost**: $\hat{J}(u) = J(\hat{y}+\mathscr{S}u,u)$ with $\hat{J}'(\bar{u}) = \kappa\bar{u}-\mathscr{B}^\star\bar{p}\in\mathscr{U}$, i.e.,

$$\big\langle \hat{J}'(\bar{u}), u(t)-\bar{u}(t)\big\rangle_{\mathscr{U}} \ge 0 \quad \forall u\in\mathscr{U}_{ad}$$

POD Galerkin for the State Variable

- **Particular solution**: $\hat{y} \in W(t_\circ, t_f)$ solves $\hat{y}(t_\circ) = y_\circ$ in H and

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \hat{y}(t), \varphi\rangle_H + a(t; \hat{y}(t), \varphi) = \langle f(t), \varphi\rangle_{V',V} \quad \forall \varphi \in V \text{ a.e. in } (t_\circ, t_f]$$

- **POD space**: $V^\ell = \operatorname{span}\{\psi_1, \ldots, \psi_\ell\} \subset V$
- **POD control-to-state mapping**: $\mathscr{S}^\ell : \mathscr{U} \to W(t_\circ, t_f)$, $w^\ell = \mathscr{S}^\ell u$ solves $w^\ell(t_\circ) = 0$ in H and

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle w^\ell(t), \psi\rangle_H + a(t; w^\ell(t), \psi) = \langle (\mathscr{B}u)(t), \psi\rangle_{V',V} \quad \forall \psi \in V^\ell \text{ a.e. in } (t_\circ, t_f]$$

  $\Rightarrow \mathscr{S}^\ell$ linear and bounded
- **POD state**: $y^\ell = \hat{y} + \mathscr{S}^\ell u$
- **Previous theorem with a-priori results for the state**:
  a) $y^\ell(0) = y_\circ$ in H, i.e., no POD error in the initial condition
  b) $\|(\mathscr{S} - \mathscr{S}^\ell)u\|^2_{W(t_\circ,t_f)} \le \sum_{i>\ell} \lambda_i(u)$
  c) $\|\mathscr{S} - \mathscr{S}^\ell\|_{\mathscr{L}(\mathscr{U}, W(t_\circ,t_f))} \to 0$ for $\ell \to \infty$

POD Galerkin for the Dual Variable (Balancing POD)

- **Adjoint/dual equation**:

$$-\frac{\mathrm{d}}{\mathrm{d}t}\langle p(t),\varphi\rangle_H + a(t;\varphi,p(t)) = 0 \;\forall\varphi\in V \text{ a.e. in } [t_\circ,t_f), \quad p(t_f) = y(t_f) - y_d$$

- **Terminal condition**: $p(t_f) = y(t_f) - y_d = (\hat{y} + \mathscr{S}u)(t_f) - y_d = \hat{y}(t_f) - y_d + (\mathscr{S}u)(t_f)$
- **Particular solution**: $\hat{p} \in W(t_\circ,t_f)$ solves

$$-\frac{\mathrm{d}}{\mathrm{d}t}\langle \hat{p}(t),\varphi\rangle_H + a(t;\varphi,\hat{p}(t)) = 0 \;\forall\varphi\in V \text{ a.e. in } [t_\circ,t_f), \quad \hat{p}(t_f) = \hat{y}(t_f) - y_d$$

- **Dual solution operator**: $\mathscr{A} : \mathscr{U} \to W(t_\circ,t_f)$, $v = \mathscr{A}u$ solves

$$-\frac{\mathrm{d}}{\mathrm{d}t}\langle v(t),\varphi\rangle_H + a(t;\varphi,v(t)) = 0 \;\forall\varphi\in V \text{ a.e. in } [t_\circ,t_f), \quad v(t_f) = (\mathscr{S}u)(t_f)$$

- **POD dual solution operator**: $\mathscr{A}^\ell : \mathscr{U} \to W(t_\circ,t_f)$, $v^\ell = \mathscr{A}^\ell u$ solves

$$-\frac{\mathrm{d}}{\mathrm{d}t}\langle v^\ell(t),\psi\rangle_H + a(t;\psi,v^\ell(t)) = 0 \;\forall\psi\in V^\ell \text{ a.e. in } [t_\circ,t_f), \quad v^\ell(t_f) = (\mathscr{S}^\ell u)(t_f) \in V^\ell$$

$\Rightarrow$ same POD basis for state and adjoint variable

POD A-Priori Analysis for the Dual Variable

- **Continuous variant of POD**: for $\ell \in \{1,\dots,d\}$ solve

$$\min \sum_{k=1}^{\wp} \int_{t_\circ}^{t_f} \Big\| y^k(t) - \sum_{i=1}^{\ell} \langle y^k(t), \psi_i \rangle_X \, \psi_i \Big\|_X^2 \mathrm{d}t \text{ s.t. } \{\psi_i\}_{i=1}^{\ell} \subset X,\ \langle \psi_i, \psi_j \rangle_X = \delta_{ij},\ 1 \le i,j \le \ell \quad (\mathbf{P}_\infty^\ell)$$

Theorem (Hinze/V.'08, Tröltzsch/V.'09, Gubisch/V.'13)

$X = V$, $\mathscr{V} = \mathrm{span}\,\{y^k(t)\,|\,t \in [t_\circ, t_f],\ 1 \le k \le \wp\}$

a) *Snapshots* $y^1 = \mathscr{S}u$, $y^2 = \mathscr{A}u$, $p = \hat{p} + \mathscr{A}u$, $p^\ell = \hat{p} + \mathscr{A}^\ell u$:

$$\|p - p^\ell\|_{W(t_\circ,t_f)}^2 \le C_1 \Big(\sum_{i>\ell} \lambda_i + \|y_t^1 - \mathscr{P}^\ell y_t^1\|_{L^2(t_\circ,t_f;V)}^2 + \|y_t^2 - \mathscr{P}^\ell y_t^2\|_{L^2(t_\circ,t_f;V')}^2 \Big)$$

b) *Snapshots* $y^1 = \mathscr{S}u$, $y^2 = \mathscr{A}u$, $y^3 = (\mathscr{S}u)_t$, $y^4 = (\mathscr{A}u)_t$, *all in* $L^2(t_\circ, t_f; V)$:

$$\|p - p^\ell\|_{W(t_\circ,t_f)}^2 \le C_2 \sum_{i>\ell} \lambda_i$$

c) *If* $\mathscr{S}\tilde{u}, \mathscr{A}\tilde{u} \in H^1(t_\circ, t_f; V)$ *for all* $\tilde{u} \in \mathscr{U}$, *then* $\lim_{\ell\to\infty} \|\mathscr{A} - \mathscr{A}^\ell\|_{\mathscr{L}(\mathscr{U}, W(t_\circ,t_f))} = 0$

In particular, $\lim_{\ell\to\infty} \|p(\tilde{u}) - p^\ell(\tilde{u})\|_{W(t_\circ,t_f)} = 0$ *for any* $\tilde{u} \in \mathscr{U}$

POD Approximation of the Variational Inequality

- **Variational inequality**:

$$\int_{t_\circ}^{t_f} \langle \kappa \bar u(t) - (\mathscr{B}^\star \bar p)(t), u(t) - \bar u(t) \rangle_U \, \mathrm{d}t \ge 0 \quad \forall u \in \mathscr{U}_{ad} \qquad \textbf{(VI)}$$

- **Optimal POD solutions**: $\bar u^\ell \in \mathscr{U}_{ad}$, $\bar y^\ell = \hat y + \mathscr{S}^\ell \bar u^\ell$, $\bar p^\ell = \hat p + \mathscr{A}^\ell \bar u^\ell$
- **POD variational inequality**:

$$\int_{t_\circ}^{t_f} \langle \kappa \bar u^\ell(t) - (\mathscr{B}^\star \bar p^\ell)(t), u(t) - \bar u^\ell(t) \rangle_U \, \mathrm{d}t \ge 0 \quad \forall u \in \mathscr{U}_{ad} \qquad (\textbf{VI}^\ell)$$

- **A-priori analysis**: choose $u = \bar u^\ell$ in **(VI)**, $u = \bar u$ in $(\textbf{VI}^\ell)$ and add

$$\begin{aligned} 0 &\le \int_{t_\circ}^{t_f} \langle \kappa(\bar u - \bar u^\ell)(t) - (\mathscr{B}^\star(\bar p - \bar p^\ell))(t), \bar u^\ell(t) - \bar u(t) \rangle_U \, \mathrm{d}t \\ &= -\kappa \|\bar u - \bar u^\ell\|_{\mathscr{U}}^2 - \underbrace{\int_{t_\circ}^{t_f} \langle (\mathscr{B}^\star(\bar p - \bar p^\ell))(t), \bar u^\ell(t) - \bar u(t) \rangle_U \, \mathrm{d}t}_{\le C \|(\mathscr{A} - \mathscr{A}^\ell)\bar u\|_{L^2(t_\circ, t_f; V)} \|\bar u^\ell - \bar u\|_{\mathscr{U}}} \end{aligned}$$

Convergence Result for the POD Suboptimal Control

- **Continuous variant of POD**: for $\ell \in \{1,\ldots,d\}$ solve

$$\min \sum_{k=1}^{\wp} \int_{t_\circ}^{t_f} \Big\| y^k(t) - \sum_{i=1}^{\ell} \langle y^k(t), \psi_i \rangle_X \, \psi_i \Big\|_X^2 \, \mathrm{d}t \text{ s.t. } \{\psi_i\}_{i=1}^{\ell} \subset X,\ \langle \psi_i, \psi_j \rangle_X = \delta_{ij},\ 1 \le i,j \le \ell \quad (\mathbf{P}_\infty^\ell)$$

Theorem (Hinze/V.'08, Tröltzsch/V.'09, Gubisch/V.'13)

$X = V$, $\mathscr{V} = \mathrm{span}\,\{y^k(t) \,|\, t \in [t_\circ, t_f],\ 1 \le k \le \wp\}$

a) *Snapshots* $y^1 = \mathscr{S}\bar{u}$, $y^2 = \mathscr{A}\bar{u}$, $y^3 = (\mathscr{S}\bar{u})_t$, $y^4 = (\mathscr{A}\bar{u})_t$, *all in* $L^2(t_\circ, t_f; V)$:

$$\|\bar{u} - \bar{u}^\ell\|_{W(t_\circ,t_f)}^2 \le C_2 \sum_{i>\ell} \lambda_i$$

b) *If* $\mathscr{S}\tilde{u}, \mathscr{A}\tilde{u} \in H^1(t_\circ, t_f; V)$ *for all* $\tilde{u} \in \mathscr{U}$*, then* $\lim_{\ell\to\infty} \|\bar{u} - \bar{u}^\ell\|_{\mathscr{U}} = 0$

Perturbation Analysis (Malanowski/Büskens/Maurer'97)

- **Variational inequality**:

$$\int_{t_\circ}^{t_f} \langle \kappa \bar{u}(t) - (\mathscr{B}^\star \bar{p})(t), u(t) - \bar{u}(t) \rangle_U \, \mathrm{d}t \geq 0 \quad \forall u \in \mathscr{U}_{ad} \qquad \textbf{(VI)}$$

- **Misfit in the variational inequality**: suboptimal $\bar{u}^\ell \in \mathscr{U}_{ad}$

$$\int_{t_\circ}^{t_f} \langle \kappa \bar{u}^\ell(t) - (\mathscr{B}^\star \tilde{p}^\ell)(t), u(t) - \bar{u}^\ell(t) \rangle_U \, \mathrm{d}t \not\geq 0 \quad \forall u \in \mathscr{U}_{ad}$$

with $\tilde{p}^\ell = \hat{p} + \mathscr{A}\bar{u}^\ell$

- **Perturbation analysis**: there exists a perturbation $\zeta^\ell \in \mathscr{U}$ satisfying

$$\int_{t_\circ}^{t_f} \langle \kappa \bar{u}^\ell(t) - (\mathscr{B}^\star \tilde{p}^\ell)(t) + \zeta^\ell(t), u(t) - \bar{u}^\ell(t) \rangle_U \, \mathrm{d}t \geq 0 \quad \forall u \in \mathscr{U}_{ad} \qquad (\widetilde{\textbf{VI}}^\ell)$$

- **A-posteriori analysis**: choose $u = \bar{u}^\ell$ in (**VI**), $u = \bar{u}$ in ($\widetilde{\textbf{VI}}^\ell$) and add

$$\kappa \|\bar{u} - \bar{u}^\ell\|_{\mathscr{U}}^2 \leq \int_{t_\circ}^{t_f} \langle (\mathscr{B}^\star \mathscr{A}(\bar{u}^\ell - \bar{u})) + \zeta^\ell(t), \bar{u}^\ell(t) - \bar{u}(t) \rangle_U \, \mathrm{d}t$$

since $\tilde{p}^\ell - \bar{p} = \mathscr{A}(\bar{u}^\ell - \bar{u})$

- **Estimate for the control**: $\|\bar{u} - \bar{u}^\ell\|_{\mathscr{U}} \leq \dfrac{1}{\kappa} \|\zeta^\ell\|_{\mathscr{U}}$

Convergence Result for the Perturbation

- **Estimate for the control**: $\|\bar{u} - \bar{u}^\ell\|_{\mathscr{U}} \leq \frac{1}{\kappa} \|\zeta^\ell\|_{\mathscr{U}}$ and $\tilde{p}^\ell = \hat{p} + \mathscr{A}\bar{u}^\ell$
- **Computation of ζ^ℓ**: $\zeta^\ell(t) = \begin{cases} -\big(\kappa\bar{u}^\ell(t) - (\mathscr{B}^\star\tilde{p}^\ell)(t)\big) & \text{if } u_a(t) < \bar{u}^\ell(t) < u_b(t) \\ -\min\big(0, \kappa\bar{u}^\ell(t) - (\mathscr{B}^\star\tilde{p}^\ell)(t)\big) & \text{if } \bar{u}^\ell(t) = u_a(t) \\ -\max\big(0, \kappa\bar{u}^\ell(t) - (\mathscr{B}^\star\tilde{p}^\ell)(t)\big) & \text{if } \bar{u}^\ell(t) = u_b(t) \end{cases}$

  i.e., $\zeta^\ell = \zeta^\ell(\bar{u}^\ell) \Rightarrow$ a-posteriori error analysis for suboptimal $\bar{u}^\ell$

Theorem (Tröltzsch/V.'09, Gubisch/V.'13)

$X = V$, $\mathscr{V} = \operatorname{span}\{y^k(t)\,|\,t \in [t_\circ, t_f],\ 1 \leq k \leq \wp\}$

a) *Snapshots* $y^1 = \mathscr{S}\bar{u}$, $y^2 = \mathscr{A}\bar{u}$, $y^3 = (\mathscr{S}\bar{u})_t$, $y^4 = (\mathscr{A}\bar{u})_t$, *all in* $L^2(t_\circ, t_f; V)$:

$$\|\zeta^\ell\|^2_{\mathscr{U}} \leq C \sum_{i>\ell} \lambda_i$$

b) *If* $\mathscr{S}\tilde{u}, \mathscr{A}\tilde{u} \in H^1(t_\circ, t_f; V)$ *for all* $\tilde{u} \in \mathscr{U}$, *then* $\lim_{\ell\to\infty} \|\zeta^\ell\|_{\mathscr{U}} = 0$

Algorithm with POD A-Posteriori Analysis

- **Estimate for the control**: $\|\bar{u}-\bar{u}^\ell\|_{\mathscr{U}} \le \frac{1}{\kappa}\|\zeta^\ell\|_{\mathscr{U}}$ and $\tilde{p}^\ell = \hat{p} + \mathscr{A}\bar{u}^\ell$
- **Computation of ζ^ℓ**: $\zeta^\ell(t) = \begin{cases} -\big(\kappa\bar{u}^\ell(t) - (\mathscr{B}^\star\tilde{p}^\ell)(t)\big) & \text{if } u_a(t) < \bar{u}^\ell(t) < u_b(t) \\ -\min\big(0, \kappa\bar{u}^\ell(t) - (\mathscr{B}^\star\tilde{p}^\ell)(t)\big) & \text{if } \bar{u}^\ell(t) = u_a(t) \\ -\max\big(0, \kappa\bar{u}^\ell(t) - (\mathscr{B}^\star\tilde{p}^\ell)(t)\big) & \text{if } \bar{u}^\ell(t) = u_b(t) \end{cases}$

Algorithmus 1 (*Optimal control with a-posteriori error estimation*)

(1) Choose $\ell_{\max}$ and POD basis $\{\psi_i\}_{i=1}^{\ell}$ for the Galerkin approximation of the LQ problem;
(2) Determine the reduced-order model for the LQ problem;
(3) Calculate suboptimal control $\bar{u}^\ell \in \mathscr{U}_{ad}$, e.g., by a semismooth Newton method;
(4) Compute perturbation $\bar{\zeta}^\ell = \zeta^\ell(\bar{u}^\ell)$;
(5) **IF** $\|\bar{\zeta}^\ell\|_{\mathscr{U}}/\kappa > \mathrm{TOL}$ **AND** $\ell < \ell_{\max}$ **THEN**
  Enlarge ℓ and go back to (2);
 ELSE
  Stop;
 ENDIF

- Applicable for **balanced-truncation** (Vossen/V.'12) or **reduced-basis method** (Tonn/Urban/V.'11)
- Error estimation between **high-** and **low-dimensional discretization** (Gubisch/Neitzel)

Numerical Example: Problem Formulation and Optimal Control (Studinger'12, Studinger/V.'13)

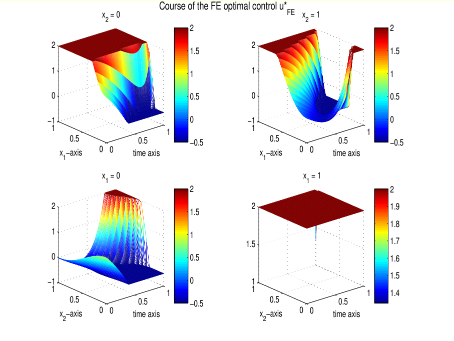
- **Consider**:

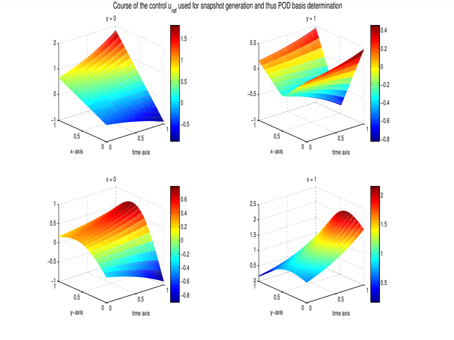
$$\min J(y,u) = \frac{1}{2}\int_\Omega |y(t_f) - y^d|^2 \,\mathrm{d}x + \frac{1}{200}\int_0^{t_f}\int_\Gamma |u|^2 \,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t$$

$$\text{s.t. } y_t + 0.1\Delta y = 0 \text{ in } Q,\ \frac{\partial y}{\partial n} + \frac{y}{100} = u \text{ on } \Sigma,\ y(0) = y_\circ \text{ in } \Omega = (0,1)^2$$

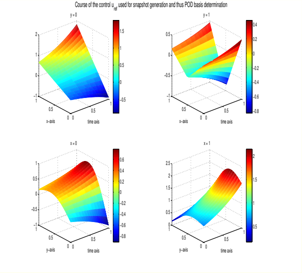
$$-0.5 \le u \le 2 \text{ on } \Sigma = (0,t_f)\times\Gamma$$

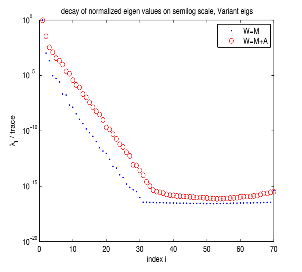
- **Method & Discretization**: semismooth Newton & implizit Euler, finite elements

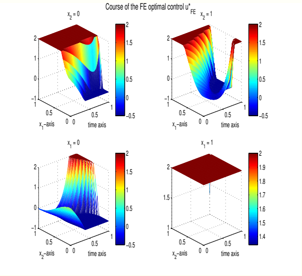




Numerical Example: POD Error Analysis (Studinger'12, Studinger/V.'13)







A-posteriori error: $\|\bar{u} - \bar{u}^\ell\|_{\mathscr{U}} \leq \dfrac{1}{\kappa}\|\zeta^\ell(\bar{u}^\ell)\|_{\mathscr{U}} =: \varepsilon_{\text{ape}}$

ℓ	ε_{ape}	$\|\bar{u}^h - \bar{u}^\ell\|$	$\frac{\varepsilon_{\text{ape}}}{\|\bar{u}-\bar{u}^\ell\|}$	ε_{ape}	$\|\bar{u}^h - \bar{u}^\ell\|$	$\frac{\varepsilon_{\text{ape}}}{\|\bar{u}-\bar{u}^\ell\|}$
5	$1.3 \cdot 10^{-0}$	$9.1 \cdot 10^{-1}$	1.32	$6.5 \cdot 10^{-1}$	$5.6 \cdot 10^{-1}$	1.16
20	$5.9 \cdot 10^{-1}$	$3.2 \cdot 10^{-1}$	1.84	$7.5 \cdot 10^{-3}$	$7.3 \cdot 10^{-3}$	1.03
60	$1.4 \cdot 10^{-2}$	$1.2 \cdot 10^{-2}$	1.17	$8.3 \cdot 10^{-5}$	$8.3 \cdot 10^{-5}$	1.00
70	$1.2 \cdot 10^{-2}$	$1.1 \cdot 10^{-2}$	1.10	$3.0 \cdot 10^{-5}$	$3.0 \cdot 10^{-5}$	1.00
90	$1.1 \cdot 10^{-2}$	$9.7 \cdot 10^{-3}$	1.13	$3.7 \cdot 10^{-6}$	$3.7 \cdot 10^{-6}$	1.00

Problem: optimal FE control $\bar{u}^h$ is unknown $\Rightarrow$ POD basis update

Optimality-System POD (OS-POD) (Kunisch/V.'08)

- **Original problem**: $\min \hat{J}(u) = J(y(u),u)$ s.t. $u \in \mathscr{U}_{ad}$
- **POD-Galerkin approximation**:

$$\min \hat{J}^\ell(u) = J(y^\ell(u),u) \quad \text{s.t.} \quad u \in \mathscr{U}_{ad} \qquad (\hat{\mathbf{P}}^\ell)$$

- **OSPOD-Problem**:

$$\min \hat{\mathscr{J}}^\ell(u) = J(y^\ell(u),u) \quad \text{s.t.} \begin{cases} y = y(u), \quad \psi_i = \psi_i(u) \text{ for } 1 \le i \le \ell \\ \mathscr{R}\psi_i = \int_{t_\circ}^{t_f} \langle y(t), \psi_i \rangle_X \, y(t)\, \mathrm{d}t = \lambda_i \psi_i, \; 1 \le i \le \ell \end{cases} \qquad (\hat{\mathbf{P}}^\ell_{\mathrm{ospod}})$$

  $\to$ more complex than the original problem
- **Numerical realization**: operator splitting
  - choose an initial control $u^{(0)}$ and a corresponding POD basis $\{\psi_i^{(0)}\}_{i=1}^\ell$
  - improve the POD basis by applying a few gradient projection steps for $(\hat{\mathbf{P}}^\ell_{\mathrm{ospod}})$
  - compute an approximate solution to $(\hat{\mathbf{P}}^\ell)$ by Algorithm 1
- **Efficient combination with a-posteriori error estimator** (Grimm'13, Grimm/Gubisch/V.'14, V.'11)

Algorithm for A-Posteriori Error with OS-POD (Grimm'13, Grimm/Gubisch/V.'14, V.'11)

- **OS-POD-Problem**:

$$\min \hat{\mathscr{J}}^\ell(u) = J(y^\ell(u), u) \quad \text{s.t.} \begin{cases} y = y(u), \quad \psi_i = \psi_i(u) \text{ for } 1 \le i \le \ell \\ \mathscr{R}\psi_i = \int_{t_\circ}^{t_f} \langle y(t), \psi_i \rangle_X \, y(t)\, \mathrm{d}t = \lambda_i \psi_i, \; 1 \le i \le \ell \end{cases} \qquad (\hat{\mathbf{P}}^\ell_{\text{ospod}})$$

Algorithmus 1 (*Optimal control with a-posteriori error estimation*)

(1) Choose initial control u^0 and number of basis elements $\ell < \ell_{\max}$;
(2) Perform k OS-POD gradient steps to get u^k and $\{\psi_i(u^k)\}_{i=1}^{\ell}$;

---

(3) Determine the reduced-order model for the LQ problem;
(4) Calculate suboptimal control $\bar{u}^\ell \in \mathscr{U}_{ad}$, e.g., by a semismooth Newton method;
(5) Compute perturbation $\bar{\zeta}^\ell = \zeta^\ell(\bar{u}^\ell)$;
(6) **IF** $\|\bar{\zeta}^\ell\|_{\mathscr{U}}/\kappa > \mathrm{TOL}$ **AND** $\ell < \ell_{\max}$ **THEN**
  Enlarge ℓ and go back to (3);
 ELSE
  Stop;
 ENDIF

- **Algorithm**: apply a few gradient steps for $(\hat{\mathbf{P}}^\ell_{\text{ospod}})$ and continue with fixed POD basis
- **Stopping criterium**: $\|\bar{\zeta}^\ell\|_{\mathscr{U}}/\kappa = \mathscr{O}(\Delta t^\alpha + \Delta x^\beta)$

OS-POD for linear-quadratic, control constrained control (Grimm'13, Grimm/Gubisch/V.'14, V.'11)

- **Consider**:

$$\min J(y,u) = \frac{1}{2}\int_\Omega \left|y(t_f) - y^d\right|^2 \mathrm{d}x + \frac{1}{20}\int_0^{t_f}\int_\Gamma |u|^2 \,\mathrm{d}\boldsymbol{x}\mathrm{d}t$$

$$\text{s.t. } y_t + 0.1\Delta y = 0 \text{ in } Q,\ \frac{\partial y}{\partial n} + \frac{y}{100} = u \text{ on } \Sigma,\ y(0) = y_\circ \text{ in } \Omega = (0,1)^2$$

$$-0 \le u \le 1 \text{ on } \Sigma = (0,t_f)\times\Gamma$$

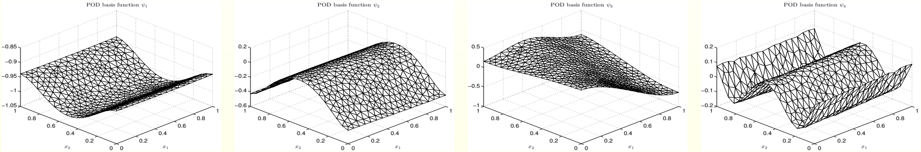
- **Method & Discretization**: semismooth Newton & implizit Euler, finite elements

	$k=0$	$k=1$	$k=2$	with u_{FE}
required ℓ	35	40	13	13
CPU	110.77 sec	147.14 sec	18.39 sec	11.48 sec
$\Vert\zeta^\ell\Vert/\sigma_u$	$3.43\cdot10^{-3}$	$1.14\cdot10^{-2}$	$2.82\cdot10^{-3}$	$1.94\cdot10^{-3}$
e^u_{abs}	$3.15\cdot10^{-3}$	$9.53\cdot10^{-3}$	$2.62\cdot10^{-3}$	$1.93\cdot10^{-3}$
e^u_{rel}	$2.45\cdot10^{-3}$	$7.73\cdot10^{-3}$	$2.15\cdot10^{-3}$	$1.59\cdot10^{-3}$
e^y_{abs}	$1.59\cdot10^{-2}$	$3.10\cdot10^{-3}$	$7.55\cdot10^{-4}$	$1.92\cdot10^{-4}$
e^y_{rel}	$5.75\cdot10^{-3}$	$1.12\cdot10^{-3}$	$2.73\cdot10^{-4}$	$6.97\cdot10^{-5}$

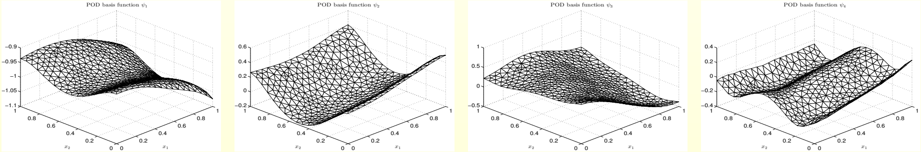
	$k=0$	$k=1$	$k=2$	with u_{FE}
$\Vert\zeta^{15}\Vert/\sigma_u$	$2.50\cdot10^{-2}$	$1.45\cdot10^{-2}$	$2.27\cdot10^{-3}$	$1.59\cdot10^{-3}$
e^u_{abs}	$2.06\cdot10^{-2}$	$1.19\cdot10^{-2}$	$2.07\cdot10^{-3}$	$1.59\cdot10^{-3}$
e^u_{rel}	$1.65\cdot10^{-2}$	$9.65\cdot10^{-3}$	$1.67\cdot10^{-3}$	$1.30\cdot10^{-3}$
e^y_{abs}	$2.59\cdot10^{-2}$	$6.34\cdot10^{-3}$	$6.42\cdot10^{-4}$	$6.91\cdot10^{-5}$
e^y_{rel}	$9.34\cdot10^{-3}$	$2.29\cdot10^{-3}$	$2.32\cdot10^{-4}$	$2.51\cdot10^{-5}$
different u_a	96	67	15	16(2233)
different u_b	63	38	6	4 (3891)

Convergence of the POD basis (Grimm'13, Grimm/Gubisch/V.'14, Kunisch/Müller'14)

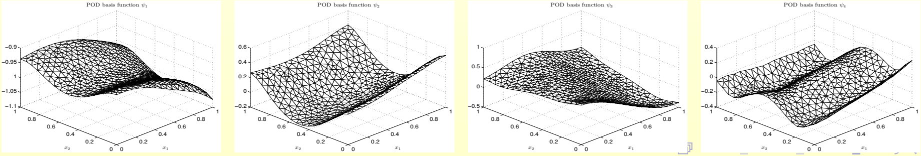
- First four POD basis functions generated from $u = 0$:



- First four POD basis functions generated from the optimal control $\bar{u}^h$:



- First four POD basis functions generated after $k = 2$ OS-POD gradient steps:



Problem with Mixed Control-State Constraints (Tröltzsch'05)

- **(Abstract) linear-quadratic problem**:

$$\min_{x=(y,u)} J(x) = \frac{1}{2}\|y(t_f)-y_d\|_H^2 + \frac{\kappa}{2}\int_{t_\circ}^{t_f}\|u(t)\|_U^2\,\mathrm{d}t$$

$$\text{s.t.}\quad \frac{\mathrm{d}}{\mathrm{d}t}\langle y(t),\varphi\rangle_H + a(t;y(t),\varphi) = \langle (f+\mathscr{B}u)(t),\varphi\rangle_{V',V}\ \forall\varphi\in V \text{ a.e. in } (t_\circ,t_f]$$

$$y(t_\circ)=y_\circ \text{ in } H \quad\text{and}\quad u_a(t)\le \varepsilon u(t)+(\mathscr{I}y)(t)\le u_b(t),\ t\in[t_\circ,t_f]$$

- **Control space**: $\mathscr{U} = L^2(t_\circ,t_f;U)$ with $U=\mathbb{R}^{N_u}$
- **Input/control operator**: $(\mathscr{B}u)(t,x) = \sum_{i=1}^{N_u} u_i(t)\chi_{\Omega_i}(x)$
- **State operator**: $(\mathscr{I}y)(t) = \big(\int_{\Omega_i} y(t,x)\,\mathrm{d}x/|\Omega_i|\big)_{1\le i\le N_u}$
- **State constraints**: $\varepsilon\to 0$
- **Particular solution**: $\hat y\in W(t_\circ,t_f)$ solves $\hat y(t_\circ)=y_\circ$ in H and

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \hat y(t),\varphi\rangle_H + a(t;\hat y(t),\varphi) = \langle f(t),\varphi\rangle_{V',V}\quad \forall\varphi\in V \text{ a.e. in } (t_\circ,t_f]$$

- **Control-to-state mapping**: $\mathscr{S}:\mathscr{U}\to W(t_\circ,t_f)$, $w=\mathscr{S}u$ solves $w(t_\circ)=0$ in H and

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle w(t),\varphi\rangle_H + a(t;w(t),\varphi) = \langle (\mathscr{B}u)(t),\varphi\rangle_{V',V}\quad \forall\varphi\in V \text{ a.e. in } (t_\circ,t_f]$$

- **Inequality constraints**: $v_a(t) := (u_a-\mathscr{I}\hat y)(t) \le (\varepsilon u+\mathscr{I}\mathscr{S}u)(t) \le (u_b-\mathscr{I}\hat y) =: v_b(t)$

Formulation as a Control Constrained Problem

- **Solution representation**: $u \mapsto y(u) = \hat{y} + \mathscr{S}u$
- **Inequality constraints**: $v_a(t) := (u_a - \mathscr{I}\hat{y})(t) \leq (\varepsilon u + \mathscr{I}\mathscr{S}u)(t) \leq (u_b - \mathscr{I}\hat{y}) =: v_b(t)$
- **Transformation of variables**: $v := \mathscr{F}u$ with $\mathscr{F} = \varepsilon + \mathscr{I}\mathscr{S}$, i.e. $y = \hat{y} + \mathscr{S}u = \hat{y} + \mathscr{S}\mathscr{F}^{-1}v$
- **Transformed, linear-quadratic problem**:

$$\min_v J(\hat{y} + \mathscr{S}\mathscr{F}^{-1}v, \mathscr{F}^{-1}v) = \cdots + \frac{\kappa}{2}\left\|\mathscr{F}^{-1}v\right\|^2$$

$$\text{s.t.} \quad v \in V_{\mathrm{ad}} = \left\{\tilde{v} \,|\, v_a(t) \leq \tilde{v}(t) \leq v_b(t) \text{ for } t \in [t_\circ, t_f]\right\}$$

$\Rightarrow$ form of the previous linear-quadratic optimal control problem

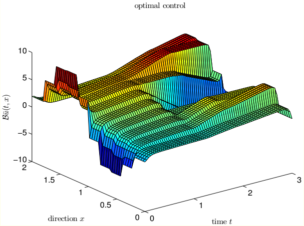
- **Variational inequality**:

$$\left\langle \kappa\mathscr{F}^{-\star}\mathscr{F}^{-1}\bar{v}(t) - \mathscr{B}^\star\bar{p}(t), v(t) - \bar{v}(t)\right\rangle_{\mathscr{U}} \geq 0 \quad \forall v \in V_{ad}$$

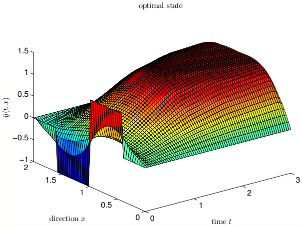
- **POD Galerkin scheme**: additional analysis for $\mathscr{F}^\ell \approx \mathscr{F}$
- **A-posteriori error estimate** (Gubisch/V'14): $\|\bar{u} - \bar{u}^\ell\| \leq \frac{1}{\kappa}\|\mathscr{F}\|_{\mathscr{L}(\mathscr{U})}\|\zeta^\ell\|$ with computable ζ^ℓ
- **Convergence result** (Gubisch/V'14): $\|\zeta^\ell\| \to 0$ for $\ell \to \infty$

Numerical Example: POD basis update (Afanasiev/Hinze'01, Gubisch/V.'14)

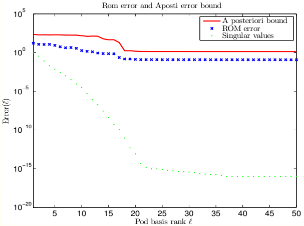
- **Optimal control problem**: heat equation, control space $\mathscr{U} = L^2(0,3;\mathbb{R}^{10})$, $\varepsilon =$1e-5



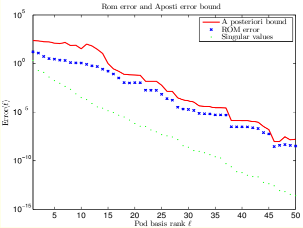
Optimal control



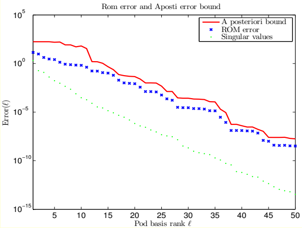
Optimal state



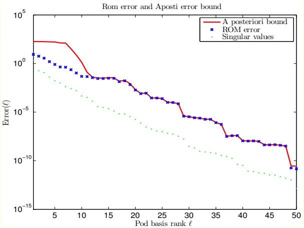
POD basis with $u = 1$



POD basis update



POD basis with $u = \bar{u}$



POD basis update ($\varepsilon =$1e-3)

State and Control Constrained Linear-Quadratic Optimal Control Problem

- **Quadratic programming (QP) problem**:

$$\min_{x=(y,u)} J(x) = \frac{1}{2}\,\|y(t_f) - y_d\|^2_{L^2(\Omega)} + \frac{\kappa}{2}\int_{t_\circ}^{t_f} \|u(t)\|_U^2 \,\mathrm{d}t$$

subject to the linear evolution problem

$$\langle y_t(t),\varphi\rangle + a(t;y(t)(t),\varphi) = \langle (f+\mathscr{B}u)(t),\varphi\rangle \quad \forall \varphi \in V \text{ in } (t_\circ, t_f]$$

with $y(t_\circ) = y_\circ$ and to bilateral control constraints

$$u \in \mathscr{U}_{ad} = \big\{ v \in \mathscr{U} \,|\, u_a(t) \le v(t) \le u_b(t) \text{ in } [t_\circ, t_f] \big\}$$

$$y \in \big\{ z \in L^2(Q) \,|\, y_a(t,\boldsymbol{x}) \le z(t,\boldsymbol{x}) \le y_b(t,\boldsymbol{x}) \text{ in } Q \big\}$$

- **Lavrentiev regularization**: $\varepsilon > 0$ and $x = (y,u)$

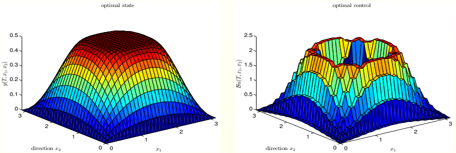
$$J(x,w) = \frac{1}{2}\,\|y(t_f) - y_d\|^2_{L^2(\Omega)} + \frac{\kappa}{2}\int_{t_\circ}^{t_f} \|u(t)\|_U^2 \,\mathrm{d}t + \frac{\sigma}{2}\int_{t_\circ}^{t_f} \|w(t)\|^2_{L^2(\Omega)} \,\mathrm{d}t$$

$$(y,w) \in \big\{ (z,v) \in L^2(Q) \in L^2(Q) \,|\, y_a(t,\boldsymbol{x}) \le \varepsilon v(t,\boldsymbol{x}) + z(t,\boldsymbol{x}) \le y_b(t,\boldsymbol{x}) \text{ in } Q \big\}$$

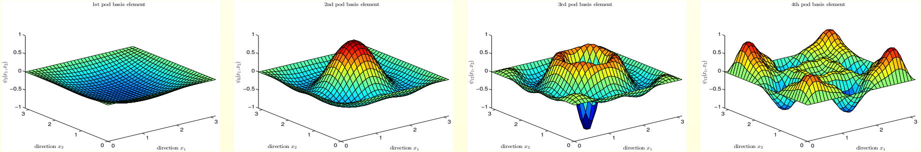
- **Regular Lagrange multipliers** (Tröltzsch'05): formulation as a control constrained problem
- **A-posteriori error** (Gubisch'14): extension of the analysis from the control-constrained case ⇒OS-POD also applicable

Numerical Example: State and Control Constraints (Gubisch'14, Grimm/Gubisch/V.'14)

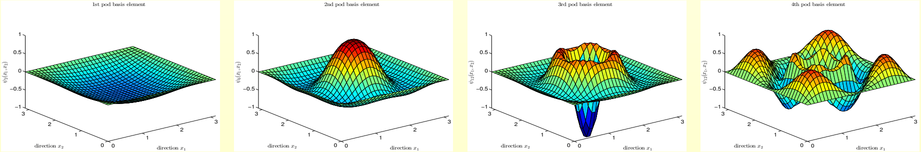
- Two-dimensional heat equation
- Distributed control
- Semismooth Newton method



- First four POD basis functions generated from the optimal control $\bar{u}$:



- First four POD basis functions generated after three OS-POD gradient steps:



Related Literature

- Afanasiev, Dede, Fahl, Grepl, Hinze, Kärcher, Manzoni, Negri, Quarteroni, Rozza, Sachs, Schu...

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Extensions to Nonlinear PDE Constrained Optimization

Topics:

- Inexact sequential quadratic programming (SQP)
- A-posteriori error analysis
- Trust-region POD

Sequential Quadratic Programming (SQP)

- **Infinite dimensional optimization**:

$$\min J(x) \quad \text{s.t.} \quad e(x) = 0,\; g(x) \leq 0 \tag{P}$$

- **Lagrange functional for (P)**: $\mathscr{L}(x,p,q) = J(x) + \langle e(x), p\rangle + \langle g(x), q\rangle$
- **(Local) SQP method**: at $z_k = (x_k, p_k, q_k)$ solve

$$\begin{cases} \min\limits_{x_\delta} \mathscr{L}_x(z_k)x_\delta + \dfrac{1}{2}\mathscr{L}_{xx}(z_k)(x_\delta, x_\delta) \\ \text{ s.t. } e(x_k) + e'(x_k)x_\delta = 0,\; g(x_k) + g'(x_k)x_\delta \leq 0 \end{cases} \tag{QP^k}$$

- **KKT system for equality constraints**: solution $\bar{x}_\delta$ to (**QP**^{k}) is characterized by

$$\underbrace{\begin{pmatrix} \mathscr{L}_{xx}(z_k) & e'(x_k)^\star \\ e'(x_k) & 0 \end{pmatrix}}_{A_k} \cdot \underbrace{\begin{pmatrix} \bar{x}_\delta \\ \bar{p}_\delta \end{pmatrix}}_{\bar{z}_\delta} = \underbrace{- \begin{pmatrix} \mathscr{L}_x(z_k) \\ e(x_k) \end{pmatrix}}_{b_k}$$

Inexact SQP by Using POD or RB

- **KKT system**: solution $\bar{x}_\delta$ to $(\mathbf{QP}^k)$ is characterized by

$$\underbrace{\begin{pmatrix} \mathscr{L}_{xx}(z_k) & e'(x_k)^\star \\ e'(x_k) & 0 \end{pmatrix}}_{A_k} \cdot \underbrace{\begin{pmatrix} \bar{x}_\delta \\ \bar{p}_\delta \end{pmatrix}}_{\bar{z}_\delta} = \underbrace{-\begin{pmatrix} \mathscr{L}_x(z_k) \\ e(x_k) \end{pmatrix}}_{b_k}$$

- **KKT system**: inexact solve of $A_k\bar{z}_\delta = b_k$ by discretization
- **Discretization**: (POD or RB or BT or...) model reduction

$$A_k^\ell \bar{z}_\delta^\ell = b_k^\ell \in \mathbb{R}^n, \quad n = n(\ell)$$

- **Convergence of (local) SQP method**: $\bar{z}_\delta^\ell$ reduced-order solution

$$\|A_k \mathscr{P} \bar{z}_\delta^\ell - b_k\| = \mathscr{O}\big(\|\mathscr{L}'(z_k)\|^q\big), \quad q \in [1,2]$$

  with prolongation $\mathscr{P}$
- **Rate of convergence**: superlinear $(1 < q < 2)$, quadratic $(q = 2)$
- **Control of reduced-order approach**:

$$\|A_k \mathscr{P} \bar{z}_\delta^\ell - b_k\| \simeq \|\bar{z}_\delta - \mathscr{P}\bar{z}_\delta^\ell\| \simeq \|\mathscr{L}'(z_k)\|^q$$

Convergence Result

- **Variables in optimal control**: $x = (y, u)$, $y = y(u)$
- **KKT system**: $z_k = (x_k, p_k)$, $x_k = (y_k, u_k)$

$$\left(\begin{array}{cc|c} \mathscr{L}_{yy}(z_k) & \mathscr{L}_{yu}(z_k) & e_y(x_k)^\star \\ \mathscr{L}_{uy}(z_k) & \mathscr{L}_{uu}(z_k) & e_u(x_k)^\star \\ \hline e_y(x_k) & e_u(x_k) & 0 \end{array}\right) \begin{pmatrix} y_\delta \\ u_\delta \\ p_\delta \end{pmatrix} = \begin{pmatrix} -\mathscr{L}_y(z_k) \\ -\mathscr{L}_u(z_k) \\ -e(x_k) \end{pmatrix}$$

- **Suboptimal solution to KKT system**: $\bar z_\delta^\ell = (\bar y_\delta^\ell, \bar u_\delta^\ell, \bar p_\delta^\ell)$
- **Prolongation $\mathscr{P}$**: $\bar z_\delta^\ell \mapsto \mathscr{P}\bar z_\delta^\ell = (\tilde y_\delta, \bar u_\delta^\ell, \tilde p_\delta)$ with

$$e_y(x_k)\tilde y_\delta = -e(x_k) - e_u(x_k)\bar u_\delta^\ell$$
$$e_y(x_k)^\star \tilde p_\delta = -\mathscr{L}_y(z_k) - \mathscr{L}_{yy}(z_k)\tilde y - \mathscr{L}_{yu}(z_k)\bar u_\delta^\ell$$

$\rightarrow$ a-posteriori error computable

Theorem (Kahlbacher/V.'12)

Second-order sufficient optimality implies

$$\lim_{k\to\infty} z_k + \mathscr{P}\bar z_\delta^\ell = \bar z \quad \textit{if} \quad \|A_k \mathscr{P}\bar z_\delta^\ell - b_k\| \simeq \|\bar u_\delta - \bar u_\delta^\ell\| < \mathrm{TOL}$$

Multilevel Approach with Reduced-Order Models

- **Convergence criterium**: $\|A_k \mathscr{P} \bar{z}_\delta^\ell - b_k\| \simeq \|\bar{u}_\delta - \bar{u}_\delta^\ell\| < \mathrm{TOL}$
- **A-posteriori error** (Tröltzsch/V.'09):

$$\|\bar{u}_\delta - \bar{u}_\delta^\ell\| \simeq \|\underbrace{\mathscr{L}_{uy}(z_k)\tilde{y}_\delta + \mathscr{L}_{uu}(z_k)\bar{u}_\delta^\ell + e_u(x_k)^\star \tilde{p}_\delta + \mathscr{L}_u(z_k)}_{:=-\bar{\zeta}^\ell}\|$$

  with $\|\bar{\zeta}^\ell\| \to 0$ for $\ell \to \infty$
- **Convergence of $\|\bar{\zeta}^\ell\|$**: no rate, basis dependent (Hinze/V.'08)
- **POD basis**: combination with Optimality-System POD (Metzdorf'15)
- **Combination with FE adaptivity**: (Clever/Lang/Ulbrich/Ziems)
- **Reduced approach**: $\min \hat{J}(u) = J(y(u), u)$
- **QP problem**: for given iterate u^k solve

$$\min q^k(u_\delta) = \hat{J}(u^k) + \hat{J}'(u^k)u_\delta + \frac{1}{2}\hat{J}''(u^k)(u_\delta, u_\delta)$$

- **Globalization by inexact trust-region**: inexact cost $q_\ell^k \approx q^k$ and inexact solution of

$$\min q_\ell^k(u_\delta) = \hat{J}_\ell(u^k) + \hat{J}_\ell'(u^k)u_\delta + \frac{1}{2}\hat{J}_\ell''(u^k)(u_\delta, u_\delta) \quad \text{s.t.} \quad \|u_\delta\| \le \Delta_k$$

- **Convergence criterium**: Carter condition $\|\hat{J}'(u^k) - \hat{J}_\ell'(u^k)\| \le \zeta \|\hat{J}_\ell'(u^k)\|$ with $\zeta \in (0,1)$
- **Trust-region POD**: (Arian/Fahl/Sachs'00, Schu/Sachs'12) and (Rogg'14)

Related Literature

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