Reduced-Order Methods in PDE Constrained Optimization

M. Hinze (Hamburg), K. Kunisch (Graz), F. Tröltzsch (Berlin)

and

E. Grimm, M. Gubisch, S. Rogg, A. Studinger, S. Trenz, S. Volkwein

University of Konstanz, Department of Mathematics and Statistics

Recent Trends and Future Developments in Computational Science & Engineering

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Motivation for our Research Areas

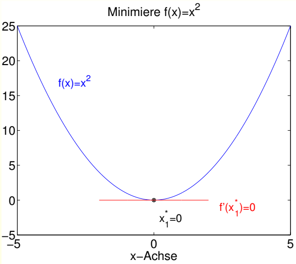
- **Problem**: time-variant, nonlinear, parametrized PDE systems
- **Efficient and reliable numerical simulation in multi-query cases**
  → finite element or finite volume discretizations too complex
- **Multi-query examples**
  - fast simulation for different parameters on small computers
  - parameter estimation, optimal design and feedback control

  → usage of a reduced-order SURROGATE MODEL
- **Time-variant, nonlinear coupled PDEs**
  → methods from linear system theory not directly applicable
- **Nonlinear model-order reduction**
  → proper orthogonal decomposition and reduced-basis method
- **Error control for reduced-order model**
  → new a-priori and a-posteriori error analysis (Martin Gubisch, Stefan Trenz, Andrea Wesche)
  → reliable PDE constrained multi-objective optimization (Laura Iapichino, Stefan Trenz)
  → economic model predicitive control (Lars Grüne, Thomas Meurer, Sabrina Rogg)
  → certified closed-loop strategies (Alessandro Alla, Maurizio Falcone)

PDE — Partial Differential Equation

Minimization with Inequality Constraints

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

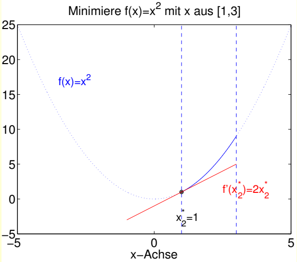


- **Problem**: min $\{f(x) = x^2 : 1 \le x \le 3\}$
- **Lagrange functional**:

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

- **Optimality condition**:

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



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

Outline of the talk

- Semilinear optimal control problems
- Proper orthogonal decomposition (POD)
- A-posteriori error for linear-quadratic optimal control
- Basis update by optimality-system POD (OS-POD)
- Extension to semilinear optimal control problems
- Conclusions and outlook

Semilinear Optimal Control Problems

Optimal Control of Semilinear Parabolic Problems (Tröltzsch'10)

- **PDE constrained optimization problem**: Minimize the quadratic cost

$$J(y,u)=\frac{\alpha_Q}{2}\int_{t_\circ}^{t_f}\int_\Omega \big|y(t,\boldsymbol{x})-y_Q(t,\boldsymbol{x})\big|^2\,\mathrm{d}\boldsymbol{x}\mathrm{d}t+\frac{\alpha_\Omega}{2}\int_\Omega\big|y(t_f,\boldsymbol{x})-y_\Omega(\boldsymbol{x})\big|^2\,\mathrm{d}\boldsymbol{x}$$
$$+\frac{\kappa^d}{2}\int_{t_\circ}^{t_f}\int_\Omega\big|u^d(t,\boldsymbol{x})-u^d_\circ(t,\boldsymbol{x})\big|^2\mathrm{d}\boldsymbol{x}\mathrm{d}t+\frac{\kappa^b}{2}\int_{t_\circ}^{t_f}\int_{\partial\Omega}\big|u^b(t,\boldsymbol{s})-u^b_\circ(t,\boldsymbol{s})\big|^2\mathrm{d}\boldsymbol{s}\mathrm{d}t$$

with respect to (y,u) subject to the semilinear evolution equation

$$\begin{aligned} c_p y_t(t,\boldsymbol{x})-\Delta y(t,\boldsymbol{x})+\mathcal{N}(y(t,\boldsymbol{x}))&=f(t,\boldsymbol{x})+u^d(t,\boldsymbol{x}), && (t,\boldsymbol{x})\in Q=(t_\circ,t_f)\times\Omega\\ \frac{\partial y}{\partial n}(t,\boldsymbol{s})+qy(t,\boldsymbol{s})&=u^b(t,\boldsymbol{s}), && (t,\boldsymbol{s})\in\Sigma=(t_\circ,t_f)\times\partial\Omega\\ y(t_\circ,\boldsymbol{x})&=y_\circ(\boldsymbol{x}), && \boldsymbol{x}\in\Omega\subset\mathbb{R}^\mathfrak{n},\ \mathfrak{n}\in\{1,2,3\} \end{aligned}\qquad\textbf{(SE)}$$

and the bilateral control constraints

$$\mathfrak{U}_{\mathrm{ad}}=\big\{u=(u^d,u^b)\,\big|\,u^d_a\le u^d\le u^d_b \text{ in } Q \text{ and } u^b_a\le u^b\le u^d_b \text{ on } \Sigma\big\}$$

- **Assumption**: for any control $u\in\mathfrak{U}_{\mathrm{ad}}$ there exists a unique state $y=y(u)$ satisfying **(SE)**
- **Reduced problem**: Setting $\hat{J}(u)=J(y(u),u)$ we consider the reduced problem

$$\min \hat{J}(u)\quad\text{subject to}\quad u\in\mathfrak{U}_{\mathrm{ad}}\qquad(\hat{\mathbf{P}})$$

$\rightarrow$ nonconvex problem $\rightarrow$ possibly many local optimal solutions

First-Order Necessary Optimality Condition (Hinze/Pinnau/Ulbrich/Ulbrich'09, Ito/Kunisch'08, Tröltzsch'10)

- **Reduced problem**: Setting $\hat{J}(u) = J(y(u), u)$ we consider the reduced problem

$$\min \hat{J}(u) \quad \text{subject to} \quad u \in \mathcal{U}_{\text{ad}} \tag{$\hat{\mathbf{P}}$}$$

- **Existence of local optimal controls $\bar{u}$**: properties of $\mathcal{N}$, regularity hypotheses
- **Optimality conditions**: based on constraint qualifications

(1) State equation $[\Rightarrow \bar{y} = y(\bar{u})]$

$$\begin{aligned} c_p \bar{y}_t - \Delta \bar{y} + \mathcal{N}(\bar{y}) &= f + \bar{u}^d && \text{in } Q = (t_\circ, t_\text{f}) \times \Omega \\ \frac{\partial \bar{y}}{\partial n} + q\bar{y} &= \bar{u}^b && \text{on } \Sigma = (t_\circ, t_\text{f}) \times \partial\Omega \\ \bar{y}(t_\circ) &= y_\circ && \text{in } \Omega \end{aligned}$$

(2) Adjoint equation $[\Rightarrow \bar{p} = p(\bar{u})]$

$$\begin{aligned} -c_p \bar{p}_t - \Delta \bar{p} + \mathcal{N}'(\bar{y})\bar{p} &= \alpha_Q (y_Q - \bar{y}), && \text{in } Q \\ \frac{\partial \bar{p}}{\partial n} + q\bar{p} &= 0 && \text{on } \Sigma \\ \bar{p}(t_\text{f}) &= \alpha_\Omega (y_\Omega - \bar{y}(t_\text{f})) && \text{in } \Omega \end{aligned}$$

(3) Variational inequality $[\bar{u} = (\bar{u}^d, \bar{u}^b) \in \mathcal{U}_{\text{ad}}]$

$$\int_{t_\circ}^{t_\text{f}} \int_\Omega \Big(\kappa^d (\bar{u}^d - u_\circ^d) - \bar{p} \Big)(u - \bar{u}^d)\, \mathrm{d}\boldsymbol{x}\mathrm{d}t + \int_{t_\circ}^{t_\text{f}} \int_{\partial\Omega} \Big(\kappa^b (\bar{u}^b - u_\circ^b) - \bar{p} \Big)(u^b - \bar{u}^b)\, \mathrm{d}\boldsymbol{s}\mathrm{d}t \geq 0$$

for all (admissible) $u = (u^d, u^b) \in \mathcal{U}_{\text{ad}}$

Computation of the Reduced Hessian (Hinze/Pinnau/Ulbrich/Ulbrich'09)

- **Reduced problem**: Setting $\hat{J}(u) = J(y(u), u)$ we consider the reduced problem

$$\min \hat{J}(u) \quad \text{subject to} \quad u \in \mathfrak{U}_{ad} \qquad (\hat{\mathbf{P}})$$

- **Reduced gradient**: $\hat{J}'(u) = \Big(\big[\kappa^d (u^d - u^d_\circ) - p\big]\big|_Q \,\Big|\, \big[\kappa^b (u^b - u^b_\circ) - p\big]\big|_\Sigma \Big)$

- **Evaluation of the reduced hessian $\hat{J}''$ at $u \in \mathfrak{U}_{ad}$ in a direction $u_\delta = (u^d_\delta, u^b_\delta)$:**

  (1) solve the linearized state equation $[\Rightarrow y_\delta = y_\delta(u_\delta; u)$ with $y = y(u)]$

$$\begin{aligned} c_p (y_\delta)_t - \Delta y_\delta + \mathcal{N}'(y) y_\delta &= u^d_\delta && \text{in } Q \\ \frac{\partial y_\delta}{\partial n} + q y_\delta &= u^b_\delta && \text{on } \Sigma \\ y_\delta(t_\circ) &= 0 && \text{in } \Omega \end{aligned}$$

  (2) solve the linearized adjoint equation $[\Rightarrow p_\delta = p_\delta(u_\delta; u)$ with $y = y(u)$, $p = p(u)]$

$$\begin{aligned} -c_p (p_\delta)_t - \Delta p_\delta + \mathcal{N}'(y) p_\delta &= -\alpha_Q y_\delta - \mathcal{N}''(y) y_\delta p, && \text{in } Q \\ \frac{\partial p_\delta}{\partial n} + q p_\delta &= 0 && \text{on } \Sigma \\ p_\delta(t_f) &= -\alpha_\Omega y_\delta(t_f) && \text{in } \Omega \end{aligned}$$

  (3) Set $\hat{J}''(u) u_\delta = \Big(\big[\kappa^d u^d_\delta - p_\delta\big]\big|_Q \,\Big|\, \big[\kappa^b u^b_\delta - p_\delta\big]\big|_\Sigma \Big)$

Numerical Solution Algorithm

- **Reduced problem**: Setting $\hat{J}(u) = J(y(u), u)$ we consider the reduced problem

$$\min \hat{J}(u) \quad \text{subject to} \quad u \in \mathcal{U}_{\text{ad}} \tag{$\hat{\mathbf{P}}$}$$

- **Newton's method**: solve at u^k with $y^k = y(u^k)$ and $p^k = p(u^k)$

$$\min \hat{J}(u^k) + \hat{J}'(u^k)u_\delta + \frac{1}{2}\hat{J}''(u^k)(u_\delta, u_\delta) \quad \text{subject to} \quad u_\delta \text{ with } u^k + u_\delta \in \mathcal{U}_{\text{ad}}$$

  with a (truncated) conjugate gradient method (Nocedal/Wright'06)

- **Reduced gradient**: $\hat{J}'(u^k) = \Big(\big[\kappa^d (u^{k,d} - u^d_\circ) - p^k\big]\big|_Q \Big| \big[\kappa^b (u^{k,b} - u^b_\circ) - p^k\big]\big|_\Sigma \Big)$

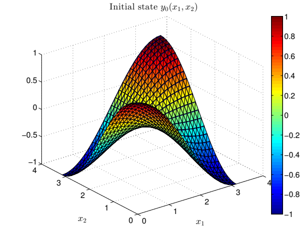
- **Evaluation of the reduced hessian at $u \in \mathcal{U}_{\text{ad}}$ in direction $u_\delta = (u^d_\delta, u^b_\delta)$:**

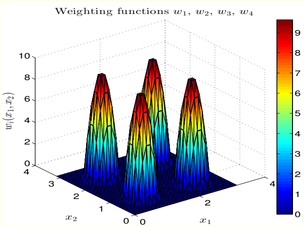
  (1) solve the linearized state equation for $y_\delta = y_\delta(u_\delta; u^k)$
  (2) solve the linearized adjoint equation for $p_\delta = p_\delta(u_\delta; u^k)$
  (3) Set $\hat{J}''(u^k)u_\delta = \Big(\big[\kappa^d u^d_\delta - p_\delta\big]\big|_Q \Big| \big[\kappa^b u^b_\delta - p_\delta\big]\big|_\Sigma \Big)$

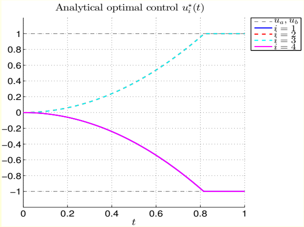
- **Globalization**: negative curvature test and Armijo line search
- **Control constraints**: projected BFGS/Newton method (Kelley'99)
- **Numerical realization**: finite elements (FE) and implicit Euler method

Numerical Example: Distributed Optimal Control (Kammann/Tröltzsch/V.'13, Trenz'15)

- **Control input**: $u^d(t,\boldsymbol{x}) = \sum_{i=1}^4 u_i(t)w_i(\boldsymbol{x})$ and $u^b \equiv 0$, start with $u^{(0)}(t,\boldsymbol{x}) = \sum_{i=1}^4 0.2w_i(\boldsymbol{x})$
- **Bilateral control bounds**: $u_a^d = -1$ and $u_b^d = 1$
- **Nonlinearity**: $\mathcal{N}(y) = y^3$ with $\mathcal{N}'(y) = 3y^2 \geq 0$
- **Discretization**: $N = 729$ FE unknown and $N_t = 120$ time instances
- **Exact optimal state**: $\bar{y}(t,\boldsymbol{x}) = \cos(x_1)\cos(x_2) = y_\circ(\boldsymbol{x})$ for $\boldsymbol{x} = (x_1,x_2) \in \Omega = (0,2\pi)^2$
- **Exact optimal control**: $\bar{u}_1 = \bar{u}_4$ and $\bar{u}_2 = \bar{u}_3$ in $[t_\circ, t_f] = [0,1]$







	Newton-CG	BFGS	BFGS-Inv
# Iterations	6	30	30
Time	59 s	40 s	48 s
$J(\bar{y}^{FE}, \bar{u}^{FE})$	3.14e-2	3.14e-2	3.14e-2
$\Vert\bar{u} - \bar{u}^{FE}\Vert$	6.69e-3	4.51e-3	5.72e-3

Proper Orthogonal Decomposition (POD)

Galerkin-Based Reduced-Order Modeling

- **Model problem (weak form of our PDE)**: $y(t_\circ) = y_\circ$ and

$$\langle c_p y_t(t), \varphi\rangle + \int_\Omega \nabla y(t) \cdot \nabla\varphi + \mathcal{N}(y(t))\varphi\,\mathrm{d}\boldsymbol{x} = \int_\Omega \big(f(t) + u^d(t)\big)\varphi\,\mathrm{d}\boldsymbol{x} + \int_{\partial\Omega} u^b(t)\varphi\,\mathrm{d}\boldsymbol{s}$$

  for all $\varphi \in V$ in $(t_\circ, t_f]$, where we write $y(t) = y(t,\cdot)$ etc.

- **Typical choices**: $H^1_0(\Omega) \subset V \subset H^1(\Omega)$ and $H = L^2(\Omega)$
- **Finite element approximation**: $y^N(t) \in V^N = \mathrm{span}\{\varphi^1,\ldots,\varphi^N\} \subset V$ with $y^N(t_\circ) = \mathscr{P}^N y_\circ$ and

$$\langle c_p y^N_t(t), \varphi\rangle + \int_\Omega \nabla y^N(t) \cdot \nabla\varphi + \mathcal{N}(y^N(t))\varphi\,\mathrm{d}\boldsymbol{x} = \int_\Omega \big(f(t) + u^d(t)\big)\varphi\,\mathrm{d}\boldsymbol{x} + \int_{\partial\Omega} u^b(t)\varphi\,\mathrm{d}\boldsymbol{s}$$

  for all $\varphi \in V^N$ in $(t_\circ, t_f]$

- **Alternatives**: finite volume or finite difference schemes
- **Reduced-order model**: $y^\ell(t) \in V^\ell = \mathrm{span}\{\psi^N_1,\ldots,\psi^N_\ell\} \subset V^N$ and $\ell \ll N$ with $y^\ell(t_\circ) = \mathscr{P}^\ell y_\circ$ and

$$\langle c_p y^\ell_t(t), \psi\rangle + \int_\Omega \nabla y^\ell(t) \cdot \nabla\psi + \mathcal{N}(y^\ell(t))\psi\,\mathrm{d}\boldsymbol{x} = \int_\Omega \big(f(t) + u^d(t)\big)\psi\,\mathrm{d}\boldsymbol{x} + \int_{\partial\Omega} u^b(t)\psi\,\mathrm{d}\boldsymbol{s}$$

  for all $\psi \in V^\ell$ in $(t_\circ, t_f]$

- **Reduced-order subspace V^ℓ**: Proper Orthogonal Decomposition or Reduced-Basis
- **Nonlinear problems**: (Discrete) Empirical Interpolation Method – (D)EIM

Proper Orthogonal Decomposition (POD)

- **Dynamical system in separable Hilbert space X** (e.g., $X = H$ or V):

$$\dot{y}(t) = F(t, y(t); \mu(t)) \quad \text{in } (t_\circ, t_\mathrm{f}], \quad y(t_\circ) = y_\circ \in X$$

  with given parameter or control $\mu(t)$, and data $y_\circ$, f
- **Given multiple snapshots**: solutions $y^k(t) \in X$, e.g., for parameters $\{\mu_k\}_{k=1}^{\wp}$
- **Snapshot subspace**: $\mathcal{V} = \mathrm{span}\,\{y^k(t)\,|\,t \in [t_\circ, t_\mathrm{f}] \text{ and } 1 \le k \le \wp\} \subset X$
- **Continuous variant of POD**: for every ℓ solve

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

- **Integral operator**: define $\mathscr{R} : X \to X$ as $\mathscr{R}\psi = \sum_{k=1}^{\wp} \int_{t_\circ}^{t_\mathrm{f}} \langle \psi, y^k(t) \rangle_X \, y^k(t)\,\mathrm{d}t$ for $\psi \in X$

Theorem (Hilbert-Schmidt, Riesz-Schauder; Perturbation theory for the spectrum)

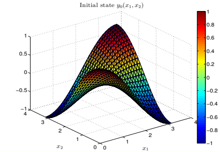
1) $\mathscr{R}$ is linear, compact, selfadjoint and nonnegative.
2) There are eigenfunctions $\{\bar\psi_i\}_{i=1}^{\infty}$ and eigenvalues $\{\bar\lambda_i\}_{i=1}^{\infty}$ with

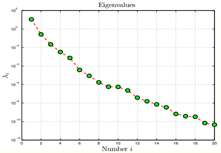
$$\mathscr{R}\bar\psi_i = \bar\lambda_i \bar\psi_i, \quad \bar\lambda_1 \ge \bar\lambda_2 \ge \ldots \ge 0, \quad \lim_{i\to\infty} \bar\lambda_i = 0$$

3) $\{\bar\psi_i\}_{i=1}^{\ell}$ solves $(*)$ and $\displaystyle\sum_{k=1}^{\wp} \int_{t_\circ}^{t_\mathrm{f}} \Big\| y^k(t) - \sum_{i=1}^{\ell} \langle y^k(t), \bar\psi_i \rangle_X \, \bar\psi_i \Big\|_X^2 \mathrm{d}t = \sum_{i=\ell+1}^{\infty} \bar\lambda_i$

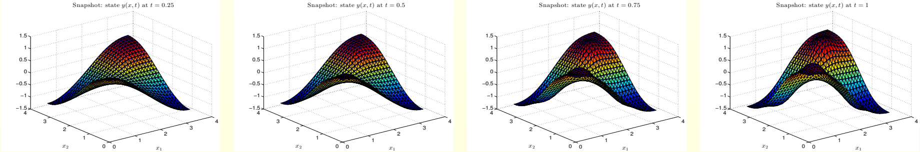
Numerical Example: POD-Basis Computation (Trenz'15)

- **Control input**: $u^d(t,\boldsymbol{x}) = \sum_{i=1}^4 0.2 w_i(\boldsymbol{x})$
- **Nonlinearity**: $\mathcal{N}(y) = y^3$
- **Discretization**: $N = 729$ FEs, $N_t = 120$
- **POD topology**: $X = L^2(\Omega)$

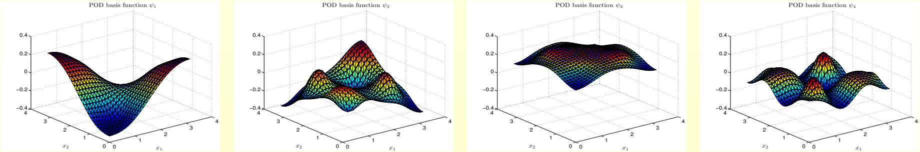




Snapshots of the state y at $t = 0.25, 0.5, 0.75$, and 1:



- First four POD basis functions:



A-Posteriori Error for Linear-Quadratic Optimal Control

Linear-Quadratic, Time-Variant Optimal Control Problems

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

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

subject to the linear evolution problem

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

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

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

- **State**: $y(t) \in V \hookrightarrow H$ with Hilbert spaces V, H
- **Control (Hilbert) space**: $\mathfrak{U} = L^2(t_\circ, t_f; U)$ with $U = \mathbb{R}^{N_u}$, $U = L^2(\Omega)$ or $U = L^2(\Gamma)$
- **Input/control**: $u \in \mathfrak{U}_{ad}$ (boundary or distributed control)
- **Bilinear form**: $a(t;\cdot,\cdot)$ continuous and $a(t;\varphi,\varphi) \ge \gamma_1\|\varphi\|_V^2 - \gamma_2\|\varphi\|_H^2$, e.g.

$$a(t;\varphi,\psi) = \int_\Omega \nabla\varphi\cdot\nabla\psi + \mathscr{N}'(y(t))\varphi\psi \,\mathrm{d}\boldsymbol{x} \quad \text{for } \varphi,\psi \in V$$

with $\mathscr{N}(y) = y^3$ or $\mathscr{N}(y) = \sinh y$

- **Control operator**: $\mathscr{B} : \mathfrak{U} \to L^2(t_\circ, t_f; V')$ linear, bounded

First-Order Necessary and Sufficient Optimality Conditions

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

$$\min_{x=(y,u)} J(x) = \frac{1}{2}\|y(t_f)-y_{t_f}\|_H^2 + \frac{\kappa}{2}\int_{t_\circ}^{t_f}\|u(t)\|_U^2\,\mathrm{d}t$$
$$\text{s.t.}\quad \langle y_t(t),\varphi\rangle + a(t;y(t),\varphi) = \langle (f+\mathscr{B}u)(t),\varphi\rangle \quad \forall\varphi\in V \text{ in } (t_\circ,t_f]$$
$$y(t_\circ)=y_\circ \quad\text{and}\quad u_a(t)\le u(t)\le u_b(t),\ t\in[t_\circ,t_f]$$

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

$$-\langle \bar{p}_t(t),\varphi\rangle + a(t;\varphi,\bar{p}(t)) = 0 \quad \forall\varphi\in V \text{ in } [t_\circ,t_f), \quad \bar{p}(t_f)=\bar{y}(t_f)-y_{t_f}$$

- **Variational inequality**:

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

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

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

POD Galerkin Scheme for the State and Dual Variable

- **State equation**:

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

- **POD space**: $V^\ell = \operatorname{span}\{\psi_1,\ldots,\psi_\ell\}\subset V$
- **Orthogonal projection**: $\mathscr{P}^\ell\varphi = \sum_{i=1}^\ell \langle\varphi,\psi_i\rangle_X\,\psi_i\in V^\ell$ for $\varphi\in V$
- **POD state**: $y^\ell = y^\ell(u)$ with $y^\ell(t)\in V^\ell$ in $[t_\circ,t_\mathrm{f}]$ solves

$$\langle y_t^\ell(t),\psi\rangle + a(t;y^\ell(t),\psi) = \langle (f+\mathscr{B}u)(t),\psi\rangle \quad \forall \psi\in V^\ell \text{ in } (t_\circ,t_\mathrm{f}], \quad y^\ell(t_\circ)=\mathscr{P}^\ell y_\circ$$

- **Adjoint/dual equation**: $p=p(y(u))$ solves

$$-\langle p_t(t),\varphi\rangle + a(t;\varphi,p(t)) = 0 \quad \forall \varphi\in V \text{ in } [t_\circ,t_\mathrm{f}), \quad p(t_\mathrm{f})=y(t_\mathrm{f})-y_{t_\mathrm{f}}$$

- **POD dual**: $p^\ell = p^\ell(y^\ell(u))$ with $p^\ell(t)\in V^\ell$ in $[t_\circ,t_\mathrm{f}]$ solves

$$-\langle p_t^\ell(t),\psi\rangle + a(t;\psi,p^\ell(t)) = 0 \quad \forall \psi\in V^\ell \text{ in } [t_\circ,t_\mathrm{f}), \quad p^\ell(t_f)=y^\ell(t_\mathrm{f})-y_{t_\mathrm{f}}$$

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

POD A-Posteriori Error Analysis (Malanowski/Büskens/Maurer'97, Tröltzsch/V.'09)

- **Variational inequality**:

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

- **Optimal POD solution**: $\bar{u}^\ell \in \mathfrak{U}_{ad}$, associated state $\bar{y}^\ell = y^\ell(\bar{u}^\ell)$ and dual $\bar{p}^\ell = p^\ell(y^\ell(\bar{u}^\ell))$
- **POD variational inequality**:

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

- **Misfit in the variational inequality**:

$$\int_{t_\circ}^{t_f} \langle \kappa\bar{u}^\ell(t) - (\mathscr{B}^\star \tilde{p}^\ell)(t), u(t) - \bar{u}^\ell(t)\rangle \,\mathrm{d}t \ngeq 0 \quad \forall u \in \mathfrak{U}_{ad}$$

  with $\tilde{y}^\ell = y(\bar{u}^\ell)$ and $\tilde{p}^\ell = p(y(\bar{u}^\ell))$
- **Perturbation analysis**: there exists a perturbation $\zeta \in \mathfrak{U}$ satisfying

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

- **A-posteriori analysis**: choose $u = \bar{u}^\ell$ in **(VI)**, $u = \bar{u}$ in $(\widetilde{\textbf{VI}}^\ell)$ and add
- **A-posteriori error estimate for the control**: $\|\bar{u} - \bar{u}^\ell\| \leq \|\zeta\|/\kappa$
- **Reduced-basis method**: related work (Dede'10, Grepl/Kärcher'14, Negri/Rozza/Manzoni/ Quarteroni'13)

Algorithm with POD A-Posteriori Analysis

- **A-posteriori error estimate**: $\|\bar{u} - \bar{u}^\ell\| \leq \|\zeta\|/\kappa$ and $\tilde{p}^\ell = p(y(\bar{u}^\ell))$
- **Computation of ζ**: $\zeta(t) = \begin{cases} -\left(\kappa\bar{u}^\ell(t) - (\mathscr{B}^\star\tilde{p}^\ell)(t)\right) & \text{if } u_a(t) < \bar{u}^\ell(t) < u_b(t) \\ -\min\left(0, \kappa\bar{u}^\ell(t) - (\mathscr{B}^\star\tilde{p}^\ell)(t)\right) & \text{if } \bar{u}^\ell(t) = u_a(t) \\ -\max\left(0, \kappa\bar{u}^\ell(t) - (\mathscr{B}^\star\tilde{p}^\ell)(t)\right) & \text{if } \bar{u}^\ell(t) = u_b(t) \end{cases}$

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

1: Choose POD basis $\{\psi_i\}_{i=1}^\ell$ for the Galerkin approximation of the QP problem;
2: Determine the reduced-order model for the QP problem;
3: Calculate suboptimal control $\bar{u}^\ell \in \mathfrak{U}_{ad}$, e.g., by a semismooth Newton method;
4: Compute perturbation $\bar{\zeta}^\ell = \zeta(\bar{u}^\ell)$;
5: **if** $\|\bar{\zeta}^\ell\|/\kappa > \mathrm{TOL}$ **then**
6: Enlarge ℓ and go back to Step 2;
7: **else**
8: Stop;
9: **end if**

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

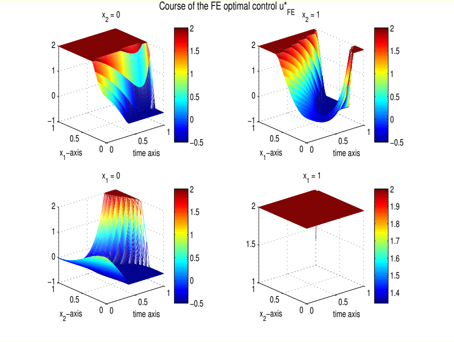
- **Consider**:

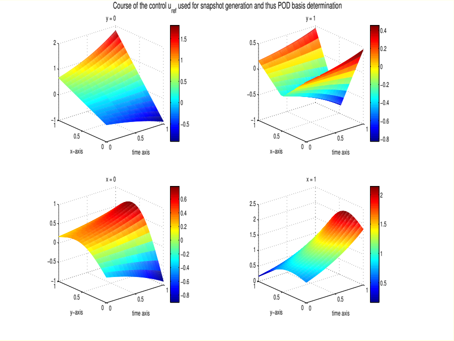
$$\min J(y,u) = \frac{1}{2}\int_\Omega |y(t_f) - y_d|^2 \,\mathrm{d}\boldsymbol{x} + \frac{1}{200}\int_0^{t_f}\int_{\partial\Omega} |u|^2 \,\mathrm{d}\boldsymbol{s}\mathrm{d}t$$

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

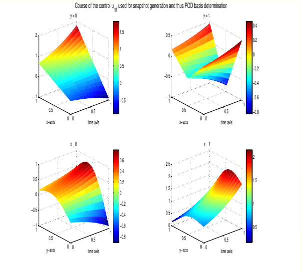
$$-0.5 \le u \le 2 \text{ on } \Sigma = (0,t_f)\times\partial\Omega$$

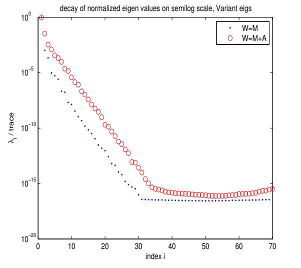
- **Method & discretization**: semismooth Newton & implizit Euler, finite elements

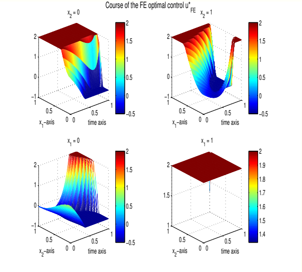




Numerical Example: POD Error Analysis (Studinger/V.'13)







- **A-posteriori error**: $\|\bar{u} - \bar{u}^\ell\| \leq \dfrac{1}{\kappa}\|\zeta(\bar{u}^\ell)\|$ (Tröltzsch/V.'09)
- **A-posteriori error within FE**: $\|\bar{u}^{FE} - \bar{u}^\ell\| \leq \dfrac{1}{\kappa}\|\zeta^{FE}(\bar{u}^\ell)\| =: \varepsilon_{\text{ape}}^{FE}$ (Gubisch/Neitzel/V.'15)

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

Difficulty: choice of 'expected' control for computation of the POD basis

Basis Update by Optimality-System POD

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

- **Optimal control problem**:

$$\min J(y,u) \quad \text{s.t.} \quad (y,u) \in \mathcal{Y}_{ad} \times \mathcal{U}_{ad},\ \dot{y}(t) = F(t,y(t),u(t)) \text{ in } (t_\circ,t_f],\ y(t_\circ) = y_\circ \qquad (\mathbf{P})$$

- **POD-Galerkin approximation**: $\{\psi_i\}_{i=1}^{\ell}$ POD basis of rank ℓ

$$\min J^\ell(y^\ell,u) \quad \text{s.t.} \quad (y^\ell,u) \in \mathcal{Y}^\ell_{ad} \times \mathcal{U}_{ad},\ \dot{y}^\ell(t) = F^\ell(t,y^\ell(t),u(t)) \text{ in } (t_\circ,t_f],\ y^\ell(t_\circ) = y^\ell_\circ \quad (\mathbf{P}^\ell)$$

- **POD basis**: eigenvalue problem with $\lambda_1 \geq \lambda_2 \geq \ldots$

$$\mathscr{R}\psi_i = \int_{t_\circ}^{t_f} \langle y(t),\psi_i\rangle\, y(t)\,\mathrm{d}t = \lambda_i\psi_i, \quad i = 1,\ldots,\ell \qquad (*)$$

$\Rightarrow y = y(u)$, i.e., $\psi_i = \psi_i(u)$ and $\lambda_i = \lambda_i(u)$

- **A-priori analysis for linear-quadratic, time-variant problems** (Hinze/V.'08):

$$\|\bar{u} - \bar{u}^\ell\|^2 = \mathscr{O}\left(\sum_{i=\ell+1}^{\infty} \lambda_i(\bar{u})\right) \text{ for } \psi_i = \psi_i(\bar{u})$$

but $\|\bar{u} - \bar{u}^\ell\| \stackrel{\ell\to\infty}{\longrightarrow} 0$ with no rate otherwise (Tröltzsch/V.'09)

- **OS-POD**: – augment $(\mathbf{P}^\ell)$ by the additional constraints $(*)$
  – improve the quality of the initial basis by applying a few gradient steps
  – proceed with a fixed basis and utilize a-posteriori error (Gubisch/V.'14, Tröltzsch/V.'09)
- **Optimization method**: variants of semismooth Newton methods

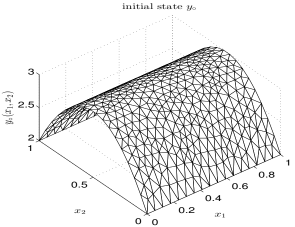
OS-POD for Linear-Quadratic, Control Constrained Control (Grimm'14, Grimm/Gubisch/V.'15)

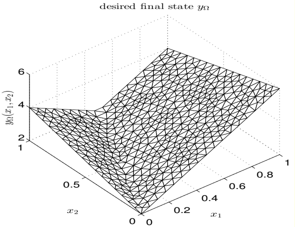
- **Optimal control problem**:

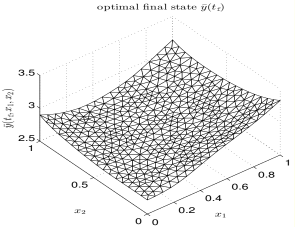
$$\min J(y,u) = \frac{1}{2}\int_\Omega \big|y(t_\mathrm{f}) - y_\Omega\big|^2\,\mathrm{d}\boldsymbol{x} + \frac{\kappa}{2}\int_0^{t_\mathrm{f}}\int_{\partial\Omega}|u|^2\,\mathrm{d}\boldsymbol{s}\mathrm{d}t$$

$$\text{s.t. } c_p y_t - \Delta y = 0 \text{ in } Q, \quad \partial_n y + qy = u \text{ on } \Sigma, \quad y(0) = y_\circ \text{ in } \Omega = (0,1)^2$$

$$u_a = 0 \le u \le 1 = u_b \text{ on } \Sigma = (0,t_\mathrm{f}) \times \partial\Omega$$





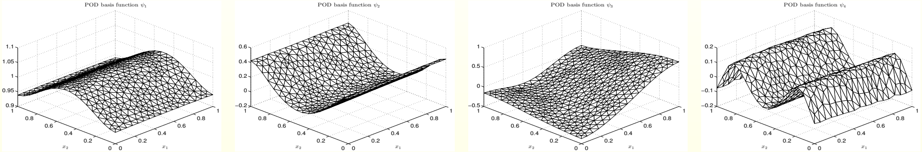


	$k=1$	$k=2$	with $\bar u^{\mathrm{FE}}$
req. ℓ	40	13	13
CPU	147.1 s	18.4 s	11.5 s
$\varepsilon_{\mathrm{ape}}^{FE}$	1.14e-2	2.82e-3	1.94e-3
$\Vert\bar u^{FE} - \bar u^\ell\Vert$	9.53e-3	2.62e-3	1.93e-3
$\Vert\bar u^{FE} - \bar u^\ell\Vert/\Vert\bar u^{FE}\Vert$	7.73e-3	2.15e-3	1.59e-3

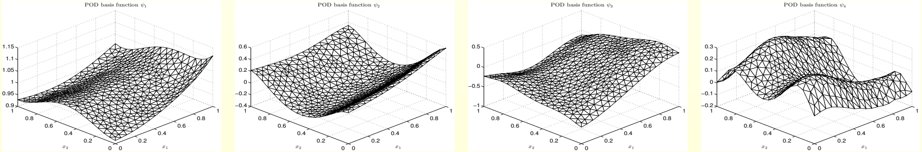
	$k=1$	$k=2$	with $\bar u^{\mathrm{FE}}$
different u_a	67	15	16 (2233)
different u_b	38	6	4 (3891)

OS-POD for Linear-Quadratic, Control Constrained Control (Grimm'14, Grimm/Gubisch/V.'15)

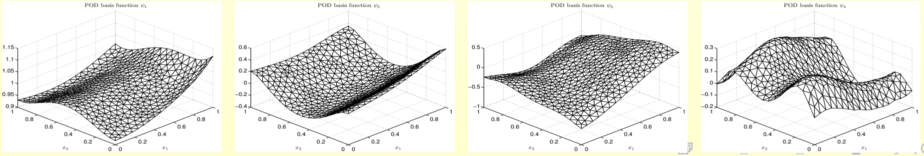
- First four POD basis functions generated from $u = 0$:



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



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



State and Control Constrained 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

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

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

$$u \in \mathcal{U}_{ad} = \{v \in \mathcal{U} \,|\, u_a(t) \le v(t) \le u_b(t) \text{ in } [t_\circ, t_f]\}$$
$$y \in \mathcal{Y}_{ad} = \{z \in L^2(Q) \,|\, y_a(t, \boldsymbol{x}) \le z(t, \boldsymbol{x}) \le y_b(t, \boldsymbol{x}) \text{ in } Q\}$$

- **Lavrentiev regularization**: $\varepsilon > 0$

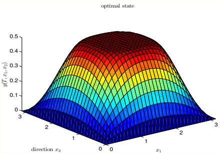
$$J(x, w) = \frac{1}{2}\|y(t_f) - y_d\|^2_{L^2(\Omega)} + \frac{\kappa}{2}\int_{t_\circ}^{t_f} \|u(t)\|_U^2 \, \mathrm{d}t + \frac{\sigma}{2}\int_{t_\circ}^{t_f} \|w(t)\|^2_{L^2(\Omega)} \, \mathrm{d}t$$

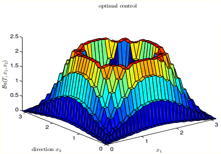
$$(y, w) \in \{z \in L^2(Q) \,|\, y_a(t, \boldsymbol{x}) \le \varepsilon w(t, \boldsymbol{x}) + z(t, \boldsymbol{x}) \le y_b(t, \boldsymbol{x}) \text{ in } Q\}$$

- **Regular Lagrange multipliers** (Tröltzsch'05): formulation as a control constrained problem
- **A-posteriori error** (Grimm/Gubisch/V.'15): extension from the control-constrained case
  → OS-POD and semismooth Newton method also applicable

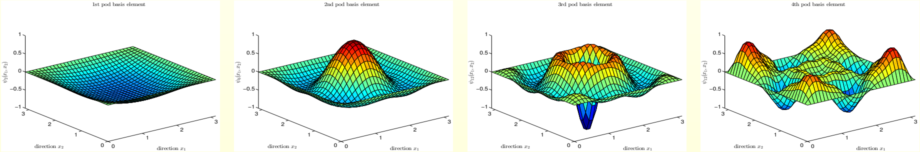
Numerical Example (Grimm/Gubisch/V.'15)

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

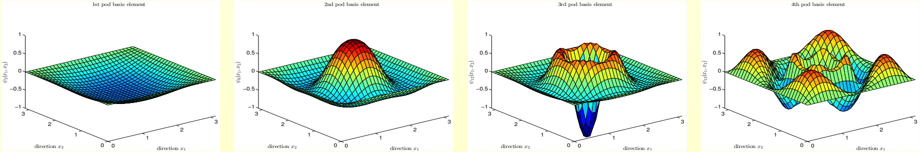




- First four POD basis functions generated from the optimal control $\bar{u}^{FE}$:



- First four POD basis functions generated after $k = 3$ OS-POD gradient steps:



Extension to Semilinear Optimal Control Problems

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

- **Reduced problem**: $\min_{u \in \mathfrak{U}_{ad}} \hat{J}(u)$ with hessian $\hat{J}''(u)$
- **First-order optimality conditions**: $\hat{J}'(\bar{u})(u-\bar{u}) \geq 0$ for all $u \in \mathfrak{U}_{ad}$
- **Second-order sufficient optimality conditions**: there is a constant $\eta = \eta(\bar{u}) > 0$ with

$$\hat{J}''(\bar{u})(u,u) \geq \eta \, \|u\|^2 \quad \forall u$$

$\Rightarrow \hat{J}''(\tilde{u})(u,u) \geq \frac{\eta}{2} \|u\|^2 \; \forall u, \forall \tilde{u} \in \mathfrak{U}_{ad}$ provided $\|\tilde{u} - \bar{u}\|$ sufficiently small

Theorem (Kammann/Tröltzsch/V.'13)

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

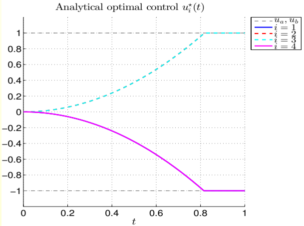
$$\|\bar{u} - \bar{u}^\ell\| \leq \varepsilon_{ape} \quad \textit{with} \quad \varepsilon_{ape} = \frac{2}{\eta} \|\zeta(\bar{u}^\ell)\|$$

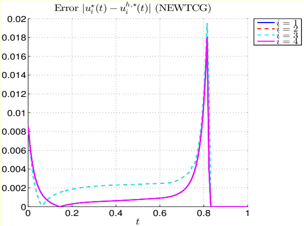
provided $\|\bar{u} - \bar{u}^\ell\|$ is sufficiently small

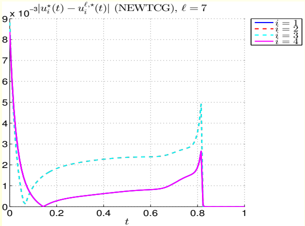
- **Computation of $\zeta(\bar{u}^\ell)$**: based on state $y = y(\bar{u}^\ell)$ and $p = p(\bar{u}^\ell)$
- **Problem**: estimate $\eta = \eta(\bar{u}) \rightarrow$ smallest eigenvalue of $\hat{J}''(\tilde{u})$

Numerical Example: Distributed Optimal Control (Kammann/Tröltzsch/V.'13, Trenz'15)

- **Control input**: $u^d(t,\boldsymbol{x}) = \sum_{i=1}^{4} u_i(t) w_i(\boldsymbol{x})$ and $u^b \equiv 0$
- **Bilateral control bounds**: $u_a^d = -1$ and $u_b^d = 1$
- **Nonlinearity**: $\mathcal{N}(y) = y^3$ with $\mathcal{N}'(y) = 3y^2 \geq 0$
- **Discretization**: $N = 729$ FE unknowns, $N_t = 120$ time instances and $\ell = 7$ PODs
- **Exact optimal state**: $\bar{y}(t,\boldsymbol{x}) = \cos(x_1)\cos(x_2) = y_\circ(\boldsymbol{x})$ for $\boldsymbol{x} = (x_1,x_2) \in \Omega = (0,2\pi)^2$
- **Exact optimal control**: $\bar{u}_1 = \bar{u}_4$ and $\bar{u}_2 = \bar{u}_3$ in $[t_\circ, t_f] = [0,1]$







POD ($\ell = 7$)	Newton-CG	BFGS	BFGS-Inv
# Iterations	9	31	31
Time	3.7 s	6.5 s	7.4 s
$J(\bar{y}^\ell, \bar{u}^\ell)$	3.15e-2	3.15e-02	3-15e-02
$\lVert \bar{u} - \bar{u}^\ell \rVert$	3.64e-3	5.17e-3	5.94e-3
ε_{ape}	3.71e-3	3.71e-3 (2.16e-3)	3.72e-3 (0.90e-3)
$\lambda_{\min}$	5.37e-3	5.37e-3 (1.72e-2)	5.37e-3 (2.22e-2)

FE ($N = 729$)	Newton-CG
# Iterations	6
Time	59 s
$J(\bar{y}^{FE}, \bar{u}^{FE})$	3.41e-2
$\lVert \bar{u} - \bar{u}^{FE} \rVert$	6.69e-3

POD Basis Update by Trust-Region Optimization (Arian/Fahl/Sachs'00, Schu'12, Rogg'14)

- **QP problem in Newton's method**:

$$\min Q^k(u_\delta) = \hat{J}(u^k) + \langle \hat{J}'(u^k), u_\delta \rangle + \frac{1}{2}\hat{J}''(u^k)(u_\delta, u_\delta) \quad \text{s.t.} \quad u_a \le u^k + u_\delta \le u_b$$

- **Expensive parts**: computation of gradient $\hat{J}'(u^k)$ and hessian $\hat{J}''(u^k)$

  $\rightarrow$ utilze POD approximations $\hat{J}'_\ell(u^k)$ and $\hat{J}''_\ell(u^k)$ in a trust region around u^k

- **Trust-region POD subproblem**:

$$\min \hat{J}(u^k) + \langle \hat{J}'_\ell(u^k), u_\delta \rangle + \frac{1}{2}\hat{J}''_\ell(u^k)(u_\delta, u_\delta) \quad \text{s.t.} \quad u_a \le u^k + u_\delta \le u_b \text{ and } \|u_\delta\| \le \Delta^k$$

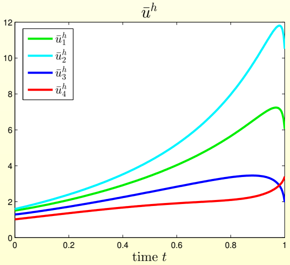
- **Convergence criterium**: Carter condition $\|\hat{J}'(u^k) - \hat{J}'_\ell(u^k)\| \le \gamma \|\hat{J}'_\ell(u^k)\|$ with $\gamma \in (0,1)$
- **Numerical experiments** (Rogg'14)
  - Steihaug CG (Nocedal/Wright'06), global convergence
  - $10\times$ faster for two-dimensional, semilinear parabolic PDE
- **Combination with a-posteriori error analysis**: use a-posteriori error for the dual

$$\|\hat{J}'(u^k) - \hat{J}'_\ell(u^k)\| = \|\mathscr{B}^\star(p(y(u^k)) - p^\ell(y^\ell(u^k))\| \le C\mathrm{err}^{\mathrm{dual}}(u^k)$$

  $\rightarrow$ efficient computation by evaluating primal and dual residuals at u^k (Rogg/Trenz/V.'15)

Numerical Example: Boundary Optimal Control (Rogg'14)

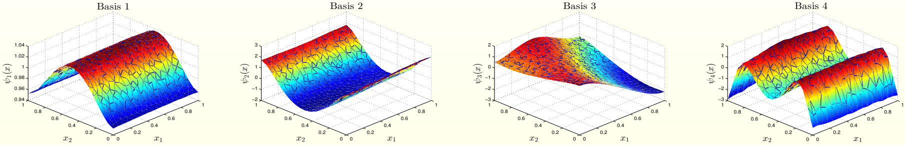
- **Boundary control**: $u^b(t,\boldsymbol{x}) = \sum_{i=1}^4 u_i(t) w_i(\boldsymbol{x})$ and $u^d \equiv 0$
- **Nonlinearity**: $\mathcal{N}(y) = y^3$ with $\mathcal{N}'(y) = 3y^2 \geq 0$
- **Discretization**: $N = 727$ FE unknowns, $N_t = 400$ time instances and $\ell = 7$ PODs



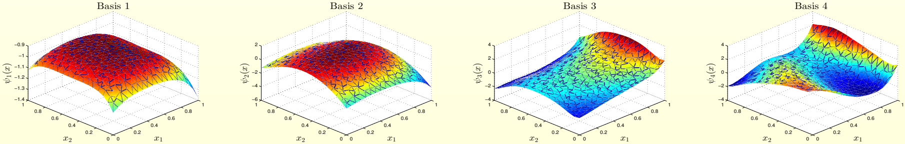
ℓ	$\hat{J}(u^k)$	$\|\hat{J}'(u^k)\|$	# CG it.	Δ^k
0	1.7667	2.4e-1	3	8.0
1	0.9377	3.6e-2	4	9.6
2	0.9029	5.7e-3	5	11.5
3	0.9022	8.5e-4		

Numerical Example (Rogg'15)

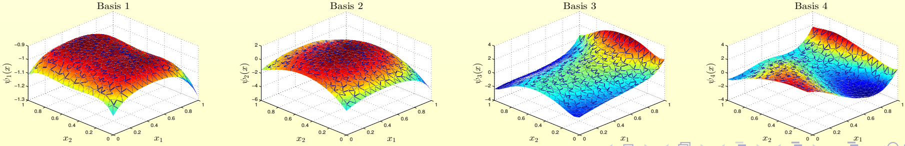
- First four POD basis functions generated from the $u = 0$:



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



- First four POD basis functions generated after one trust-region step:



Summary and Ongoing Research

- POD method for **constrained optimal control problems**
- **A-priori and a-posteriori error analysis** for the controls
- Change of the POD basis by **OS-POD** and **TR-POD**
- POD basis updates by **optimality conditions** (OS-POD)
- POD basis updates by **trust region constraints** (TR-POD)

- Combination of **SQP and OS-POD** (Metzdorf/V.)
- Reduced-order method in **PDE constrained multiobjective optimization** (Iapichino/Trenz/V.)
- **Model predictive control** in pharmaceutical application (Renal Research Institute New York & Rogg/V.)
- A-priori error analysis for **closed-loop control** (Hamilton-Jacobi-Bellman) (Alla/Falcone/V.'15)

Are **YOU** interested in ...

- Reduced Basis Methods
- Model Reduction for Parametrized Systems
- Balanced Truncation
- POD Methods
- Optimization
- Low Rank Tensor Approximation

Reduced Basis Summer School 2015

`http://www.math.uni-konstanz.de/numerik/pod/rbss_2015`

Literature

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