PDE Constrained Optimization Utilizing Reduced-Order Modeling

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Outline of Lecture 2

- Quadratic Programming (QP) Problems
- 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**:

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

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

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

- 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**:

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

- **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**: $V^\ell = \mathrm{span}\,\{\psi_1, \ldots, \psi_\ell\} \subset V$
- **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) $\|(\mathscr{S} - \mathscr{S}^\ell)u\|^2_{W(t_\circ, t_f)} \leq \sum_{i>\ell} \lambda_i(u)$
  c) $\|\mathscr{S} - \mathscr{S}^\ell\|_{\mathscr{L}(\mathscr{U}, V)} \to 0$ 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

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

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

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

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

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

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* $L^2(t_\circ, t_f; V)$:

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

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* $\lim_{\ell\to\infty} \|\mathscr{A} - \mathscr{A}^\ell\|_{\mathscr{L}(\mathscr{U},V)} = 0$

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**:

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

- **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**:

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

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

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

Convergence Result for the POD Suboptimal Control

- **Continuous variant of POD**: for $\ell \in \{1,\dots,d\}$ 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* $y^1 = \mathscr{S}\bar{u}$, $y^2 = \mathscr{A}\bar{u}$, $y^3 = (\mathscr{S}\bar{u})_t$, $y^4 = (\mathscr{A}\bar{u})_t$, *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**: $\|\bar u - \bar u^\ell\|_{\mathscr U} \le \frac{1}{\kappa}\|\zeta^\ell\|_{\mathscr U}$ and $\tilde p^\ell = \hat p + \mathscr A \bar u^\ell$
- **Computation of ζ^ℓ**: $\zeta^\ell(t) = \begin{cases} -\big(\kappa \bar u^\ell(t) - (\mathscr B^\star \tilde p^\ell)(t)\big) & \text{if } u_a(t) < \bar u^\ell(t) < u_b(t) \\ -\min\big(0, \kappa \bar u^\ell(t) - (\mathscr B^\star \tilde p^\ell)(t)\big) & \text{if } \bar u^\ell(t) = u_a(t) \\ -\max\big(0, \kappa \bar u^\ell(t) - (\mathscr B^\star \tilde p^\ell)(t)\big) & \text{if } \bar u^\ell(t) = u_b(t) \end{cases}$

  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)

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

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* $L^2(t_\circ, t_f; V)$:

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

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**: $\zeta^\ell(t) = \begin{cases} -\left(\kappa\bar{u}^\ell(t) - (\mathscr{B}^\star\tilde{p}^\ell)(t)\right) & \text{if } u_a(t) < \bar{u}^\ell(t) < u_b(t) \\ -\min\left(0, \kappa\bar{u}^\ell(t) - (\mathscr{B}^\star\tilde{p}^\ell)(t)\right) & \text{if } \bar{u}^\ell(t) = u_a(t) \\ -\max\left(0, \kappa\bar{u}^\ell(t) - (\mathscr{B}^\star\tilde{p}^\ell)(t)\right) & \text{if } \bar{u}^\ell(t) = u_b(t) \end{cases}$

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/V.'13)

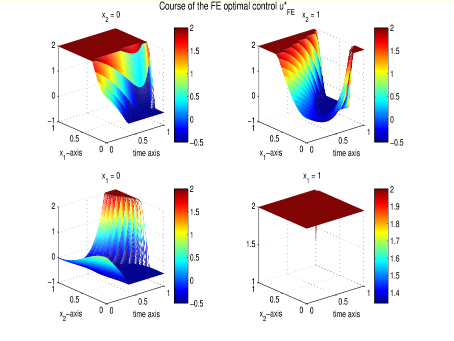
- **Consider**:

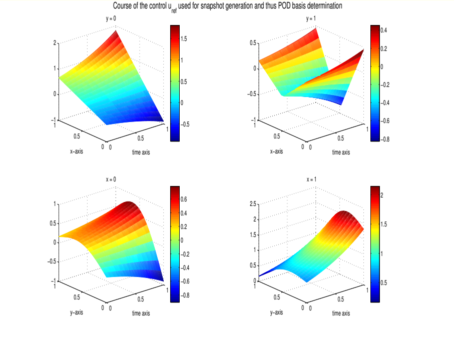
$$\min J(y,u) = \frac{1}{2}\int_\Omega |y(t_f) - y^d|^2\,\mathrm{d}x + \frac{1}{200}\int_0^{t_f}\int_\Gamma |u|^2\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t$$

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

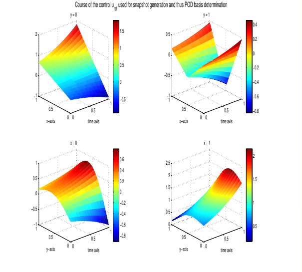
$$-0.5 \le u \le 2 \text{ on } \Sigma = (0,t_f) \times \Gamma$$

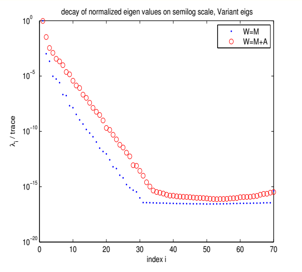
- **Method & Discretization**: semismooth Newton & implizit Euler, finite elements

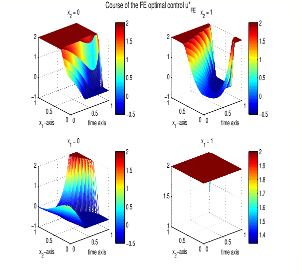




Numerical Example: POD Error Analysis (Studinger/V.'13)







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

ℓ	$\varepsilon_{\mathrm{ape}}$	$\|\bar u^h - \bar u^\ell\|$	$\frac{\varepsilon_{\mathrm{ape}}}{\|\bar u - \bar u^\ell\|}$	$\varepsilon_{\mathrm{ape}}$	$\|\bar u^h - \bar u^\ell\|$	$\frac{\varepsilon_{\mathrm{ape}}}{\|\bar u - \bar u^\ell\|}$
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

Optimality-System POD (OSPOD) (Grimm/V.'13, Kunisch/V.'08, V.'11)

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

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

- **OSPOD-Problem**:

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

  $\rightarrow$ 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/V.'13, V.'13)

Numerical example for A-Posteriori Error with OSPOD Basis Update (Grimm/V.'13)

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

- **Algorithm**: apply a few gradient steps for $(\hat{\mathbf{P}}^\ell_{\text{ospod}})$ and continue by Algorithm 1
- **Stopping criterium**: $\|\bar{\zeta}^\ell\|_{\mathscr{U}}/\kappa < \mathrm{TOL} = \min(\Delta t, \Delta x^2) = 1\text{e-}4$, $\ell_{\max} = 30$
- **No basis update**: $\ell = 10 \nearrow 30$, $\|\bar{\zeta}^{30}\|_{\mathscr{U}}/\kappa \approx 1.2\text{e-}2$, 48 s for Alg. 1
- **1 OSPOD gradient step**: $\ell = 10 \nearrow 30$, $\|\bar{\zeta}^{30}\|_{\mathscr{U}}/\kappa \approx 5\text{e-}3$, 4.0 s (OSPOD) + 47 s for Alg. 1
- **2 OSPOD gradient steps**: $\ell = 10 \nearrow 13$, $\|\bar{\zeta}^{13}\|_{\mathscr{U}}/\kappa < \mathrm{TOL}$, 6.3 s (OSPOD) + 8.1 s for Alg. 1

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

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

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

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

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

- **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**:

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

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

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

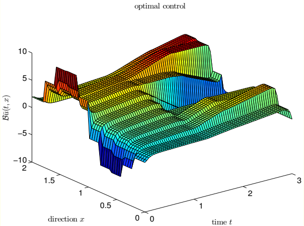
- **Variational inequality**:

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

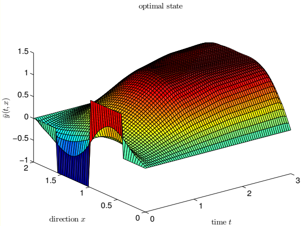
- **POD Galerkin scheme**: additional analysis for $\mathscr{F}^\ell \approx \mathscr{F}$
- **A-posteriori error estimate**: $\|\bar{u} - \bar{u}^\ell\| \leq \frac{1}{\kappa}\|\mathscr{F}\|_{\mathscr{L}(\mathscr{U})}\|\zeta^\ell\|$ with computable ζ^ℓ
- **Convergence result**: $\|\zeta^\ell\| \to 0$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

Numerical Example: POD basis update (Afanasiev/Hinze'01, Gubisch/V.'13)

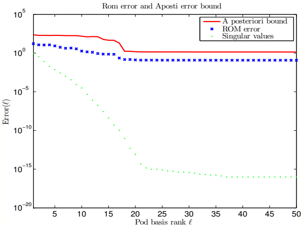
- **Optimal control problem**: heat equation, control space $\mathscr{U} = L^2(0,3;\mathbb{R}^{10})$, $\varepsilon =$1e-5



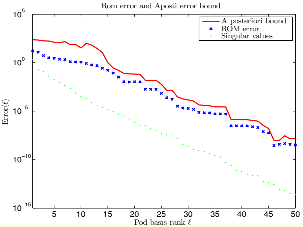
Optimal control



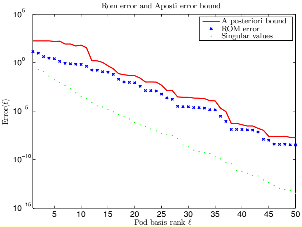
Optimal state



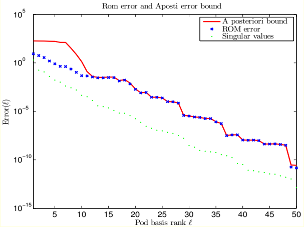
POD basis with $u = 1$



POD basis update



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



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

Related Literature

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

- M. Gubisch and S. Volkwein: *POD a-posteriori error analysis for optimal control problems with mixed control-state constraints*, 2013
- M. Hinze, S. V.: *Error estimates for abstract linear-quadratic optimal control problems using POD*, 2008
- M. Kahlbacher, S.V.: *POD a-posteriori error based inexact SQP method for bilinear elliptic optimal control problems*, 2012
- A. Studinger, S.V.: *Numerical analysis of POD a-posteriori error estimation for optimal control*, 2013
- T. Tonn, K. Urban, S.V.: *Comparison of the reduced-basis and POD a-posteriori error estimators for an elliptic linear-quadratic optimal control problem*, 2011
- F. Tröltzsch, S. V.: *POD a-posteriori error estimates for linear-quadratic optimal control problems*, 2009
- S.V.: *Optimality system POD and a-posteriori error analysis for linear-quadratic problems*, 2011

Nonlinear PDE Constrained Optimization

Topics:

- Inexact sequential quadratic programming (SQP)
- A-posteriori error control for nonlinear problems

Sequential Quadratic Programming (SQP)

- **Infinite dimensional optimization**:

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

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

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

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

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

Inexact SQP by Using POD or RB

- **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**: $z_k = (x_k, p_k)$, $x_k = (y_k, u_k)$

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

- **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

$$e_y(x_k)\tilde{y}_\delta = -e(x_k) - e_u(x_k)\bar{u}_\delta^\ell$$

$$e_y(x_k)^\star\tilde{p}_\delta = -\mathcal{L}_y(z_k) - \mathcal{L}_{yy}(z_k)\tilde{y} - \mathcal{L}_{yu}(z_k)\bar{u}_\delta^\ell$$

$\rightarrow$ a-posteriori error computable

Theorem (Kahlbacher/V.'12)

Second-order sufficient optimality implies

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

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 (V.'11)
- **Nonlinear optimization approach**: Trust-Region POD (Arian/Fahl/Sachs'00, Schu/Sachs'07)
- **Combination with FE adaptivity**: (Clever/Lang/Ulbrich/Ziems)

Numerical experiments (Kahlbacher/V.'12)

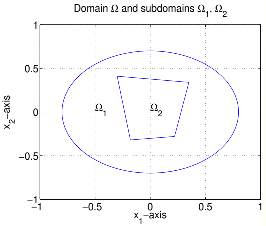
- **Optimal control problem**:

$$\min \frac{1}{2}\int_{\Omega_m} |y-y^d|^2\,\mathrm{d}x + \frac{\kappa}{2}\sum_{i=1}^{n_\Omega} |\Omega_i||u_i-u_i^\circ|^2$$

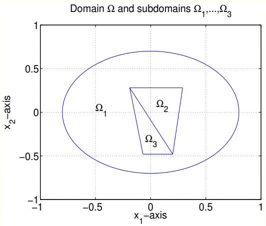
$$\text{s.t. } u_i \geq 0, \quad -\Delta y + y\sum_{i=1}^{n_\Omega} u_i\chi_{\Omega_i} = f \text{ in } \Omega,\ \frac{\partial y}{\partial n} + y = g \text{ on } \Gamma$$

- **Given data**: y^d, u_i°, $\kappa > 0$, f, g
- **Globalisation of SQP**:
  - modification of the hessian
  - Armijo linesearch with ℓ_1 merit function
- **Equality constraint case**: $\bar{x} = (\bar{y}, \bar{u})$ with inactive $\bar{u} > 0$

Numerical examples (Kahlbacher/V.'12)



Reference control: u°
Desired state: $y(u^\circ)+$ noise
Measurement domain: $\Omega_m \subsetneq \Omega$



SQP it.	$\Vert\mathscr{L}'(z_k)\Vert$	a-post.
$k=0$	1.38e-0	1.16e−3
$k=1$	8.53e-1	8.36e−2
$k=2$	2.57e-1	7.87e−5
$k=3$	4.65e-3	5.67e−6
$k=4$	3.05e-5	1.90e−6
$k=5$	4.66e-9	—

SQP it.	$\Vert\mathscr{L}'(z_k)\Vert$	a-post.
$k=0$	3.01e-2	1.58e-3
$k=1$	4.48e-1	7.44e-4
$k=2$	3.63e-1	3.46e-4
$k=3$	5.16e-2	4.04e-5
$k=4$	1.48e-2	4.98e-4
$k=5$	1.62e-3	6.56e-4
$k=6$	7.51e-7	—

Elliptic-Parabolic Systems Arising in Battery Models (DFN'96, WXZ'06)

- **Coupled nonlinear parameterized PDE system**: $\Omega = (0, L)$

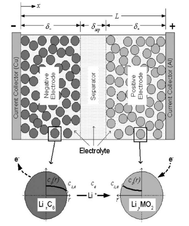
$$\begin{aligned} y_t - \nabla \cdot (D \nabla y) - \mathscr{F}(y,p,q;\mu) &= 0 && \text{in } Q = (t_\circ, t_f) \times \Omega \\ -\nabla \cdot (\kappa(y;\mu) \nabla p) - \mathscr{F}(y,p,q;\mu) &= 0 && \text{in } Q \\ -\nabla \cdot (\sigma \nabla q) + \mathscr{F}(y,p,q;\mu) &= 0 && \text{in } Q \end{aligned}$$

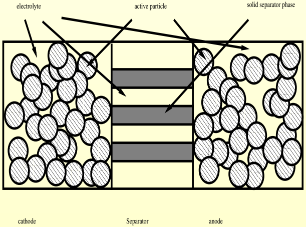
$\rightarrow$ concentration y and potentials p, q

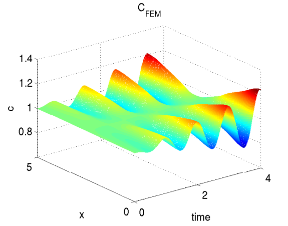
- **Parameterized nonlinearities**: $\mu = (\mu_1, \mu_2, \mu_3, \mu_4) \in \mathbb{R}^4$

$$\kappa(y;\mu) = (1 + \mu_4 y)^3, \quad \mathscr{F}(y,p,q;\mu) = \begin{cases} \mu_2 \sqrt{y} \sinh(\mu_1 (q - p - \ln y)) & \text{in } \Omega_s^1 \\ 0 & \text{in } \Omega_e \\ \mu_3 \sqrt{y} \sinh(\mu_1 (q - p - \ln y)) & \text{in } \Omega_s^2 \end{cases}$$

- **Boundary conditions**: $y_x(t,\cdot) = p_x(t,\cdot) = 0$, $q(t,0) = 0$ (uniqueness), $\sigma q_x(t,L) = I(t)$







Variational Formulation of the PDEs

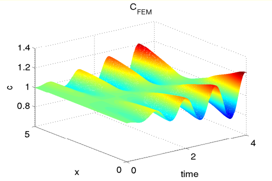
- **Coupled nonlinear parameterized PDE system**: $\Omega = (0, L)$

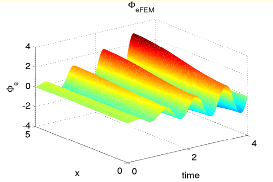
$$
\begin{aligned}
y_t - \nabla \cdot (D \nabla y) - \mathscr{F}(y, p, q; \mu) &= 0 && \text{in } Q = (t_\circ, t_f) \times \Omega \\
-\nabla \cdot (\kappa(y; \mu) \nabla p) - \mathscr{F}(y, p, q; \mu) &= 0 && \text{in } Q \\
-\nabla \cdot (\sigma \nabla q) + \mathscr{F}(y, p, q; \mu) &= 0 && \text{in } Q
\end{aligned}
$$

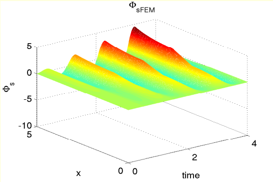
  and boundary conditions

- **Variational formulation**: $V_0 = \{\varphi \in V : \varphi(0) = 0\} \subset V = H^1(\Omega)$

$$
\begin{aligned}
\int_\Omega y_t \varphi + D \nabla y \cdot \nabla \varphi - \mathscr{F}(y, p, q; \mu) \varphi \, \mathrm{d}x &= 0 && \forall \varphi \in V \\
\int_\Omega \kappa(y; \mu) \nabla p \cdot \nabla \varphi - \mathscr{F}(y, p, q; \mu) \varphi \, \mathrm{d}x &= 0 && \forall \varphi \in V \\
\int_\Omega \sigma \nabla q \cdot \nabla \chi + \mathscr{F}(y, p, q; \mu) \chi \, \mathrm{d}x &= I \chi(L) && \forall \chi \in V_0
\end{aligned}
$$







Finite Element (FE) Galerkin Model (Lass/V.'13)

- **Nonlinear FE-Galerkin scheme**: $y^{\mathcal{N}}(t) = \sum_{j=1}^{\mathcal{N}} \underline{y}_j(t)\varphi_j^{\mathcal{N}}$ etc.

$$\int_\Omega y_t^{\mathcal{N}}\varphi^{\mathcal{N}} + D\nabla y^{\mathcal{N}}\cdot\nabla\varphi^{\mathcal{N}} - \mathscr{F}(y^{\mathcal{N}},p^{\mathcal{N}},q^{\mathcal{N}};\mu)\varphi^{\mathcal{N}}\,\mathrm{d}x = 0 \qquad \forall\varphi^{\mathcal{N}}\in V^{\mathcal{N}}$$
$$\int_\Omega \kappa(y^{\mathcal{N}};\mu)\nabla p^{\mathcal{N}}\cdot\nabla\varphi^{\mathcal{N}} - \mathscr{F}(y^{\mathcal{N}},p^{\mathcal{N}},q^{\mathcal{N}};\mu)\varphi^{\mathcal{N}}\,\mathrm{d}x = 0 \qquad \forall\varphi^{\mathcal{N}}\in V^{\mathcal{N}}$$
$$\int_\Omega \sigma\nabla q^{\mathcal{N}}\cdot\nabla\chi^{h} + \mathscr{F}(y^{\mathcal{N}},p^{\mathcal{N}},q^{\mathcal{N}};\mu)\chi^{\mathcal{N}}\,\mathrm{d}x = I\chi^{\mathcal{N}}(L) \qquad \forall\chi^{\mathcal{N}}\in V_0^{\mathcal{N}}$$

- **High-dimensional** (large $\mathcal{N}$) **nonlinear ODE system**:

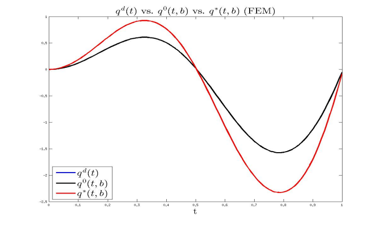
$$\mathrm{M}\underline{y}'(t)+\mathrm{S}_D\underline{y}(t)-\mathrm{F}\big(\underline{y}(t),\underline{p}(t),\underline{q}(t);\mu\big)=0, \qquad t\in(t_\circ,t_f]$$
$$\mathrm{S}_\kappa\big(\underline{y}(t);\mu\big)\underline{p}(t)-\mathrm{F}\big(\underline{y}(t),\underline{p}(t),\underline{q}(t);\mu\big)=0, \qquad t\in(t_\circ,t_f]$$
$$\mathrm{S}_\sigma\underline{q}(t)+\mathrm{F}\big(\underline{y}(t),\underline{p}(t),\underline{q}(t);\mu\big)=\underline{I}(t), \qquad t\in(t_\circ,t_f]$$

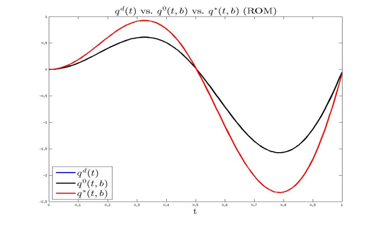
M ... mass matrix, S_* ... stiffness matrices depending on the diffusion parameters D, $\kappa(y;\mu)$, σ
$\mathrm{F}(\underline{z}(t);\mu) = \big(\int_\Omega \mathscr{F}(y^{\mathcal{N}}(t),p^{\mathcal{N}}(t),q^{\mathcal{N}}(t);\mu)\varphi_j^{\mathcal{N}}\,\mathrm{d}x\big)_j$ with coeffizient vector $\underline{z}=(\underline{y},\underline{p},\underline{q})$

- **Model reduction**: replace $\{\varphi_i^{\mathcal{N}}\}_{i=1}^{\mathcal{N}}$ by $\{\psi_i\}_{i=1}^{\ell}$ with $\ell \ll \mathcal{N}$

Parameter Estimation without Noise (Lass'13)

- **Optmization problem**: estimate $\mu = (\mu_1, \ldots, \mu_4)$ from boundary potential data $q^d(t)$
- **Cost functional**: $\hat{J}(\mu) = \frac{1}{2} \int_{t_\circ}^{t_f} |q(t, L; \mu) - q^d(t)|^2 \, \mathrm{d}x$
- **Subset selection method**: determine parameters, which can be identified (Kappel et al.'12)



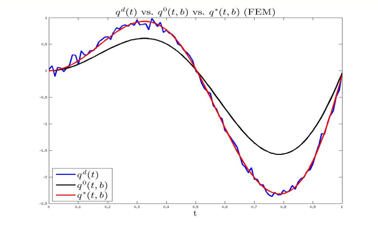


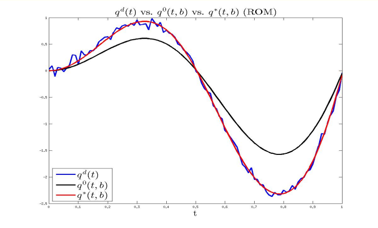
- **Numerical algorithm**: Gauss-Newton method (regularisation by subset selection)
- **Computation times** (Noise: 0%):

	CPU time	optimal parameters
FE	358.8 s	(0.80000, −0.90000, −0.20000, 0.10000)
POD	9.9 s	(0.79995, −0.90000, −0.20003, 0.10001)

Parameter Estimation with Noise (Lass'13)

- **Optmization problem**: estimate $\mu = (\mu_1, \ldots, \mu_4)$ from boundary potential data $q^d(t)$
- **Cost functional**: $\hat{J}(\mu) = \frac{1}{2} \int_{t_\circ}^{t_f} |q(t, L; \mu) - q^d(t)|^2 \, \mathrm{d}x$
- **Subset selection method**: determine parameters, which can be identified (Kappel et al.'12)





- **Numerical algorithm**: Gauss-Newton method (regularisation by subset selection)
- **Computation times** (Noise: 5%):

	CPU time	optimal parameters
FE	314.6 s	(0.77324, −0.90000, −0.19157, 0.15786)
POD	9.3 s	(0.77310, −0.90000, −0.19156, 0.15806)

A-Posteriori Analysis for Nonlinear Optimal Control Problems (Kammann/Tröltzsch/V.'12, DFG grant)

- **Reduced problem**: $\min_{\mu \in \mathfrak{D}} \hat{J}(\mu)$ with hessian $\nabla^2 \hat{J}(\mu)$
- **First-order optimality conditions**: $\nabla \hat{J}(\bar{\mu})^\top (\mu - \bar{\mu}) \geq 0$ for all $\mu \in \mathfrak{D}$
- **Second-order sufficient optimality conditions**: there is a constant $\eta = \eta(\bar{\mu}) > 0$ with

$$\mu^\top \hat{J}''(\bar{\mu})\mu \geq \eta \, \|\mu\|_2^2 \quad \forall \mu \in \mathbb{R}^4$$

$\Rightarrow \mu^\top \nabla^2 \hat{J}(\tilde{\mu})\mu \geq \frac{\eta}{2} \, \|\mu\|_2^2 \; \forall \mu \in \mathbb{R}^4, \forall \tilde{\mu} \in \mathfrak{D}_{ad}$ provided $\|\tilde{\mu} - \bar{\mu}\|_2$ sufficiently small

Theorem (Kammann/Tröltzsch/V.'13)

$\bar{\mu}$ optimal control, $\bar{\mu}^\ell$ suboptimal control. Then, second-order sufficient optimality implies

$$\|\bar{\mu} - \bar{\mu}^\ell\|_2 \leq \varepsilon_{ape} \quad \text{with} \quad \varepsilon_{ape} = \frac{2}{\eta} \, \|\zeta(\bar{\mu}^\ell)\|_2$$

provided $\|\bar{\mu} - \bar{\mu}^\ell\|_2$ is sufficiently small

- **Problem**: $\eta = \eta(\bar{\mu})$

A-Posteriori Error Analysis (Lass/V.'13)

- **Theory**: $\|\bar\mu - \bar\mu^\ell\|_2 \le \varepsilon_{\mathrm{ape}}$ with $\varepsilon_{\mathrm{ape}} = 2\|\zeta(\bar\mu^\ell)\|_2/\eta$ and $\eta = \lambda_{\min}(\nabla^2\hat J(\bar\mu))$
- **A-posteriori error**:

$$\|\bar\mu^{\mathcal N} - \bar\mu^\ell\|_2 \le \frac{2}{\lambda_{\min}(\nabla^2\hat J(\bar\mu^\ell))}\|\nabla\hat J(\bar\mu^\ell)\|_2 =: \Delta^{\mathcal N}(\bar\mu^\ell)$$

- **Results (CPU time $\approx$ 30 seconds)**:

Noise	$\|\bar\mu^{\mathcal N} - \bar\mu^\ell\|_2$	$\Delta^{\mathcal N}(\bar\mu^\ell)$
0%	5.10e-5	8.94e-2
5%	2.53e-4	3.70e-2

- **CPU times for the optimization**:

	0% noise	5% noise
FE	358.8 seconds	314.6 seconds
POD	9.9 seconds	9.3 seconds

- **Different approach**: utilize Kantorovich theory (Dihlmann/Haasdonk'13)

Related Literature

- Alla, Dihlmann, Haasdonk, Heinkenschloss, Hinze, Manzoni, Quarteroni, Rozza, Sachs, Ulbrich, Ziems...

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- E. Kammann, F. Tröltzsch, S.V.: *A method of a-posteriori error estimation with application to POD*, 2013
- K. Kunisch, S.V.: *POD for optimality systems*, 2008
- E.W. Sachs, S.V.: *POD-Galerkin approximations in PDE-constrained optimization*, 2010
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