

Mathematics of PDE constrained optimization

CPDE summerschool, Bertinoro

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Outline

- **Motivation: PDE model-based simulation to PDE model-based design.**
- **A multiphysics example: Optimal control of crystal growth.**
- **Motivation: Interface motion planning in multiphase flows.**
- **Model predictive control - the general concept.**
- **Mathematics of PDE constrained optimization for model problems → main part of the presentation.**
 - **Basic concepts.**
 - **Discretization.**
 - **Algorithms.**
 - **Numerical analysis.**
 - **Incorporation of state constraints.**
- **Applications and further aspects (Sunday).**

Motivation

Mathematical model of a real world process available

- predict process behaviour for given inputs,
- analyse the sensitivity of the process at certain states,

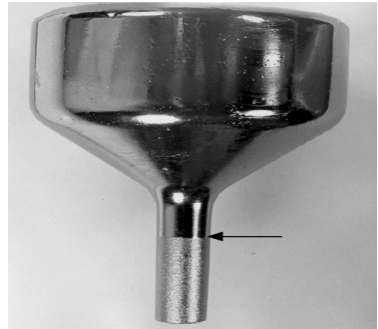
Mathematical model of a real world process available

- design your process through inputs; this is optimization,
- consider the inverse problem: given observations of the system, which input delivers the best reconstruction of the observations?. In other words: how should I choose the input to achieve a prescribed output.
- keep your process on track; control the mathematical model so that it stays in the vicinity of a desired state

For systems governed by PDEs the basic building block here is

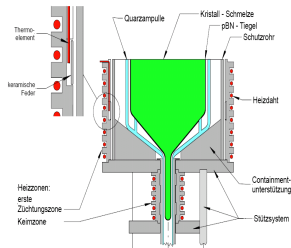
Optimization with PDE constraints

Vertical gradient freeze growth - oven and crystal

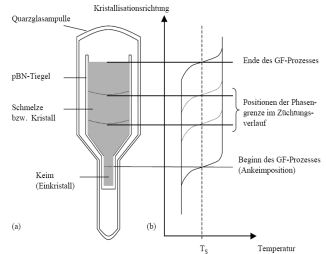


VGF-Oven with coil system for the application of travelling magnetic fields, courtesy Olf Pätzold

VGF schematic and principle



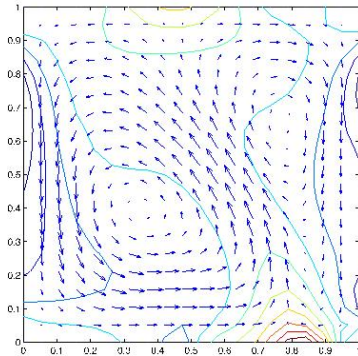
Sectional drawing of the seed zone and the bottom growth zone. The thermocouple arrangement is shown in detail on the left hand side. Courtesy: H. Krause, O. Pätzold, U. Wunderwald, M. Hermann



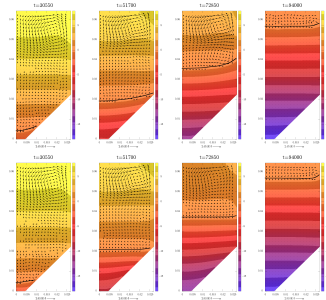
Principle of VGF-growth in closed ampoules: (a) Sketch of the growth ampoule; (b) Thermal profiles during the process (T_S ... melting temperature). Courtesy: H. Krause, O. Pätzold, U. Wunderwald, M. Hermann

VGF crystal growth - subproblems

Flow control



Control of solidification (H., Ziegenbalg J. Comput. Phys. 223, ZAMM 87, 2007; H., Pätzold, Ziegenbalg J. Crystal Growth 311, 2009)



Why optimization? And which kind of optimization?

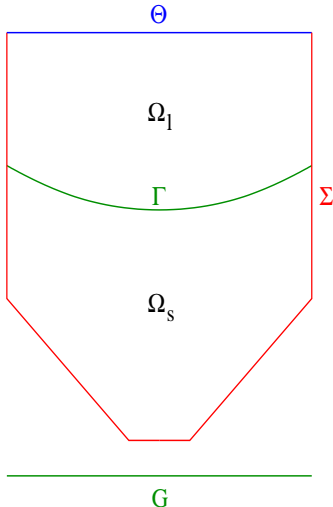
Why optimization?

- Large radial temperature gradients cause thermal stresses → striations in the crystal.
- Remedy: flat fluid-liquid interface.

Which kind of optimization?

- Closed-loop optimization desirable. But process hard to observe.
- Growth-system is closed → open loop (optimal) control.

Modeling of the crystal-melt complex



- 2-phase Stefan problem with flow driven by convection and Lorentz forces.
- Interface (free boundary) is modeled as a graph.
- Free boundary motion control by wall temperature and the Lorentz forces.
- Control goal: tracking a prescribed evolution of the free boundary.
- Achieve this goal by minimizing an appropriate cost functional.
- Express derivatives with the help of the adjoint calculus.
- Consider physical constraints on controls and states.

Mathematical model

Interface: $\Gamma(t) = \{(x, f(t, x))^T; x \in G\}.$

$$\partial_t u = \frac{k_s}{c_s \rho} \Delta u \quad \text{in } \Omega_s^T,$$

$$\partial_t u + \vec{v} \cdot \nabla u = \frac{k_l}{c_l \rho} \Delta u \quad \text{in } \Omega_l^T,$$

$$\partial_t \vec{v} + (\nabla \vec{v}) \vec{v} - \frac{\varepsilon}{\rho} \Delta \vec{v} + \frac{1}{\rho} \nabla p = -\vec{g} \gamma(u - u_M) + \vec{A}(A_c) \quad \text{in } \Omega_l^T,$$

$$\frac{k_{s/l}}{\alpha_{s/l}} \partial_{\vec{v}} u = u_b - u \quad \text{on } \Sigma,$$

$$u = u_M \quad \text{on } \Gamma(t),$$

$$\nabla \cdot \vec{v} = 0 \quad \text{in } \Omega_l^T,$$

$$L\rho \frac{f_t}{\sqrt{1+|\nabla f|^2}} = \frac{k_s}{\rho} \partial_{\vec{\mu}} u_s - \frac{k_l}{\rho} \partial_{\vec{\mu}} u_l \quad \text{on } G^T,$$

+IC +BC.

Optimization problem

By \bar{f} the desired evolution of the free boundary is denoted. The control goal mathematically is formulated as a pde-constrained optimization problem;

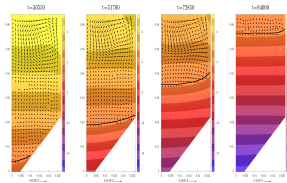
$$(P) \begin{cases} \min_{f, u_b, A_c} J(f, u_b, \vec{A}_c) := \frac{1}{2T} \int_0^T \int_G \left(f(t, y) - \bar{f}(t, y) \right)^2 dy dt + S(u_b, \vec{A}_c) \\ \text{s.t. mathematical model} + \text{constraints on controls and/or states.} \end{cases}$$

The functional J models the objective of reducing the mismatch between the interface and the desired free boundary in the mean square sense.

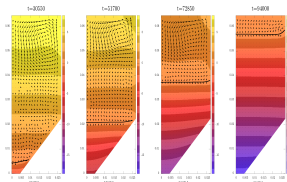
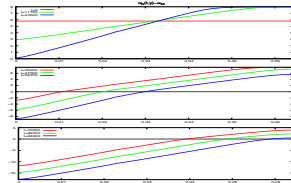
The function f is coupled to the controls through the mathematical model.
 S penalizes control costs.

Numerical experiment, results (Implementation Stefan Ziegenbalg)

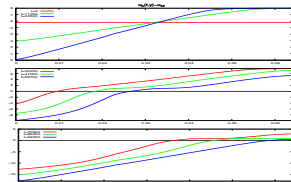
Temperature $u - u_M$ (colored stripes), velocity (arrows) and free boundary (black line) at four time instances



without optimization

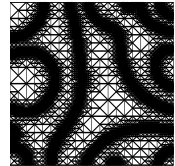
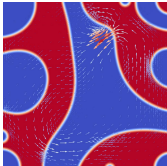


with optimization

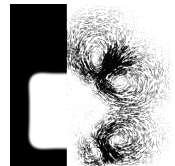
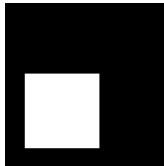
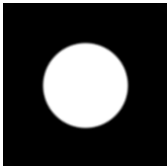


Simulation and control of multiphase flows

- **Develop numerics for hydrodynamics of multiphase flows, including efficient, reliable, fully automatic adaptive concepts to resolve interface**



- **Develop control concepts for multiphase flows**



- **Use of diffuse interface approach to cope e.g. with topology changes**

Aim of closed-loop control of nonlinear systems

Given some initial state x_0 , find a **control law** $\mathcal{B}u(t) = K(x(t))$ which steers the state $x(t)$ towards a given trajectory \bar{x} :

$$x(t) \xrightarrow{!} \bar{x}(t) \quad t \rightarrow \infty$$

Mathematical model:

$$\begin{aligned} \dot{x}(t) + Ax(t) &= b(x, t) + \mathcal{B}u(t) \text{ state,} \\ y(t) &= Cx(t) \text{ observation,} \\ x(0) &= x_0 \end{aligned}$$

Here

- \bar{x} desired stationary state, or
- \bar{x} a reference trajectory obtained from open loop optimal control.

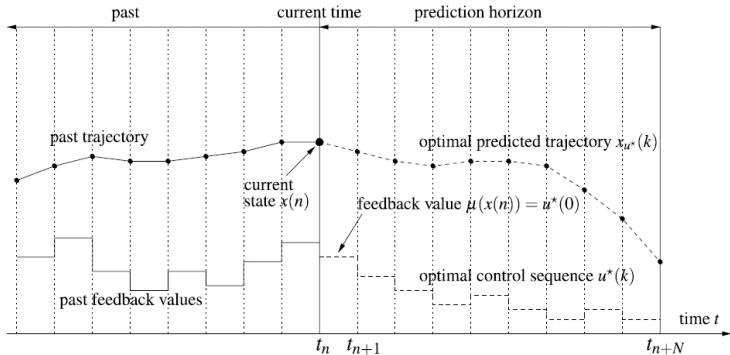
System theoretic point of view (H. SICON 44, 2005)

In practice feedback control (closed loop control) based on observations is needed. If a mathematical model is available, Model Predictive Control (MPC) may be applied.

- 1 At time t_k compute an **optimal** time discrete control strategy u_{k+1}, \dots, u_{k+l} .
- 2 Apply u_{k+1} and proceed to t_{k+1} .
- 3 Set $k = k + 1$.
- 4 Goto 1

Idea: apply **suboptimal variant called instantaneous control**; solve the optimal control problem only approximately by e.g. applying a few steepest descent steps (for $l = 1$ proposed by H. Choi, 1995).

MPC schematic (from Grüne & Pannek)



With $t = t_n$, $t_p = t_{n+N}$ and $t_c = t_{n+1}$ perform

- 1 Prediction step: solve optimization problem on $[t, t + t_p]$,
- 2 Control step: apply control on $[t, t + t_c]$,
- 3 Receding horizon step: $t = t + t_c$, goto 1.

MPC with $t_c = t_p \equiv h$, discretization

Discretize the state equation w.r.t. time (your favorite scheme!)

$$(I + hA)x^{k+1} = x^k + hb^k$$

and minimize at every time step an instantaneous version of the cost

$$(P_k) \quad \begin{cases} \min J(u^{k+1}) = \frac{\gamma}{2}|u^{k+1}|^2 + \frac{1}{2}|\mathcal{C}(x^{k+1} - \bar{x}^k)|^2 \\ \text{s.t.} \\ (I + hA)x^{k+1} = x^k + hb^k + \mathcal{B}u^{k+1}. \end{cases}$$

Time discretization here with implicit Euler.

- (P_k) is an optimization problem with PDE constraints!

Feedback oracle

- 1 Set $x^0 = \phi$, $k = 0$ and $t_0 = 0$.
- 2 Given an initial control u_0^k , set

$$u^{k+1} = \text{RECIPE}(u_0^k, x^k, \bar{x}^k, t_k)$$

- 3 Solve

$$(I + hA)x^{k+1} = x^k + hb(x^k, t_k) + \mathcal{B}u^{k+1}.$$

- 4 Set $t_{k+1} = t_k + h$, $k = k + 1$. If $t_k < T$ goto 2.

Instantaneous control

For instantaneous control the oracle RECIPE is given by

$$u = \text{RECIPE}(v, x^k, z, t_k)$$

iff

- Solve $(I + hA)x = x^k + hb(x^k, t_k) + \mathcal{B}v$,
- solve $(I + hA)^* \lambda = -\mathcal{C}^*(\mathcal{C}x - z)$,
- set $d = \alpha v + \mathcal{B}^* \lambda$.
- determine $\rho > 0$,
- set $\text{RECIPE} = v - \rho d$ ($= P_{ad}(v - \rho d)$ in case of constraints).

This oracle realizes steepest descent for problem (P_k) .

Feedback operators: Instantaneous control

$$u = \text{RECIPE}(0, x^k, \bar{x}^k, t_k), \quad E := (I + hA)^{-1}.$$

Instantaneous control rewritten

$$\begin{aligned}
 (I + hA)x^{k+1} = & \\
 x^k + hb^k & - \underbrace{\rho \mathcal{B}\mathcal{B}^* E^* C^* C E (x^k - \bar{x}^k) - h\rho \mathcal{B}\mathcal{B}^* E^* C^* C E (b(x^k) - A\bar{x}^k)}_{\mathcal{B}u^{k+1} =: K_I^d(x^k)}.
 \end{aligned}$$

This is the semi-discrete version of

$$\begin{aligned}
 \dot{x} + Ax = b - & \underbrace{\frac{\rho}{h} \mathcal{B}\mathcal{B}^* E^* C^* C E (x - \bar{x}) - \rho \mathcal{B}\mathcal{B}^* E^* C^* C E (b(x) - A\bar{x})}_{\mathcal{B} \frac{u}{h} =: K_I(x)}, \\
 x(0) = & x_0.
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 \end{aligned}$$

Model predictive control

For model predictive control the oracle RECIPE is given by

$$u = \text{RECIPE}(x^k, z, t_k)$$

iff

- Solve the optimality system for u

$$\begin{aligned}(I + hA)x &= x^k + hb(x^k, t_k) + \mathcal{B}u \\ (I + hA)^*\lambda &= -\mathcal{C}^*(\mathcal{C}x - z) \\ \gamma u + \mathcal{B}^*\lambda &= 0 \quad (\gamma u + \mathcal{B}^*\lambda \geq 0) \text{ in case of constraints.}\end{aligned}$$

- set $\text{RECIPE} = u$

This oracle realizes solution of problem (P_k) .

Feedback operators: MPC

With $\mathcal{C} \equiv Id$ and $\mathcal{B} = id$ let $S := \gamma(E^*E + \gamma I)^{-1}E^*E$.
 Model predictive control rewritten

$$(I + hA)x^{k+1} = x^k + hb(x^k) - \underbrace{\frac{1}{\gamma}S(x^k - \bar{x}^k + hb(x^k) - hA\bar{x}^k)}_{u^{k+1} =: K_O^d(x^k)}.$$

This is the semi-discrete version of

$$\dot{x} + Ax = b(x) - \underbrace{\frac{1}{\gamma h}S(x - \bar{x} + hb(x) - hA\bar{x})}_{\frac{u}{h} =: K_O(x)}, \quad x(0) = x_0.$$

Feedback operators: MPC

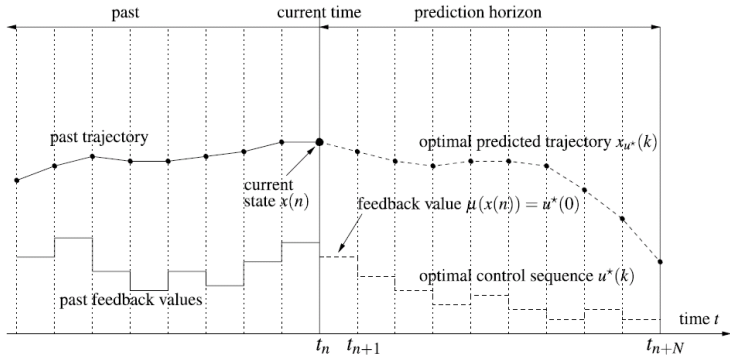
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MPC schematic revisited



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MPC with $t_c = h, t_p = Nh$

Discretize the state equation w.r.t. time (your favorite scheme!)

Set $x_0 := x^k$, $x_i \approx x(t_k + ih)(i = 1, \dots, N)$.

$$(*) \quad T \begin{bmatrix} x_1 \\ \vdots \\ x_N \end{bmatrix} = \begin{bmatrix} x_0 \\ \vdots \\ x_{N-1} \end{bmatrix} + h \begin{bmatrix} b(x_0) \\ \vdots \\ b(x_{N-1}) \end{bmatrix} + \mathcal{B} \begin{bmatrix} u_1 \\ \vdots \\ u_N \end{bmatrix}$$

and minimize at every time step an instantaneous version of the cost; with $X := (x_1, \dots, x_N)^t$ and $U := (u_1, \dots, u_N)^t$ solve

$$(P_k) \quad \left\{ \begin{array}{l} \min J(U) = \frac{\gamma}{2} \|U\|^2 + \frac{1}{2} \|\mathcal{C}X - z\|^2 \\ \text{s.t. } (*) \equiv \text{transition constraints} \end{array} \right.$$

Controller construction now along the lines of the previous slides.

- (P_k) is an optimization problem with nonlinear PDE constraints!

Comments on controller construction

- **Optimal control problem in MPC approach need not admit a (unique) solution. Thus MPC controller need not be well defined.**
- Transition constraints (often) guarantee a well defined control to state mapping. An instantaneous controller in this case is well defined.
- Time marching scheme for the state and discretization of the state in prediction step may differ.
- Analysis (stability, decay, length of prediction horizon) of MPC schemes for PDEs is emerging (Altmüller, Grüne & Worthmann). Results for instantaneous control available in special situations ($\mathcal{C} = Id, \mathcal{B} = Id$).
- Promising approach: combine controller construction introduced here with techniques developed by Altmüller, Grüne, and Worthmann (GAMM Mitteilungen 35(2):131–145, 2012)
- It is *very easy* to include pointwise bounds on the control and/or the state within the MPC setting!
- Optimization problems with PDE constraints (and pointwise bounds on the control and/or state form the central building block in MPC!

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PDE constrained optimization for mother problems



Mother Problem

$$(\mathbb{P}) \quad \left\{ \begin{array}{l} \min_{(y,u) \in Y \times U} J(y,u) := \frac{1}{2} \|y - z\|_{L^2(\Omega)}^2 + \frac{\alpha}{2} \|u\|_U^2 \\ \text{s.t.} \\ \begin{array}{rcl} -\Delta y & = & Bu \quad \text{in } \Omega, \\ y & = & 0 \quad \text{on } \partial\Omega, \end{array} \\ \text{and} \\ u \in U_{\text{ad}} \subseteq U. \end{array} \right. \quad (0.1)$$

Here,

- $\Omega \subset \mathbb{R}^n$ denotes an open, bounded sufficiently smooth (polyhedral) domain,
- $Y := H_0^1(\Omega)$,
- the operator $B : U \rightarrow H^{-1}(\Omega) \equiv Y^*$ denotes the (linear, continuous) control operator, and
- U_{ad} is assumed to be a closed and convex subset of the Hilbert space U .
- Later we will also add state constraints $y \in Y_{\text{ad}}$.

Exercises 1

- Explain the spaces $L^2(\Omega)$, $H_0^1(\Omega)$, and $H^{-1}(\Omega)$.
- In which sense is the PDE understood if the solution space is $H_0^1(\Omega)$?
- How is the weak solution of the Poisson problem defined?
- Does the Poisson equation possess a unique solution?
- Does problem (\mathbb{P}) admit a solution for all $\alpha \geq 0$?

Examples for control spaces and operators

1 $U := L^2(\Omega)$, $B : L^2(\Omega) \rightarrow H^{-1}(\Omega)$ Injection, , $U_{\text{ad}} := \{v \in L^2(\Omega); a \leq v(x) \leq b \text{ a.e. in } \Omega\}$, $a, b \in L^\infty(\Omega)$.

2 $U := H^1(\Omega)$, $B : H^1(\Omega) \rightarrow H^{-1}(\Omega)$ Injection, , $U_{\text{ad}} := \{v \in L^2(\Omega); a \leq v(x) \leq b \text{ a.e. in } \Omega\}$, $a, b \in L^\infty(\Omega)$.

3 $U := \mathbb{R}^m$, $B : \mathbb{R}^m \rightarrow H^{-1}(\Omega)$, $Bu := \sum_{j=1}^m u_j F_j$, $F_j \in H^{-1}(\Omega)$ given ,
 $U_{\text{ad}} := \{v \in \mathbb{R}^m; a_j \leq v_j \leq b_j\}$, $a < b$.

Reduced cost functional

We have that

- the Poisson problem for given right hand side Bu admits a unique solution $y = y(u)$,
- Problem (\mathbb{P}) admits a unique solution $(y, u) \in H_0^1(\Omega) \times U$, with $y = y(u)$.

Thus, problem (\mathbb{P}) can be equivalently rewritten as the optimization problem

$$(\hat{\mathbb{P}}) \quad \min_{u \in U_{\text{ad}}} \hat{J}(u) \tag{0.2}$$

for the reduced functional

$$\hat{J}(u) := J(y(u), u) \equiv J(SBu, u)$$

over the set U_{ad} , where $S : Y^* \rightarrow Y$ denotes the weak solution operator associated with $-\Delta$.

First order necessary optimality condition

- The first order necessary (and here also sufficient) optimality conditions take the form

$$\langle \hat{J}'(u), v - u \rangle_{U^*, U} \geq 0 \text{ for all } v \in U_{ad}. \quad (0.3)$$

- Here

$$\hat{J}'(u) = \alpha(u, \cdot)_U + B^* S^*(SBu - z) \equiv \alpha(u, \cdot)_U + B^* p,$$

with

- $p := S^*(SBu - z) \in Y^{**}$ denoting the adjoint variable. The function p in our reflexive setting satisfies

$$\begin{aligned} -\Delta p &= y - z && \text{in } \Omega, \\ p &= 0 && \text{on } \partial\Omega. \end{aligned}$$

- With the Riesz isomorphism $R : U^* \rightarrow U$ and the orthogonal projection $P_{U_{ad}} : U \rightarrow U_{ad}$ we have that (0.4) is equivalent to

$$u = P_{U_{ad}} \left(u - \sigma \nabla \hat{J}(u) \right) \text{ for all } \sigma > 0, \quad (0.4)$$

where

$$\nabla \hat{J}(u) = R \hat{J}'(u)$$

denotes the gradient of $\hat{J}(u)$.

Exercises 2

- Prove the optimality condition.
- How can we obtain the formula for $\hat{J}'(u)$?
- Discuss the adjoint variable p ?
- How is the Riesz isomorphism in a Hilbert space defined?
- Discuss examples for the Riesz isomorphism, e.g. the cases $U = L^2(\Omega)$ and $U = H_0^1(\Omega)$.
- Is the gradient *smoother* than the derivative?
- How is the orthogonal projection $P_{U_{\text{ad}}} : U \rightarrow U_{\text{ad}}$ defined?
- How can we obtain the fixpoint formula for the optimal control?

To discretize (\mathbb{P}) we concentrate on Finite Element approaches and make the following assumptions.

Assumption

- $\Omega \subset \mathbb{R}^n$ denotes a polyhedral domain,
- $\bar{\Omega} = \cup_{j=1}^{nt} \bar{T}_j$,
- with admissible quasi-uniform sequences of partitions $\{T_j\}_{j=1}^{nt}$ of Ω , i.e. with $h_{nt} := \max_j \text{diam } T_j$ and $\sigma_{nt} := \min_j \{\sup \text{diam } K; K \subseteq T_j\}$ there holds

$$c \leq \frac{h_{nt}}{\sigma_{nt}} \leq C$$

uniformly in nt with positive constants $0 < c \leq C < \infty$ independent of nt .

- We abbreviate $\tau_h := \{T_j\}_{j=1}^{nt}$.

In order to tackle (\mathbb{P}) numerically we shall distinguish two different approaches.
The first is called

First discretize, then optimize,

the second

First optimize, then discretize.

It will turn out that both approaches under certain circumstances lead to the same numerical results. However, from a structural point of view they are completely different.

- We later will highlight a special variant of the FDTO approach which is called *variational discretization*.

First discretize, then optimize

All quantities in (\mathbb{P}) are discretized:

- replace Y and U by finite dimensional subspaces Y_h and U_d ,
- the set U_{ad} by some discrete counterpart U_{ad}^d , and
- the functionals, integrals and dualities by appropriate discrete surrogates.

Finite element space: For $k \in \mathbb{N}$

$$W_h := \{v \in C^0(\bar{\Omega}); v|_{T_j} \in \mathbb{P}_k(T_j) \text{ for all } 1 \leq j \leq nt\} =: \langle \phi_1, \dots, \phi_{ng} \rangle, \text{ and}$$

$$Y_h := \{v \in W_h, v|_{\partial\Omega} = 0\} =: \langle \phi_1, \dots, \phi_n \rangle \subseteq Y,$$

with some $0 < n < ng$.

Ansatz for discrete state: $y_h(x) = \sum_{i=1}^n y_i \phi_i$.

Discrete control space: with $u^1, \dots, u^m \in U$, we set

- $U_d := \langle u^1, \dots, u^m \rangle$, and
- $U_{\text{ad}}^d := P_{U_{\text{ad}}}^d(U_d)$, where
- $P_{U_{\text{ad}}}^d : U \rightarrow U_{\text{ad}}$ is a sufficiently smooth (nonlinear) mapping.

With $C \subset \mathbb{R}^m$ denoting a convex closed set we assume

$$U_{\text{ad}}^d = \left\{ u \in U; u = \sum_{j=1}^m s_j u^j, s \in C \right\}.$$

Finally let $z_h := Q_h z = \sum_{i=1}^{ng} z_i \phi_i$, where $Q_h : L^2(\Omega) \rightarrow W_h$ denotes a continuous projection operator.

Now we replace problem (\mathbb{P}) by

$$(\mathbb{P}_{(h,d)}) \left\{ \begin{array}{ll} \min_{(y_h, u_d) \in Y_h \times U_d} J_{(h,d)}(y, u) := \frac{1}{2} \|y_h - z_h\|_{L^2(\Omega)}^2 + \frac{\alpha}{2} \|u_d\|_U^2 \\ \text{s.t.} \\ a(y_h, v_h) = \langle B u_d, v_h \rangle_{Y^*, Y} \quad \text{for all } v_h \in Y_h, \\ \text{and} \\ u_d \in U_{ad}^d. \end{array} \right. \quad (0.5)$$

Here, we have set $a(y, v) := \int_{\Omega} \nabla y \nabla v dx$.

Introduce Finite Element matrices:

- Stiffness matrix: $A := (a_{ij})_{i,j=1}^n$, $a_{ij} := a(\phi_i, \phi_j)$,
- mass matrix $M := (m_{ij})_{i,j=1}^{ng}$, $m_{ij} := \int_{\Omega} \phi_i \phi_j dx$, the
- control matrix $E := (e_{ij})_{i,j=1}^{n,m}$, $e_{ij} = \langle Bu^j, \phi_i \rangle_{Y^*, Y}$, and the
- control mass matrix $F := (f_{ij})_{i,j=1}^m$, $f_{ij} := (u^i, u^j)_U$.

Using these quantities allows us to rewrite $(\mathbb{P}_{(h,d)})$ as finite-dimensional optimization problem:

$$(\mathbb{P}_{(n,m)}) \quad \begin{cases} \min_{(y,s) \in \mathbb{R}^n \times \mathbb{R}^m} Q(y, s) := \frac{1}{2}(y - z)^t M (y - z) + \frac{\alpha}{2} s^t F s \\ \text{s.t.} \\ \mathbf{A}y = \mathbf{E}s \\ \text{and} \\ s \in C. \end{cases} \quad (0.6)$$

Admissibility is characterized by the closed, convex set $C \subset \mathbb{R}^m$.

Since the matrix A is spd, problem $(\mathbb{P}_{(n,m)})$ is equivalent to minimizing the reduced functional

$$\hat{Q}(s) := Q(A^{-1}Es, s)$$

over the set C .

Problem $(\mathbb{P}_{(n,m)})$ admits a unique solution $(y(s), s) \in \mathbb{R}^n \times C$ which is characterized by the finite dimensional variational inequality

$$(\nabla \hat{Q}(s), t - s)_{\mathbb{R}^m} \geq 0 \text{ for all } t \in C, \quad (0.7)$$

with

$$\nabla \hat{Q}(s) = \alpha F s + E^t A^{-t} M(A^{-1}Es - z) \equiv \alpha F s + E^t p,$$

where

$$p := A^{-t} M(A^{-1}Es - z).$$

Comparing

$$\nabla \hat{Q}(s) = \alpha F s + E^t A^{-t} M (A^{-1} E s - z) \equiv \alpha F s + E^t p$$

with

$$\nabla \hat{J}(u) = \alpha u + R B^* S^* (S B u - z) \equiv \alpha u + R B^* p$$

from the infinite-dimensional problem, we note that transposition takes the role of the Riesz isomorphism R ,

- the matrix F takes the role of the identity in U ,
- the matrix M takes the role of the identity in $L^2(\Omega)$,
- the matrix E takes the role the control operator B , and
- the matrix A^{-1} that of the solution operator S .

Problem $(\mathbb{P}_{(n,m)})$ now can be solved numerically with the help of appropriate solution algorithms, which should exploit the structure of the problem. We fix the following

Remark

In the **First discretize, then optimize** approach the discretization of the adjoint variable \mathbf{p} is determined by the test space for the discrete state \mathbf{y}_h .

In the **First optimize, then discretize** approach discussed next, this is different.

Exercises 3

- Is the finite element space W_h a subset of $H^1(\Omega)$?
- How are the functions ϕ_i ($i = 1, \dots, ng$) defined?
- Show that the matrices A , M , and F are spd.
- Does $(\mathbb{P}_{n,m})$ admit a unique solution?
- What is (0.7) in the case $C \equiv \mathbb{R}^m$?

First optimize, the discretize

Starting point: the first order necessary optimality conditions for problem (\mathbb{P}) ;

$$(\text{OS}) \quad \left\{ \begin{array}{lll} -\Delta y & = & Bu \quad \text{in } \Omega, \\ y & = & 0 \quad \text{on } \partial\Omega, \\ -\Delta p & = & y - z \quad \text{in } \Omega, \\ p & = & 0 \quad \text{on } \partial\Omega, \\ (\alpha u + RB^*p, v - u)_U & \geq & 0 \quad \text{for all } v \in U_{\text{ad}}. \end{array} \right. \quad (0.8)$$

- Discretize everything related to the state y , the control u , and to functionals, integrals, and dualities as in the **First discretize, then optimize** approach.
- In addition, we have the freedom to also select an appropriate discretization of the adjoint variable p .

For p we choose continuous Finite Elements of order l on τ , which leads to the Ansatz

$$p_h(x) = \sum_{i=1}^q p_i \chi_i(x),$$

where

$$\langle \chi_1, \dots, \chi_q \rangle \subset Y$$

denotes the Ansatz space for the adjoint variable.

Matrices:

- adjoint stiffness matrix $\tilde{A} := (\tilde{a}_{ij})_{i,j=1}^q$, $\tilde{a}_{ij} := a(\chi_i, \chi_j)$,
- the matrix $\tilde{E} := (\tilde{e}_{ij})_{i,j=1}^{q,m}$, $\tilde{e}_{ij} = \langle Bu^j, \chi_i \rangle_{Y^*, Y}$,
- and the matrix $T := (t_{ij})_{i,j=1}^{n,q}$, $t_{ij} := \int_{\Omega} \phi_i \chi_j dx$.

The discrete analogon to (OS) reads

$$(\text{OS})_{(n,q,m)} \quad \left\{ \begin{array}{ll} Ay & = Es, \\ \tilde{A}p & = T(y - z), \\ (\alpha Fs + \tilde{E}^t p, t - s)_{\mathbb{R}^m} & \geq 0 \text{ for all } t \in C. \end{array} \right. \quad (0.9)$$

Since the matrices A and \tilde{A} are spd, this system is equivalent to the variational inequality

$$(\alpha Fs + \tilde{E}^t \tilde{A}^{-1} T(A^{-1} Es - z), t - s)_{\mathbb{R}^m} \geq 0 \text{ for all } t \in C. \quad (0.10)$$

Examples

- 1 $U := L^2(\Omega)$, $B : L^2(\Omega) \rightarrow H^{-1}(\Omega)$ Injection, $U_{ad} := \{v \in L^2(\Omega); a \leq v(x) \leq b \text{ a.e. in } \Omega\}$, $a, b \in L^\infty(\Omega)$. Further let $k = l = 1$ (linear Finite Elements for y and p), $U_d := \langle u^1, \dots, u^{nt} \rangle$, where $u^k|_{T_i} = \delta_{ki}$ ($k, i = 1, \dots, nt$) are piecewise constant functions (i.e. $m = nt$), $C := \prod_{i=1}^{nt} [a_i, b_i]$, where $a_i := a(\text{barycenter}(T_i))$, $b_i := b(\text{barycenter}(T_i))$.
- 2 As in 1., but $U_d := \langle \phi_1, \dots, \phi_{ng} \rangle$ (i.e. $m = ng$), $C := \prod_{i=1}^{ng} [a_i, b_i]$, where $a_i := a(P_i)$, $b_i := b(P_i)$, with P_i ($i = 1, \dots, ng$) denoting the vertices of the triangulation τ .
- 3 As in 1., but $U := \mathbb{R}^m$, $B : \mathbb{R}^m \rightarrow H^{-1}(\Omega)$, $Bu := \sum_{j=1}^m u_j F_j$, $F_j \in H^{-1}(\Omega)$ given, $U_{ad} := \{v \in \mathbb{R}^m; a_j \leq v_j \leq b_j\}$, $a < b$, $U_d := \langle e_1, \dots, e_m \rangle$ with $e_i \in \mathbb{R}^m$ ($i = 1, \dots, m$) denoting the i -th unitvector, $C := \prod_{i=1}^{ng} [a_i, b_i] \equiv U_d$.

Discussion and implications

- Choosing the same Ansatz spaces for the state y and the adjoint variable p in the **First optimize, then discretize** approach leads to an optimality condition which is identical to that of the **First discretize, then optimize** approach, since then $T \equiv M$.
- Choosing a different approach for p in general leads to a non-symmetric matrix T , with the consequence that the matrix $\alpha F + \tilde{E}^t \tilde{A}^{-1} T A^{-1} E$ no longer represents a symmetric matrix (and thus no Hessian), and
- the expression $\alpha F s + \tilde{E}^t \tilde{A}^{-1} T (A^{-1} E s - z)$ in general does not represent a gradient.
- There is up to now no general recipe which approach has to be preferred, and it should depend on the application and computational resources which approach to take for tackling the numerical solution of the optimization problem.
- However, the numerical approach taken should to some extent reflect and preserve the structure which is inherent in the infinite dimensional optimization problem (\mathbb{P}) .

Structure exploiting discretization

This can be best explained in the case without control constraints, i.e. $U_{\text{ad}} \equiv U$. Then the first order necessary optimality conditions for (\mathbb{P}) read

$$\nabla \hat{J}(u) = \alpha u + RB^* S^*(SBu - z) \equiv \alpha u + RB^* p = 0 \text{ in } U.$$

For proceeding on the numerical level this identity clearly gives us the advice to relate to each other the discrete Ansätze for the control u and the adjoint variable p .

This remains true also in the presence of control constraints, for which this smooth operator equation has to be replaced by the nonsmooth operator equation

$$u = P_{U_{\text{ad}}} (u - \sigma(\alpha u + RB^* p)) \equiv_{\sigma=\frac{1}{\alpha}} P_{U_{\text{ad}}} \left(-\frac{1}{\alpha} RB^* p \right) \text{ in } U, \quad (0.11)$$

where $P_{U_{\text{ad}}}$ denotes the orthogonal projection in U onto the admissible set of controls.

In any case, optimal control and corresponding adjoint state are related to each other, and this should be reflected by numerical approaches to be taken for the solution of problem (\mathbb{P}) .

Remark

Controls should be discretized conservative, i.e. according to the relation between the adjoint state and the control given by the first order optimality condition. This rule should be obeyed in both, the **First discretize, then optimize**, and in the **First optimize, then discretize** approach.

A structure exploiting discretization concept

Let us closer investigate (0.11) in terms of the simple fixpoint iteration given next.

Algorithm

- u given
- do until convergence
$$u^+ = P_{U_{ad}} \left(-\frac{1}{\alpha} RB^* p(u) \right), u = u^+.$$

In this algorithm $p(u)$ is obtained by first solving $y = SBu$, and then $p = S^*(SBu - z)$.

To obtain a discrete algorithm we now replace the solution operators S, S^* by their discrete counterparts S_h, S_h^* obtained by a Finite Element discretization, say. The discrete algorithm then reads

Algorithm

- u given
- do until convergence
$$u^+ = P_{U_{ad}} \left(-\frac{1}{\alpha} RB^* p_h(u) \right), \quad u = u^+,$$

where $p_h(u)$ is obtained by first solving $y = S_h Bu$, and then solving $p_h = S_h^*(S_h Bu - z)$.

We note that in this algorithm the control is not discretized. Only state and adjoint state are discretized.

Two questions immediately arise.

- ❶ Is Algorithm 4 numerically implementable?
- ❷ Do Algorithms 3, 4 converge?

Let us first discuss question (2). Since both algorithms are fixpoint algorithms, sufficient conditions for convergence are given by the relations

$$\alpha > \|RB^*S^*SB\|_{\mathcal{L}(U)}$$

for Algorithm 3, and by

$$\alpha > \|RB^*S_h^*S_hB\|_{\mathcal{L}(U)}$$

for Algorithm 4, since $P_{U_{\text{ad}}} : U \rightarrow U_{\text{ad}}$ denotes the orthogonal projection which is Lipschitz continuous with Lipschitz constant $L = 1$.

Question (1) admits the answer **Yes**, whenever for given u it is possible to numerically evaluate the expression

$$P_{U_{\text{ad}}} \left(-\frac{1}{\alpha} RB^* p_h(u) \right)$$

in the $i - th$ iteration of Algorithm 4 with an numerical overhead which is **independent** of the iteration counter of the algorithm.

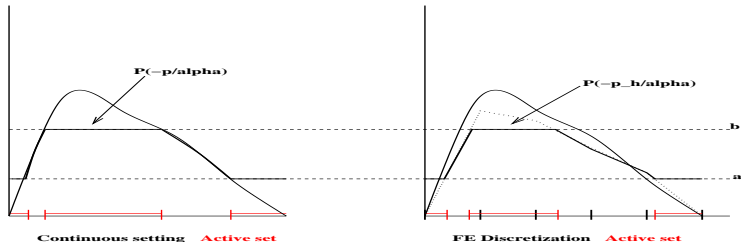
To illustrate this fact let us consider the case $U = L^2(\Omega)$ and $B : U \rightarrow H^{-1}(\Omega)$ denoting the injection, with $a \equiv \text{const}1$, $b \equiv \text{const}2$. In this case it is easy to verify that

$$P_{U_{\text{ad}}}(v)(x) = P_{[a,b]}(v(x)) = \max\{a, \min\{v(x), b\}\},$$

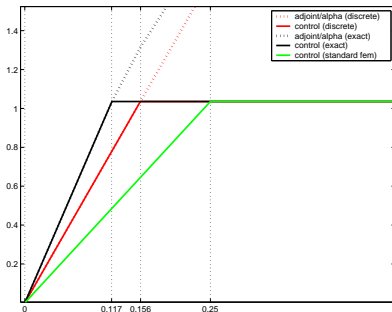
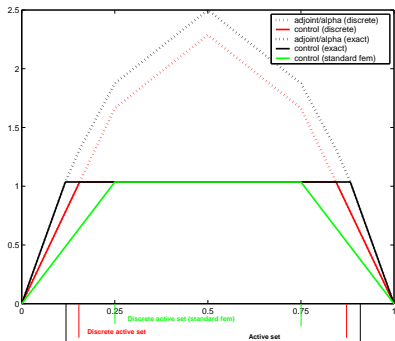
so that in every iteration of Algorithm 4 we have to form the control

$$u^+(x) = P_{[a,b]}\left(-\frac{1}{\alpha}p_h(x)\right), \quad (0.12)$$

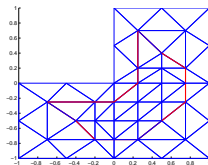
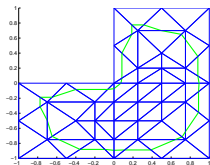
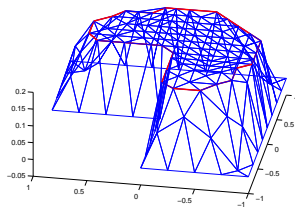
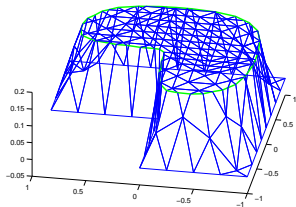
which for in the onedimensional setting is illustrated in Figure 54.



A 1-d example



A 2-d example



To construct the function u^+ it is sufficient to characterize the intersection of the bounds a, b (understood as constant functions) and the function $-\frac{1}{\alpha}p_h$ on every simplex T of the triangulation $\tau = \tau_h$. For piecewise linear finite element approximations of p we have the following theorem.

Theorem

Let u^+ denote the function of (0.12), with p_h denoting a piecewise linear, continuous finite element function, and constant bounds $a < b$. Then there exists a partition $\kappa_h = \{K_1, \dots, K_{l(h)}\}$ of Ω such that u^+ restricted to K_j ($j = 1, \dots, l(h)$) is a polynomial either of degree zero or one. For $l(h)$ there holds

$$l(h) \leq Cnt(h),$$

with a positive constant $C \leq 3$ and $nt(h)$ denoting the number of simplexes in τ_h . In particular, the vertices of the discrete active set associated to u^+ need not coincide with finite element nodes.

Proof: Abbreviate $\xi_h^a := -\frac{1}{\alpha}p_h^* - a$, $\xi_h^b := b - \frac{1}{\alpha}p_h^*$ and investigate the zero level sets 0_h^a and 0_h^b of ξ_h^a and ξ_h^b , respectively.

Case $n = 1$: $0_h^a \cap T_i$ is either empty or a point $S_i^a \in T_i$. Every point S_i^a subdivides T_i into two sub-intervals. Analogously $0_h^b \cap T_i$ is either empty or a point $S_i^b \in T_i$. Further $S_i^a \neq S_i^b$ since $a < b$. The maximum number of sub-intervals of T_i induced by 0_h^a and 0_h^b therefore is equal to three. Therefore, $l(h) \leq 3nt(h)$, i.e. $C = 3$.

Case $n \in \mathbb{N}$: $0_h^a \cap T_i$ is either empty or a part of a k -dimensional hyperplane ($k < n$) $L_i^a \subset T_i$, analogously $0_h^b \cap T_i$ is either empty or a part of k -dimensional hyperplane ($k < n$) $L_i^b \subset T_i$. Since $a < b$ the surfaces L_i^a and L_i^b do not intersect. Therefore, similar considerations as in the case $n = 1$ yield $C = 3$.

- It is now clear that the proof of the previous theorem easily extends to functions p_h which are piecewise polynomials of degree $k \in \mathbb{N}$, and bounds a, b which are piecewise polynomials of degree $l \in \mathbb{N}$ and $m \in \mathbb{N}$, respectively, since the difference of a, b and p_h in this case also represents a piecewise polynomial function whose projection on every element can be (easily ?) characterized.
- We now have that Algorithm 4 is numerically implementable, but only converges for a certain parameter range of α . A locally fast (superlinear) convergent algorithm for the numerical solution of equation (0.13) is the semi-smooth Newton method, if the function G is semi-smooth in the sense of [HIK03],[MU03, Example 5.6].

Let us recall that (0.11) for every $\sigma > 0$ is equivalent to the equation

$$\begin{aligned} G(u) = u - P_{U_{\text{ad}}} \left(u - \sigma \nabla \hat{J}(u) \right) &\equiv u - P_{U_{\text{ad}}} \left(u - \sigma(\alpha u + RB^*p) \right) \equiv \\ &\equiv_{\sigma=\frac{1}{\alpha}} u - P_{U_{\text{ad}}} \left(-\frac{1}{\alpha} RB^*p \right) = 0 \text{ in } U, \quad (0.13) \end{aligned}$$

so that we may apply a semi-smooth Newton algorithm, or a primal-dual active set strategy to its numerical solution.

Remark

For the choice $\sigma = \frac{1}{\alpha}$ we in certain situations obtain that the semi-smooth Newton method and the primal-dual active set strategy are equivalent, and are both numerically implementable in the discrete case.

Exercises 4

- Why is the orthogonal projection in a Hilbert space Lipschitz continuous with constant $L = 1$?

- Show for constant box constraints $a < b$ that

$$P_{U_{\text{ad}}}(v)(x) = P_{[a,b]}(v(x)) = \max\{a, \min\{v(x), b\}\}$$

holds.

- Why is the bound $\alpha > \|RB^*S^*SB\|_{\mathcal{L}(U)}$ sufficient for convergence of the fixpoint iteration?

What is the underlying discrete problem?

Let us define

$$\hat{J}_h(u) := J(S_h B u, u), \quad u \in U$$

and consider the following infinite dimensional optimization problem

$$\min_{u \in U_{\text{ad}}} \hat{J}_h(u). \tag{0.14}$$

According to (0.2) this problem admits a unique solution $u_h \in U_{\text{ad}}$ which is characterized by the variational inequality

$$(\nabla \hat{J}_h(u_h), v - u_h)_U \geq 0 \text{ for all } v \in U_{\text{ad}}, \tag{0.15}$$

This variational inequality is equivalent to the non-smooth operator equation (compare (0.13))

$$\begin{aligned} G_h(u) = u - P_{U_{\text{ad}}} \left(u - \sigma \nabla \hat{J}_h(u) \right) &\equiv u - P_{U_{\text{ad}}} \left(u - \sigma(\alpha u + RB^* p_h) \right) \equiv_{\sigma=\frac{1}{\alpha}} \\ &\equiv_{\sigma=\frac{1}{\alpha}} u - P_{U_{\text{ad}}} \left(-\frac{1}{\alpha} RB^* p_h \right) = 0 \text{ in } U, \end{aligned}$$

where similar as above

$$\nabla \hat{J}_h(u) = \alpha u + RB^* S_h^*(S_h B u - z) \equiv \alpha u + RB^* p_h(u).$$

The considerations made above now imply that the unique solution u_h of the infinite dimensional optimization problem (0.14) can be numerically computed either by Algorithm 4 (for α large enough), or by a semi-smooth Newton method (which for $\sigma = \frac{1}{\alpha}$ coincides with the primal-dual active set strategy) (since the function G_h also is semi-smooth), however in both cases **without** a further discretization step.

Primal-dual active set strategy

Solve ($B \equiv Id$)

$$(\alpha + S_h^* S_h)u + \hat{\lambda} = S_h^* z = -r$$

$$\Psi(u, \hat{\lambda}; u) := \max(\hat{\lambda} + \sigma(u - b), 0) + \min(\hat{\lambda} + \sigma(u - a), 0) = \hat{\lambda}$$

Primal-dual active set strategy:

Initialize $u_0 = 0$, $\hat{\lambda}_0 = -r$; set $l = 1$, $\epsilon > 0$ small.

Loop l

$$\mathcal{A}_l^a := \{\hat{\lambda}_{l-1} + \sigma(u_{l-1} - a) < 0\} (= \{-r - S_h^* S_h u_{l-1} - \alpha a < 0\}, \text{ if } \sigma = \alpha),$$

$$\mathcal{A}_l^b := \{\hat{\lambda}_{l-1} + \sigma(u_{l-1} - b) > 0\} (= \{-r - S_h^* S_h u_{l-1} - \alpha b > 0\}, \text{ if } \sigma = \alpha),$$

$$\mathcal{I}_l := \Omega \setminus (\mathcal{A}_l^a \cup \mathcal{A}_l^b).$$

$$l \geq 2, \mathcal{A}_l^a = \mathcal{A}_{l-1}^a, \mathcal{A}_l^b = \mathcal{A}_{l-1}^b, \text{ or } \|\Psi(u_{l-1}, \hat{\lambda}_{l-1}) - \hat{\lambda}_{l-1}\| \leq \epsilon:$$

$u = u_{l-1}$, $\hat{\lambda} = \hat{\lambda}_l$, RETURN.

Otherwise

$$u_l = a \text{ on } \mathcal{A}_l^a, u_l = b \text{ on } \mathcal{A}_l^b, \hat{\lambda}_l = 0 \text{ on } \mathcal{I}_l$$

$$\text{Solve for } u_l|_{\mathcal{I}_l}, \hat{\lambda}_l|_{\mathcal{A}_l^a \cup \mathcal{A}_l^b}$$

$$(\alpha + S_h^* S_h)u_l + \hat{\lambda}_l = -r$$

$l := l + 1.$

Semi-smooth Newton method

- u given, solve until convergence

$$G'_h(u)u^+ = -G_h(u) + G'_h(u)u, \quad u = u^+.$$

1. This algorithm is implementable whenever the fix-point iteration is, since

$$\begin{aligned} -G_h(u) + G'_h(u)u &= \\ &= -P_{U_{\text{ad}}} \left(-\frac{1}{\alpha} RB^* p_h(u) \right) - \frac{1}{\alpha} P'_{U_{\text{ad}}} \left(-\frac{1}{\alpha} RB^* p_h(u) \right) RB^* S_h^* S_h B u. \end{aligned}$$

2. In certain settings this algorithm for every $\alpha > 0$ is locally fast convergent.

Neumann (Robin) boundary control

$U = L^2(\Gamma)$, $Bu := \int_{\Gamma} u \cdot d\Gamma \in (H^1)^*(\Omega)$, $R : U^* \rightarrow U$ with $R(u, \cdot)_U = u$.

Discrete weak form

$$a(y_h, v_h) = \int_{\Gamma} u v_h d\Gamma \text{ for all } v_h \in W_h,$$

discrete adjoint equation

$$a(v_h, p_h) = \int_{\Omega} (y_h - z) v_h dx \text{ for all } v_h \in W_h.$$

Thus

$RB^* p_h = (p_h)_{\Gamma}$ piecewise polynomial, continuous on the boundary grid.

With $U_{ad} = \{a \leq u \leq b\}$ we have for the variational discrete $u_h \in U_{ad}$

$$u_h = \max\{a, \min\{-\frac{1}{\alpha}(p_h)_{\Gamma}, b\}\} \text{ simple cut-off at the bounds.}$$

Dirichlet boundary control

$U = L^2(\Gamma)$, $Bu := - \int_{\Gamma} u \partial_{\eta} \cdot d\Gamma \in (H_0^1(\Omega) \cap H^2(\Omega))^*$, $R : U^* \rightarrow U$ with $R(u, \cdot)_U = u$.

Discrete weak form; find $y_h \in W_h$ with

$$a(y_h, v_h) = 0 \text{ for all } v_h \in Y_h, \text{ and } y_h = \Pi(u) \in \text{Trace}(W_h),$$

where Π denotes the L^2 -projection. Discrete adjoint equation for $p_h \in Y_h$

$$a(v_h, p_h) = \int_{\Omega} (y_h - z) v_h dx \text{ for all } v_h \in Y_h.$$

Thus

$$u_h = P_{U_{ad}}\left(\frac{1}{\alpha} \kappa_h\right),$$

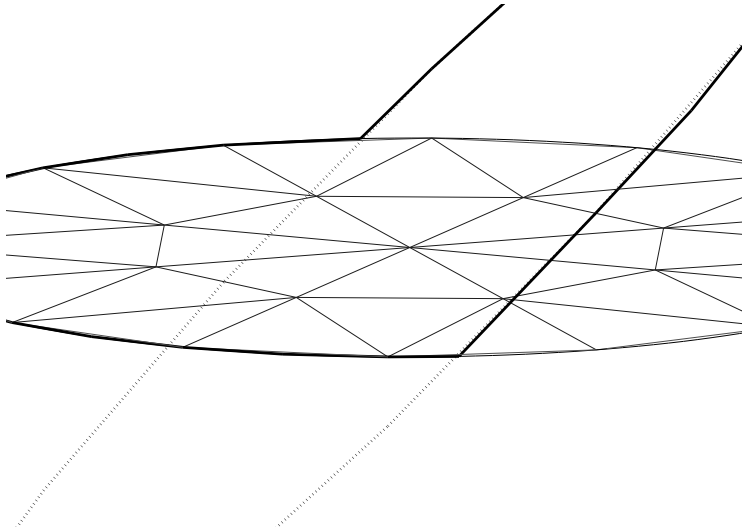
where $\kappa_h \in \text{Trace}(W_h)$ denotes the discrete adjoint flux satisfying

$$\int_{\Gamma} \kappa_h w_h d\Gamma = a(w_h, p_h) - \int_{\Omega} (y_h - z) w_h dx \text{ for all } w_h \text{ in } W_h.$$

With $U_{ad} = \{a \leq u \leq b\}$ we have for the variational discrete $u_h \in U_{ad}$

$$u_h = \max\{a, \min\{\frac{1}{\alpha} \kappa_h, b\}\} \text{ simple cut-off at the bounds.}$$

Dirichlet boundary control



Exercises 5

- In the case of box constraints, what is a canonical choice of $P'_{U_{ad}}$?
- $\Pi : L^2(\Gamma) \rightarrow W_h$, the L^2 —projection, is how defined?
- Show that in the case of Dirichlet boundary control

$$u_h = P_{U_{ad}}\left(\frac{1}{\alpha}\kappa_h\right),$$

where $\kappa_h \in \text{Trace}(W_h)$ denotes the discrete adjoint flux satisfying

$$\int_{\Gamma} \kappa_h w_h d\Gamma = a(w_h, p_h) - \int_{\Omega} (y_h - z) w_h dx \text{ for all } w_h \text{ in } W_h.$$

- If one would like to approximate the Dirichlet boundary control problem with piecewise constant controls. How could one achieve this? Tip: Discretize the state with mixed finite elements (lowest order Raviart-Thomas elements).

Error estimates

Theorem

Let \mathbf{u} denote the unique solution of (0.2), and \mathbf{u}_h the unique solution of (0.14). Then there holds

$$\begin{aligned} \alpha \|\mathbf{u} - \mathbf{u}_h\|_{\mathbf{U}}^2 + \frac{1}{2} \|y(\mathbf{u}) - y_h\|^2 &\leq \\ &\leq \langle B^*(p(\mathbf{u}) - \tilde{p}_h(\mathbf{u})), \mathbf{u}_h - \mathbf{u} \rangle_{\mathbf{U}^*, \mathbf{U}} + \frac{1}{2} \|y(\mathbf{u}) - y_h(\mathbf{u})\|^2, \quad (0.16) \end{aligned}$$

where $\tilde{p}_h(\mathbf{u}) := \mathbf{S}_h^*(\mathbf{S}B\mathbf{u} - z)$, $y_h(\mathbf{u}) := \mathbf{S}_h B\mathbf{u}$, and $y(\mathbf{u}) := \mathbf{S}B\mathbf{u}$.

Proof: We switch back to the variational inequalities

$$\langle \hat{J}'(u), v - u \rangle_{U^*, U} \geq 0 \text{ for all } v \in U_{\text{ad}},$$

and

$$\langle \hat{J}'_h(u_h), v - u_h \rangle_{U^*, U} \geq 0 \text{ for all } v \in U_{\text{ad}}.$$

Crucial:

The unique solution u of the continuous problem (upper inequality) is an admissible test function for the discrete problem (lower inequality).

Let us emphasize, that this is different for approaches, where the control space is discretized explicitly. In this case we may only expect that u_h is an admissible test function for the continuous problem (if ever).

So let us test the optimality condition for u with u_h , and the optimality condition for u_h with u , and then add the resulting variational inequalities. This leads to

$$\langle \alpha(u - u_h) + B^* S^*(SBu - z) - B^* S_h^*(S_h B u_h - z), u_h - u \rangle_{U^*, U} \geq 0.$$

This inequality is equivalent to

$$\alpha \|u - u_h\|_U^2 \leq \langle B^*(p(u) - \tilde{p}_h(u)) + B^*(\tilde{p}_h(u) - p_h(u_h)), u_h - u \rangle_{U^*, U}.$$

Let us investigate the second addend on the right hand side of this inequality. By definition of the adjoint variables there holds

$$\begin{aligned} \langle B^*(\tilde{p}_h(u) - p_h(u)), u_h - u \rangle_{U^*, U} &= \langle \tilde{p}_h(u) - p_h(u), B(u_h - u) \rangle_{Y, Y^*} = \\ &= a(y_h - y_h(u), \tilde{p}_h(u) - p_h(u)) = \int_{\Omega} (y_h(u_h) - y_h(u))(y(u) - y_h(u)) dx = \\ &= -\|y_h - y\|^2 + \int_{\Omega} (y - y_h)(y - y_h(u)) dx \leq -\frac{1}{2}\|y_h - y\|^2 + \frac{1}{2}\|y - y_h(u)\|^2 \end{aligned}$$

so that the claim of the theorem follows.

What are the consequences of this Theorem?

From the structure of this estimate we immediately infer that an error estimate for $\|u - u_h\|_U$ is at hand, if

- an error estimate for $\|B^*(p(u) - \tilde{p}_h(u))\|_{U^*}$ is available, and**
- an error estimate for $\|y(u) - y_h(u)\|_{L^2(\Omega)}$ is available.**

This means, that the error of $\|u - u_h\|_U$ is completely determined by the approximation properties of the discrete solution operators S_h and S_h^* .

Remark

The error $\|\mathbf{u} - \mathbf{u}_h\|_{\mathbf{U}}$ between the solutions \mathbf{u} and \mathbf{u}_h is completely determined by the approximation properties of the discrete solution operators \mathbf{S}_h and \mathbf{S}_h^ .*

Let us revisit our first example with $U = L^2(\Omega)$ and B denoting the injection. Then $y = SBu \in H^2(\Omega) \cap H_0^1(\Omega)$ (if for example $\Omega \in C^{1,1}$ or Ω polygonal, convex). Let us estimate the right side of our error estimate. There holds

$$\begin{aligned} (RB^*(p(u) - \tilde{p}_h(u)), u - u_h)_U &= \int_{\Omega} (p(u) - \tilde{p}_h(u))(u - u_h) dx \leq \\ &\leq \|p(u) - \tilde{p}_h(u)\|_{L^2(\Omega)} \|u - u_h\|_{L^2(\Omega)} \leq \\ &\leq ch^2 \|y(u) - z\|_{L^2(\Omega)} \|u - u_h\|_{L^2(\Omega)}, \end{aligned}$$

and

$$\|y(u) - y_h(u)\|_{L^2} \leq ch^2 \|u\|_{L^2(\Omega)}.$$

Theorem

Let \mathbf{u} and \mathbf{u}_h denote the solutions of the continuous and the discrete problem, respectively in the setting of the first example,(1). Then there holds

$$\|\mathbf{u} - \mathbf{u}_h\|_{L^2(\Omega)} \leq ch^2 \left\{ \|y(\mathbf{u}) - z\|_{L^2(\Omega)} + \|\mathbf{u}\|_{L^2(\Omega)} \right\}.$$

And this theorem is also valid for the setting of this example,(2) if we require $F_j \in L^2(\Omega)$ ($j = 1, \dots, m$). This is an easy consequence of the fact that for a function $z \in Y$ there holds $B^*z \in \mathbb{R}^m$ with $(B^*z)_i = \langle F_i, z \rangle_{Y^*, Y}$ for $i = 1, \dots, m$.

Theorem

Let \mathbf{u} and \mathbf{u}_h denote the solutions of problem (0.2) and (0.14), respectively in the setting of Example ??(2). Then there holds

$$\|\mathbf{u} - \mathbf{u}_h\|_{\mathbb{R}^m} \leq ch^2 \left\{ \|y(\mathbf{u}) - z\|_{L^2(\Omega)} + \|\mathbf{u}\|_{\mathbb{R}^m} \right\},$$

where the positive constant now depends on the functions F_j ($j = 1, \dots, m$).

Proof:

It suffices to estimate

$$\begin{aligned}
 (RB^*(p(u) - \tilde{p}_h(u)), u - u_h)_{\mathbb{R}^m} &= \\
 &= \sum_{j=1}^m \left\{ \int_{\Omega} F_j(p(u) - \tilde{p}_h(u)) dx (u - u_h)_j \right\} \leq \\
 &\leq \|p(u) - \tilde{p}_h(u)\|_{L^2(\Omega)} \left(\sum_{j=1}^m \int_{\Omega} |F_j|^2 dx \right)^{\frac{1}{2}} \|u - u_h\|_{\mathbb{R}^m} \leq \\
 &\leq ch^2 \|y(u) - z\|_{L^2(\Omega)} \|u - u_h\|_{\mathbb{R}^m}.
 \end{aligned}$$

The reminder terms can be estimated as above.

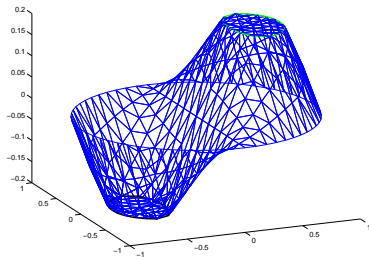
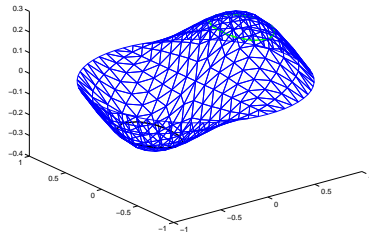
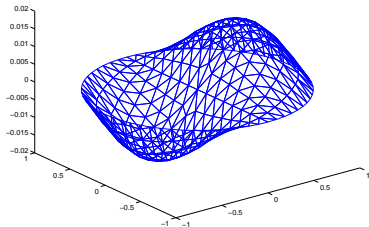
Numerical example distributed control

We consider our optimal control problem with Ω denoting the unit circle,

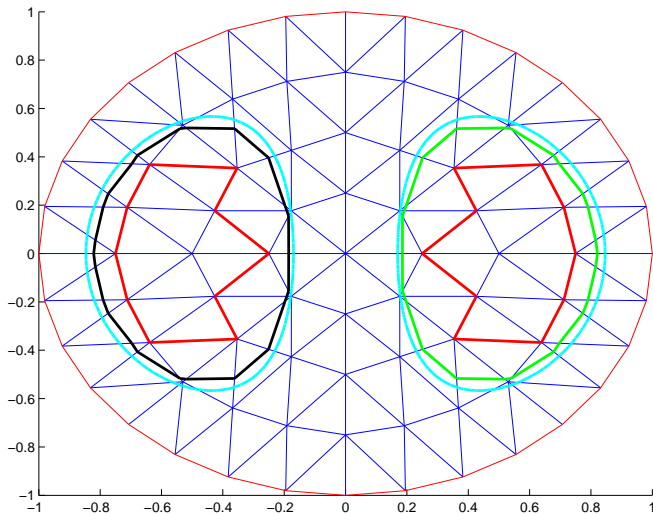
$$U_{\text{ad}} := \{v \in L^2(\Omega); -0.2 \leq u \leq 0.2\} \subset L^2(\Omega)$$

and $B : L^2(\Omega) \rightarrow Y^*(\equiv H^{-1}(\Omega))$ the injection. Further we set $z(x) := (1 - |x|^2)x_1$ and $\alpha = 0.1$. The numerical discretization of state and adjoint state is performed with linear, continuous finite elements.

Here we consider the scenario that the exact solution of the problem is not known in advance (although it is easy to construct example problems where exact state, adjoint state and control are known, see [T05]). Instead we use the numerical solutions computed on a grid with $h = \frac{1}{256}$ as references.



$$h = \frac{1}{4}, \alpha = 0.01$$



$$h = \frac{1}{8}, \alpha = 0.1$$

To present numerical results it is convenient to introduce the **Experimental Order of Convergence**, brief EOC, which for some positive error functional E is defined by

$$\text{EOC} := \frac{\ln E(h_1) - \ln E(h_2)}{\ln h_1 - \ln h_2}.$$

EOC for the state y

h	E_{yL2}	E_{ysup}	E_{ysem}	E_{yH_1}	EOC_{yL2}	EOC_{ysup}	EOC_{yH_1}
1/1	1.47e-2	1.63e-2	5.66e-2	5.85e-2	-	-	-
1/2	5.61e-3	6.02e-3	2.86e-2	2.92e-2	1.39	1.44	1.00
1/4	1.47e-3	1.93e-3	1.38e-2	1.39e-2	1.93	1.64	1.08
1/8	3.83e-4	5.02e-4	6.89e-3	6.90e-3	1.94	1.95	1.01
1/16	9.65e-5	1.26e-4	3.44e-3	3.45e-3	1.99	2.00	1.00
1/32	2.40e-5	3.14e-5	1.71e-3	1.71e-3	2.01	2.00	1.01
1/64	5.73e-6	7.78e-6	8.37e-4	8.37e-4	2.06	2.01	1.03
1/128	1.16e-6	1.85e-6	3.74e-4	3.74e-4	2.30	2.07	1.16

EOC for the adjoint state p

h	$E_{p_{L2}}$	$E_{p_{sup}}$	$E_{p_{sem}}$	$E_{p_{H_1}}$	$EOC_{p_{L2}}$	$EOC_{p_{sup}}$	$EOC_{p_{H_1}}$
1/1	2.33e-2	2.62e-2	8.96e-2	9.26e-2	-	-	-
1/2	6.14e-3	7.75e-3	4.36e-2	4.40e-2	1.92	1.76	1.07
1/4	1.59e-3	2.50e-3	2.17e-2	2.18e-2	1.95	1.64	1.02
1/8	4.08e-4	6.52e-4	1.09e-2	1.09e-2	1.97	1.94	0.99
1/16	1.03e-4	1.64e-4	5.48e-3	5.48e-3	1.99	1.99	1.00
1/32	2.54e-5	4.14e-5	2.73e-3	2.73e-3	2.01	1.99	1.01
1/64	6.11e-6	1.04e-5	1.33e-3	1.33e-3	2.06	1.99	1.03
1/128	1.27e-6	2.61e-6	5.96e-4	5.96e-4	2.27	1.99	1.16

EOC for the control u

h	$E_{u_{L2}}$	$E_{u_{sup}}$	$E_{u_{sem}}$	$E_{u_{H_1}}$	$EOC_{u_{L2}}$	$EOC_{u_{sup}}$	$EOC_{u_{H_1}}$
1/1	2.18e-1	2.00e-1	8.66e-1	8.93e-1	-	-	-
1/2	5.54e-2	7.75e-2	4.78e-1	4.81e-1	1.97	1.37	0.89
1/4	1.16e-2	2.30e-2	2.21e-1	2.22e-1	2.25	1.75	1.12
1/8	3.02e-3	5.79e-3	1.15e-1	1.15e-1	1.94	1.99	0.95
1/16	7.66e-4	1.47e-3	6.09e-2	6.09e-2	1.98	1.98	0.92
1/32	1.93e-4	3.67e-4	2.97e-2	2.97e-2	1.99	2.00	1.03
1/64	4.82e-5	9.38e-5	1.41e-2	1.41e-2	2.00	1.97	1.07
1/128	1.17e-5	2.37e-5	6.40e-3	6.40e-3	2.04	1.98	1.14

EOC for the control u , conventional approach

h	$E_{u_{L2}}$	$E_{u_{sup}}$	$E_{u_{sem}}$	$E_{u_{H_1}}$	$EOC_{u_{L2}}$	$EOC_{u_{sup}}$	$EOC_{u_{H_1}}$
1/1	2.18e-1	2.00e-1	8.66e-1	8.93e-1	-	-	-
1/2	6.97e-2	9.57e-2	5.10e-1	5.15e-1	1.64	1.06	0.79
1/4	1.46e-2	3.44e-2	2.39e-1	2.40e-1	2.26	1.48	1.10
1/8	4.66e-3	1.65e-2	1.53e-1	1.54e-1	1.65	1.06	0.64
1/16	1.57e-3	8.47e-3	9.94e-2	9.94e-2	1.57	0.96	0.63
1/32	5.51e-4	4.33e-3	6.70e-2	6.70e-2	1.51	0.97	0.57
1/64	1.58e-4	2.09e-3	4.05e-2	4.05e-2	1.80	1.05	0.73
1/128	4.91e-5	1.07e-3	2.50e-2	2.50e-2	1.68	0.96	0.69

$$E_a := |(A \setminus A_h) \cup (A_h \setminus A)|$$

denotes the symmetric difference of discrete and continuous active sets. EOC with the corresponding subscripts denotes the associated experimental order of convergence.

h	EOC for active set			
	conventional E_a	approach EOC_a	our E_a	approach EOC_a
1/1	5.05e-1	-	5.11e-1	-
1/2	5.05e-1	0.00	3.38e-1	0.60
1/4	5.05e-1	0.00	1.25e-1	1.43
1/8	2.60e-1	0.96	2.92e-2	2.10
1/16	1.16e-1	1.16	7.30e-3	2.00
1/32	4.98e-2	1.22	1.81e-3	2.01
1/64	1.88e-2	1.41	4.08e-4	2.15
1/128	6.98e-3	1.43	8.51e-5	2.26

Postprocessing

Let us note that similar numerical results can be obtained by an approach of Meyer and Rösch presented in [MR04]. The authors in a preliminary step compute a piecewise constant optimal control \bar{u} and with its help compute in a post-processing step a projected control u through

$$u = P_{U_{\text{ad}}} \left(-\frac{1}{\alpha} RB^* p_h(\bar{u}) \right).$$

The numerical analysis requires the assumption, that the measure of the set of elements intersected by the boarder of the active set of the control can be bounded in terms of the grid size.

Bang–Bang control

$$\begin{aligned} \min_{u \in U_{ad}} J(u) &= \frac{1}{2} \int_{\Omega} |y - y_0|^2 \\ \text{subject to } y &= \mathcal{G}(u). \end{aligned}$$

Here,

$$U_{ad} := \{v \in L^2(\Omega); a \leq v \leq b\} \subseteq L^2(\Omega)$$

with $a < b$ constants, and $y = \mathcal{G}(Bu)$ iff

$$-\Delta y = u \text{ in } \Omega, \text{ and } y = 0 \text{ on } \partial\Omega.$$

More general elliptic operators may be considered, and also control operators which map abstract controls to feasible right-hand sides of the elliptic equation.

Existence and uniqueness, optimality conditions

The optimal control problems admits a unique solution.

The function $u \in U_{ad}$ is a solution of the optimal control problem iff there exists an adjoint state p such that $y = \mathcal{G}(u)$, $p = \mathcal{G}(y - y_0)$ and

$$(p, v - u) \geq 0 \text{ for all } v \in U_{ad}.$$

There holds

$$u(x) \quad \begin{cases} = a, & p(x) > 0, \\ \in [a, b], & p(x) = 0, \\ = b, & p(x) < 0. \end{cases}$$

Strict complementarity requirement for the solution u :

$$\exists C > 0 \forall \epsilon > 0 : \mathcal{L}(\{x \in \bar{\Omega}; |p(x)| \leq \epsilon\}) \leq C\epsilon$$

Variational discretization

Discrete optimal control problem:

$$\begin{aligned} \min_{u \in U_{ad}} J_h(u) &:= \frac{1}{2} \int_{\Omega} |y_h - y_0|^2 \\ \text{subject to } y_h &= \mathcal{G}_h(u). \end{aligned}$$

Here, $\mathcal{G}_h(u)$ denotes the piecewise linear and continuous finite element approximation to $y(u)$, i.e.

$$a(y_h, v_h) := (\nabla y_h, \nabla v_h) = (u, v_h) \text{ for all } v_h \in X_h,$$

where on a given, quasi-uniform triangulation \mathcal{T}_h

$$X_h := \{w \in C^0(\bar{\Omega}); w|_{\partial\Omega} = 0, w|_T \text{ linear for all } T \in \mathcal{T}_h\}.$$

This problem is still ∞ -dimensional.

Ritz projection $R_h : H_0^1(\Omega) \rightarrow X_h$,

$$a(R_h w, v_h) = a(w, v_h) \text{ for all } v_h \in X_h$$

Existence and uniqueness, optimality conditions for discrete problem

The variational-discrete optimal control problems admits a solution. The solution is unique, if $\text{meas}\{p_h = 0\} = 0$.

The function $u_h \in U_{ad}$ is a solution of the optimal control problem iff there exists an adjoint state p_h such that $y_h = \mathcal{G}_h(u_h)$, $p_h = \mathcal{G}_h(y_h - y_0)$ and

$$(p_h, v - u_h) \geq 0 \text{ for all } v \in U_{ad}.$$

There holds

$$u_h(x) \quad \begin{cases} = a, & p_h(x) > 0, \\ \in [a, b], & p_h(x) = 0, \\ = b, & p_h(x) < 0. \end{cases}$$

Error estimate

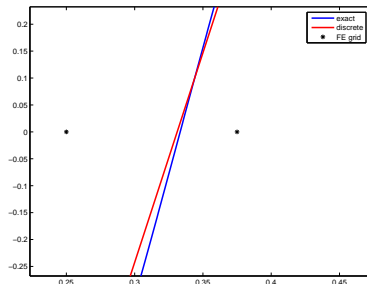
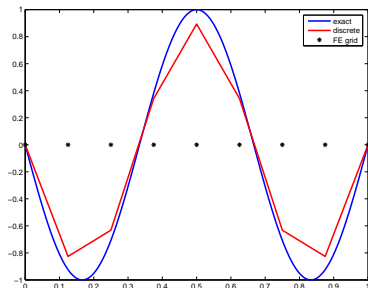
Let u, u_h denote the unique solutions of the optimal control problems with corresponding states $y = \mathcal{G}(u)$ and $y_h = \mathcal{G}_h(u_h)$, resp. Then

$$\|u - u_h\|_{L^1}, \|y - y_h\|, \|p - p_h\|_{L^\infty} \leq C \left\{ h^2 + \|p - R_h p\|_{L^\infty} \right\}$$

Sketch of proof:

- $\|u - u_h\|_{L^1} \leq (b - a) \mathcal{L}(\{p > 0, p_h \leq 0\} \cup \{p < 0, p_h \geq 0\})$
- $\{p > 0, p_h \leq 0\} \cup \{p < 0, p_h \geq 0\} \subseteq \{|p(x)| \leq \|p - p_h\|_\infty\} \Rightarrow$
- $\|u - u_h\|_{L^1} \leq C \|p - p_h\|_\infty$
- $\|p - p_h\|_\infty \leq \|p - R_h p\|_\infty + \|R_h p - p_h\|_\infty$
- $\|R_h p - p_h\|_\infty \leq C \|y - y_h\|.$
- Combine these estimates with $(p, u_h - u) \geq 0$ and $(p_h, u - u_h) \geq 0$ (note that u is admissible as testfunction for the discrete problem!).

Numerical example with 2 switching points



Experimental order of convergence:

- Active set 3.00073491, (here \approx) $\|u - u_h\|_{L^1}$: 3.00077834
- Function values 1.99966106
- $\|p - p_h\|_{L^\infty}$: 1.99979367
- $\|y - y_h\|_{L^\infty}$: 1.9997965
- $\|p - p_h\|_{L^2}$: 1.99945711

Homotopy in α with semi-smooth Newton, Tröltzsch checkerboard

D. & G. Wachsmuth (ESAIM: COCV 2011 (Preprint 2009)), von Daniels (Diploma Thesis 2010):

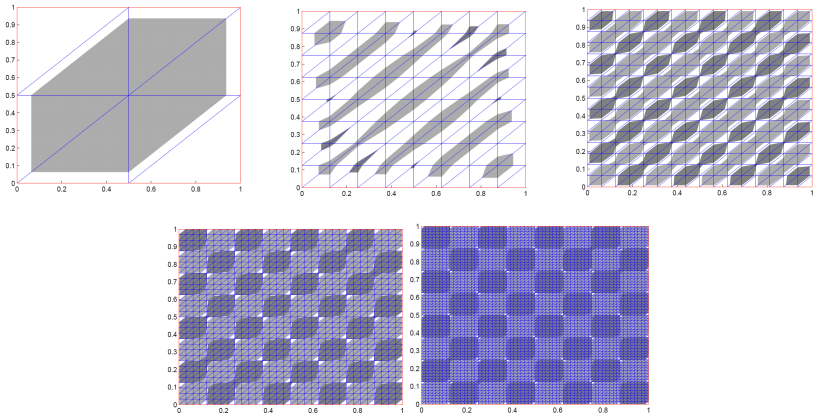
- $\|u_0 - u_\alpha\| \sim \sqrt{\alpha}$,
- $\|u_\alpha - u_{\alpha,h}\| \sim h^2 \alpha^{-1}$, thus
- $\|u_0 - u_{\alpha,h}\| \sim h^{\frac{2}{3}}$

$$u(x) = -\text{sign } p(x), p(x) = -\frac{1}{128\pi^2} \sin(8\pi x_1) \sin(8\pi x_2), y(x) = \sin(\pi x_1) \sin(\pi x_2).$$

Loop i	$\ u - u_h\ _{L^1}$	$\ u - u_h\ _{L^2}$	$EOC_{L^1}(u)$	$EOC_{L^2}(u)$	Nit
3	2.5008e-001	4.7416e-001	1.10	0.61	4
4	1.2045e-001	3.4864e-001	1.05	0.44	5
5	3.6487e-002	1.9368e-001	1.72	0.85	4
6	5.8124e-003	6.2070e-002	1.33	0.82	3
7	2.1287e-003	3.7590e-002	1.45	0.72	3
mean			1.33	0.69	

Numerical example by Nicolaus von Daniels

Checkerboard example, plots



Time-dependent problems

For the time-dependent case we sketch the analysis of Discontinuous Galerkin approximations w.r.t. time for an abstract linear-quadratic model problem. The underlying analysis turns out to be very similar to that of the previous section for the stationary model problem.

Let V, H denote separable Hilbert spaces, so that $(V, H = H^*, V^*)$ forms a Gelfand triple. We denote by $a : V \times V \rightarrow \mathbb{R}$ a bounded, coercive (and symmetric) bilinear form, and again by U the Hilbert space of controls, and by $B : U \rightarrow L^2(V^*)$ the linear control operator. Here, $T > 0$. For $y_0 \in H$ we consider the state equation

$$\left. \begin{aligned} \int_0^T \langle y_t, v \rangle_{V^*, V} + a(y, v) dt &= \int_0^T \langle (Bu)(t), v \rangle_{V^*, V} dt & \forall v \in L^2(V), \\ (y(0), v)_H &= (y_0, v)_H & \forall v \in V, \end{aligned} \right\} : \Leftrightarrow y = \mathcal{T}Bu,$$

which for every $u \in U$ admits a unique solution $y = y(u) \in W := \{w \in L^2(V), w_t \in L^2(V^*)\}$.

Optimization problem

$$(TP) \quad \begin{cases} \min_{(y,u) \in W \times U_{\text{ad}}} J(y, u) := \frac{1}{2} \|y - z\|_{L^2(H)}^2 + \frac{\alpha}{2} \|u\|_U^2 \\ \text{s.t. } y = \mathcal{T}Bu, \end{cases} \quad (0.17)$$

where $U_{\text{ad}} \subseteq U$ denotes a closed, convex subset. Introducing the reduced cost functional

$$\hat{J}(u) := J(y(u), u),$$

the necessary (and in the present case also sufficient) optimality conditions take the form

$$\langle \hat{J}'(u), v - u \rangle_{U^*, U} \geq 0 \text{ for all } v \in U_{\text{ad}}.$$

Here

$$\nabla \hat{J}(u) = \alpha u + B^* p(y(u)),$$

where the adjoint state p solves the adjoint equation

$$\begin{aligned} \int_0^T \langle -p_t, w \rangle_{V^*, V} + a(w, p) dt &= \int_0^T (y - z, w)_H \quad \forall w \in W, \\ (p(T), v)_H &= 0, \quad v \in V. \end{aligned}$$

This variational inequality is equivalent to the semi-smooth operator equation

$$u = P_{U_{\text{ad}}} \left(-\frac{1}{\alpha} R B^* p(y(u)) \right).$$

Discretization

Let $V_h \subset V$ denote a finite dimensional subspace, and let

$0 = t_0 < t_1 < \dots < t_m = T$ denote a time grid with grid width δt . We set $I_n := (t_{n-1}, t_n]$ for $n = 1, \dots, m$ and seek discrete states in the space

$$V_{h,\delta t} := \{\phi : [0, T] \times \Omega \rightarrow \mathbb{R}, \phi(t, \cdot)|_{\bar{\Omega}} \in V_h, \phi(\cdot, x)|_{I_n} \in \mathbb{P}_r \text{ for } n = 1, \dots, m\}.$$

i.e. $y_{h,\delta t}$ is a polynomial of degree $r \in \mathbb{N}$ w.r.t. time. Possible choices of V_h in applications include polynomial finite element spaces, and also wavelet spaces, say. We define the discontinuous Galerkin w.r.t. time approximation (dG(r)-approximation) $\tilde{y} = y_{h,\delta t}(u) \equiv \mathcal{T}_{h,\delta t} Bu \in V_{h,\delta t}$ of the state y as unique solution of

$$\begin{aligned}
 A(\tilde{y}, v) &:= \sum_{n=1}^m \int_{I_n} (\tilde{y}_t, v)_H + a(\tilde{y}, v) dt + \sum_{n=1}^m ([\tilde{y}]^{n-1}, v^{n-1+})_H + (\tilde{y}^{0+}, v^{0+})_H = \\
 &= (y_0, v^{0+})_H + \int_0^T \langle (Bu)(t), v \rangle_{V^*, V} dt \text{ for all } v \in V_{h,\delta t}. \quad (0.18)
 \end{aligned}$$

Here,

$$v^{n+} := \lim_{t \searrow t_n} v(t, \cdot), \quad v^{n-} := \lim_{t \nearrow t_n} v(t, \cdot), \text{ and } [v]^n := v^{n+} - v^{n-}.$$

Discrete optimal control problem

The discrete counterpart of the optimal control problem reads for the variational approach

$$(P_{h,\delta t}) \quad \min_{u \in U_{\text{ad}}} \hat{J}_{h,\delta t}(u) := J(y_{h,\delta t}(u), u)$$

and it admits a unique solution $u_{h,\delta t} \in U_{\text{ad}}$. We further have

$$\nabla \hat{J}_{h,\delta t}(v) = \alpha v + B^* p_{h,\delta t}(y_{h,\delta t}(v)),$$

where $p_{h,\delta t}(y_{h,\delta t}(v)) \in V_{h,\delta t}$ denotes the unique solution of

$$A(v, p_{h,\delta t}) = \int_0^T (y_{h,\delta t} - z, v)_H dt \text{ for all } v \in V_{h,\delta t}.$$

Further, the unique discrete solution $u_{h,\delta t}$ satisfies

$$\langle u_{h,\delta t} + B^* p_{h,\delta t}, v - u_{h,\delta t} \rangle_{U^*, U} \geq 0 \text{ for all } v \in U_{\text{ad}}.$$

As in the continuous case this variational inequality is equivalent to a semi-smooth operator equation, namely

$$u_{h,\delta t} = P_{U_{\text{ad}}} \left(-\frac{1}{\alpha} R B^* p_{h,\delta t}(y_{h,\delta t}(u_{h,\delta t})) \right).$$

Error estimate

Theorem

Let $\mathbf{u}, \mathbf{u}_{h,\delta t}$ denote the unique solutions of (P) and $(P_{h,\delta t})$, respectively. Then

$$\begin{aligned} \alpha \|\mathbf{u} - \mathbf{u}_{h,\delta t}\|_U^2 + \|y_{h,\delta t}(\mathbf{u}_{h,\delta t}) - y_{h,\delta t}(\mathbf{u})\|_{L^2(H)}^2 &\leq \\ &\leq \langle B^*(p(\mathbf{u}) - \tilde{p}_{h,\delta t}(\mathbf{u})), \mathbf{u}_{h,\delta t} - \mathbf{u} \rangle_{U^*,U} + \|y(\mathbf{u}) - y_{h,\delta t}(\mathbf{u})\|_{L^2(H)}^2, \quad (0.19) \end{aligned}$$

where $\tilde{p}_{h,\delta t}(\mathbf{u}) := \mathcal{T}_{h,\delta t}^*(\mathcal{T}B\mathbf{u} - z)$, $y_{h,\delta t}(\mathbf{u}) := \mathcal{T}_{h,\delta t}B\mathbf{u}$, and $y(\mathbf{u}) := \mathcal{T}B\mathbf{u}$.

As a result of estimate (0.19) we have that error estimates for the variational discretization are available if error estimates for the $dg(r)$ -approximation to the state and the adjoint state are available. With $dG(0)$ in time and piecewise linear and continuous finite elements in space one gets

$$\alpha \|\mathbf{u} - \mathbf{u}_{h,\delta t}\|_U^2 + \|y_{h,\delta t}(\mathbf{u}_{h,\delta t}) - y_{h,\delta t}(\mathbf{u})\|_{L^2(H)}^2 \leq C\{\delta t + h^2\}.$$

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Incorporation of state constraints

Optimal control of pdes with pointwise constraints:

$$\min_{u \in U_{\text{ad}}, y \in Y_{\text{ad}}} J(y, u) \text{ s.t. } PDE(y) = B(u)$$

Analysis: Casas 85,93 (pointwise state constraints), Casas & Fernandez 93 (pointwise constraints on gradient)

Numerical analysis (pointwise state constraints):

A priori:

Original problem: Casas & Mateos; Deckelnick & H.; Meyer; ...

Relaxation: Group of Rösch; Group of Tröltzsch; Hintermüller & H.; H. & Meyer; H. & Schiela; ...

A posteriori: Benedix, Vexler & Wollner; Günther & H.; Hintermüller, Hoppe & Kieweg.

Numerical analysis (pointwise constraints on gradient): Deckelnick, Günther, & H.

State and control constraints

Model problem

$$\begin{aligned}
 \min_{u \in U_{ad}} J(u) &= \frac{1}{2} \int_D |y - z|^2 + \frac{\alpha}{2} \|u\|_U^2 \\
 \text{subject to } y &= \mathcal{G}(Bu) \text{ and } y \leq b \text{ in } D.
 \end{aligned}$$

Here, $U_{ad} \subseteq U$ closed and convex, $\alpha > 0$, z , b , sufficiently smooth, and $y = \mathcal{G}(Bu)$ iff

$$Ay = Bu \text{ in } D, \text{ plus b.c. (plus i.c.)}$$

- elliptic case: $D = \Omega$ and $Ay := -\sum_{i,j=1}^d \partial_{x_j}(a_{ij}y_{x_i}) + \sum_{i=1}^d b_i y_{x_i} + cy$ uniformly elliptic operator,
- parabolic case: $D = (0, T] \times \Omega$ and $Ay := y_t - \sum_{i,j=1}^d \partial_{x_j}(a_{ij}y_{x_i}) + \sum_{i=1}^d b_i y_{x_i} + cy$ with strongly elliptic leading part.

Slater condition: $\exists \tilde{u} \in U_{ad}$ such that $\mathcal{G}(B\tilde{u}) < b$ in \bar{D} .

Optimality conditions (Casas 86,93)

Let $u \in U_{ad}$ denote the unique optimal control and $y = \mathcal{G}(Bu)$. Then there exist $\mu \in \mathcal{M}(\bar{D})$ and some p such that there holds

$$\begin{aligned}
 \int_D p A v &= \int_D (y - z) v + \int_{\bar{D}} v d\mu \quad \forall v \in X, \\
 \langle B^* p + \alpha u, v - u \rangle_{U^*, U} &\geq 0 \quad \forall v \in U_{ad}, \\
 \mu &\geq 0, \quad y \leq b \text{ in } D \text{ and } \int_{\bar{D}} (b - y) d\mu = 0,
 \end{aligned}$$

where

- elliptic case: $p \in W^{1,s}(\Omega)$ for all $s < d/(d-1)$ and $X = H^2(\Omega)$ with $\sum_{i,j=1}^d a_{ij} v_{x_i} v_j = 0$ on $\partial\Omega$,
- parabolic case: $p \in L^s(W^{1,\sigma})$ for all $s, \sigma \in [1, 2)$ with $2/s + d/\sigma > d+1$ and $X = \{v \in C^0(\bar{Q}); v(0, \cdot) = 0\} \cap \{v \in L^2(H^2), v_t \in L^2(H^1)\}$.

Discretization – a variational concept

Discrete optimal control problem:

$$\begin{aligned} \min_{u \in U_{ad}} J_h(u) &:= \frac{1}{2} \int_D |y_h - z|^2 + \frac{\alpha}{2} \|u\|_U^2 \\ \text{subject to } y_h &= \mathcal{G}_h(Bu) \text{ and } y_h \leq l_h b. \end{aligned}$$

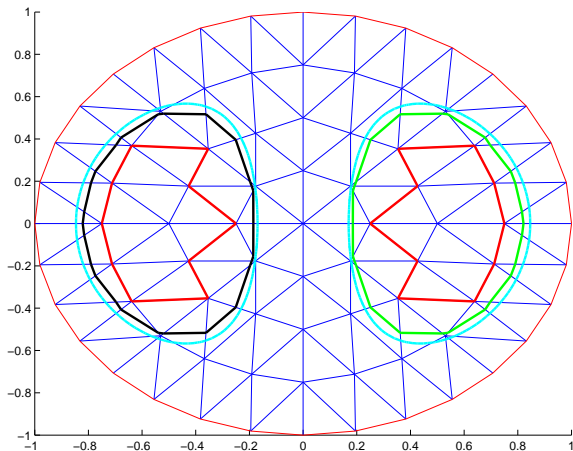
Here, $y_h(u) = \mathcal{G}_h(Bu)$ denotes the

- p.l. and continuous fe approximation to $y(u)$ (elliptic case),
- $dg(0)$ in time and p.l. and continuous fe in space approximation to $y(u)$ (parabolic case), i.e.

$$a(y_h, v_h) = \langle Bu, v_h \rangle \text{ for all } v_h \in X_h.$$

We do not discretize the control!

Variational versus conventional discretization



Variational discretization for time-dependent problems

Movie time-dependent problems

Discrete optimality conditions

Let $u_h \in U_{ad}$ denote the unique variational-discrete optimal control, $y_h = \mathcal{G}(Bu_h)$. There exist $\mu \in \mathbb{R}^k$ and $p_h \in X_h$ such that with

- $\mu_h = \sum_{j=1}^{nv} \mu_j \delta_{x_j}$ (elliptic case, x_i fe nodes, $k = nv$),
- $\mu_h = \sum_{i=1}^m \sum_{j=1}^{nv} \mu_{ij} \delta_{x_j} \circ \frac{1}{|I_i|} \int_{I_i} \bullet dt$ (parabolic case, x_i fe nodes, I_i dg intervals, $k = nv + m$),

we have

$$\begin{aligned}
 a(v_h, p_h) &= \int_D (y_h - z) v_h + \int_{\bar{D}} v_h d\mu_h \quad \forall v_h \in X_h, \\
 \langle B^* p_h + \alpha u_h, v - u_h \rangle_{U^*, U} &\geq 0 \quad \forall v \in U_{ad}, \\
 \mu_j &\geq 0, y_h \leq l_h b, \text{ and } \int_{\bar{D}} (l_h b - y_h) d\mu_h = 0.
 \end{aligned}$$

Here, δ_x denotes the Dirac measure concentrated at x and l_h is the usual Lagrange interpolation operator.

Results

Let $u_h \in U_{ad}$ denote the variational-discrete optimal solution with corresponding state $y_h \in X_h$ and $\mu_h \in \mathcal{M}(\bar{D})$. Then for h small enough

$$\|y_h\|, \|u_h\|_U, \|\mu_h\|_{\mathcal{M}(\bar{D})} \leq C.$$

For the proof a discrete counterpart to the Slater condition is needed, which is deduced from uniform convergence of the discrete states associated to the Slater point $B\tilde{u}$.

Results, cont.

Let u denote the solution of the continuous problem and u_h the variational discrete optimal control. Then

$$\begin{aligned} \alpha \|u - u_h\|^2 + \|y - y_h\|^2 &\leq \\ &\leq C(\|\mu\|_{\mathcal{M}(\bar{D})}, \|\mu_h\|_{\mathcal{M}(\bar{D})}) \left\{ \|y - y_h(u)\|_\infty + \|y^h(u_h) - y_h\|_\infty \right\} + \\ &\quad + C(\|u\|, \|u_h\|) \left\{ \|y - y_h(u)\| + \|y^h(u_h) - y_h\| \right\}. \end{aligned}$$

Here, $y_h(u) = \mathcal{G}_h(Bu)$, $y^h(u_h) = \mathcal{G}(Bu_h)$.

We need uniform estimates for discrete approximations.

Error estimates, parabolic case

Deckelnick, H. (JCM 2010)

Controls $u \in L^2(0, T)^m$, and $f_i \in H^1(\Omega)$ given actuations.

$$Bu := \sum_{i=1}^m u_i(t) f_i(x), \quad y_0 \in H^2(\Omega).$$

Then $y = \mathcal{G}(Bu) \in \{v \in L^\infty(H^2), v_t \in L^2(H^1)\}$ and we have with $y_h = \mathcal{G}_h(Bu)$ and time stepping $\delta t \sim h^2$

$$\|y - y_h\|_\infty \leq C \begin{cases} h\sqrt{|\log h|}, & (d = 2) \\ \sqrt{h}, & (d = 3) \end{cases}$$

This is not an *off-the-shelf* result! It yields

$$\alpha \|u - u_h\|^2 + \|y - y_h\|^2 \leq C \begin{cases} h\sqrt{|\log h|}, & (d = 2) \\ \sqrt{h}, & (d = 3). \end{cases}$$

Error estimates, elliptic case

Deckelnick, H. (SINUM 2007, ENUMATH 2007)

- $Bu \in L^2(\Omega)$:

$$\|u - u_h\|_U, \|y - y_h\|_{H^1} = \begin{cases} O(h^{\frac{1}{2}}), & \text{if } d = 2, \\ O(h^{\frac{1}{4}}), & \text{if } d = 3, \end{cases}$$

- $Bu \in W^{1,s}(\Omega)$:

$$\|u - u_h\|_U, \|y - y_h\|_{H^1} \leq Ch^{\frac{3}{2} - \frac{d}{2s}} \sqrt{|\log h|}.$$

- $Bu \in L^\infty(\Omega)$:

$$\|u - u_h\|_U, \|y - y_h\|_{H^1} \leq Ch |\log h|.$$

- $U = L^2(\Omega)$, $U_{ad} = \{u \leq d\}$, u_h p.c.:

$$\|u - u_h\|_U, \|y - y_h\|_{H^1} \leq C \begin{cases} h |\log h|, & \text{if } d = 2, \\ \sqrt{h}, & \text{if } d = 3. \end{cases}$$

Similar results obtained by C. Meyer for discrete controls.

Numerical experiment 1

$$\Omega := B_1(0), \alpha > 0,$$

$$z(x) := 4 + \frac{1}{\pi} - \frac{1}{4\pi}|x|^2 + \frac{1}{2\pi} \log |x|, \quad b(x) := |x|^2 + 4,$$

$$\text{and } u_0(x) := 4 + \frac{1}{4\alpha\pi}|x|^2 - \frac{1}{2\alpha\pi} \log |x|.$$

$$J(u) := \frac{1}{2} \int_{\Omega} |y - z|^2 + \frac{\alpha}{2} \int_{\Omega} |u - u_0|^2,$$

where $y = \mathcal{G}(u)$.

Unique solution $u \equiv 4$ with corresponding state $y \equiv 4$ and multipliers

$$p(x) = \frac{1}{4\pi}|x|^2 - \frac{1}{2\pi} \log |x| \quad \text{and} \quad \mu = \delta_0.$$

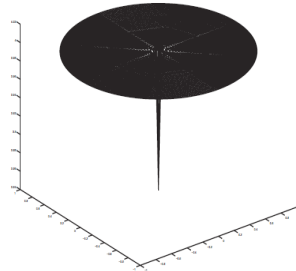
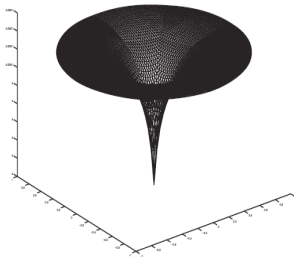
Experimental order of convergence

Recall

$$\text{EOC} = \frac{\ln E(h_1) - \ln E(h_2)}{\ln h_1 - \ln h_2}.$$

<i>RL</i>	$\ u - u_h\ $	$\ y - y_h\ $
1	0.788985	0.536461
2	0.759556	1.147861
3	0.919917	1.389378
4	0.966078	1.518381
5	0.986686	1.598421

State and control for Dirac example



Relaxing constraints – Lavrentiev (H., Meyer COAP 2008)

Lavrentiev Regularization: relax $y \leq b$ to $\lambda u + y \leq b$ ($\lambda > 0$). Numerical analysis yields

- $Bu^\lambda \in L^2(\Omega)$ uniformly:

$$\|u - u_h^\lambda\| \sim \|u - u^\lambda\| + \|u^\lambda - u_h^\lambda\| \sim \sqrt{\lambda} + h^{1-d/4},$$

- $Bu^\lambda \in W^{1,s}(\Omega)$ uniformly for all $s \in (1, \frac{d}{d-1})$:

$$\|u - u_h^\lambda\| \sim \|u - u^\lambda\| + \|u^\lambda - u_h^\lambda\| \sim \sqrt{\lambda} + h^{2-d/2-\epsilon},$$

- $Bu^\lambda \in L^\infty(\Omega)$, $Bu_h^\lambda \in L^\infty(\Omega)$ uniformly:

$$\|u - u_h^\lambda\| \sim \|u - u^\lambda\| + \|u^\lambda - u_h^\lambda\| \sim \sqrt{\lambda} + h |\log h|.$$

Relaxing constraints – penalization (Hintermüller, H.)

Relax $y \leq b$ with $\frac{\gamma}{2} \int_{\Omega} |(y - b)^+|^2 dx$ in cost functional.

- $Bu^\gamma \in L^2(\Omega)$ uniformly:

$$\begin{aligned}
 \|u - u_h^\gamma\| &\sim \|u - u^\gamma\| + \|u^\gamma - u_h^\gamma\| \sim \\
 &\sim \left(h^{1-d/p} + \frac{1}{\sqrt{\gamma}} h^{-d/2} \right)^{1/2} + h^{1-d/4},
 \end{aligned}$$

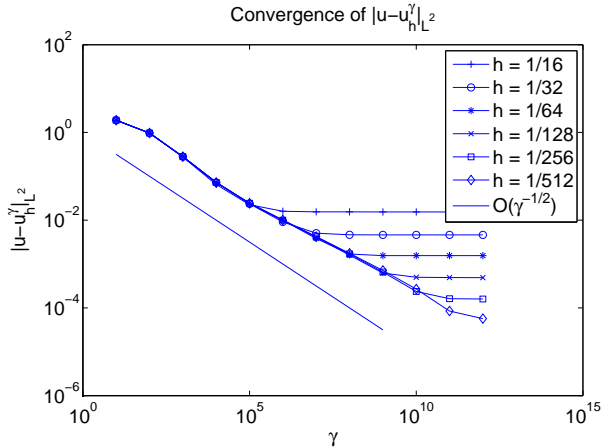
- $Bu^\gamma \in W^{1,s}(\Omega)$ for all $s \in (1, \frac{d}{d-1})$ uniformly:

$$\begin{aligned}
 \|u - u_h^\gamma\| &\sim \|u - u^\gamma\| + \|u^\gamma - u_h^\gamma\| \sim \\
 &\sim \left(h^{1-d/p} + \frac{1}{\sqrt{\gamma}} h^{-d/2} \right)^{1/2} + h^{2-d/2-\epsilon},
 \end{aligned}$$

- $Bu^\gamma \in L^\infty(\Omega), Bu_h^\gamma \in L^\infty(\Omega)$ uniformly:

$$\begin{aligned}
 \|u - u_h^\gamma\| &\sim \|u - u^\gamma\| + \|u^\gamma - u_h^\gamma\| \sim \\
 &\sim \left(h^{1-d/p} + \frac{1}{\sqrt{\gamma}} h^{-d/2} \right)^{1/2} + h |\log h|.
 \end{aligned}$$

Relaxing constraints – penalization, numerical results



Relaxing constraints – barriers (H., Schiela 2008)

Barriers: relax $y \leq b$ by adding $-\mu \int_{\Omega} \log(b - y) dx$ to cost functional ($\mu > 0$).
Numerical analysis yields

- $Bu^{\mu} \in L^2(\Omega)$ uniformly:

$$\|u - u_h^{\mu}\| \sim \|u - u^{\mu}\| + \|u^{\mu} - u_h^{\mu}\| \sim \sqrt{\mu} + h^{1-d/4},$$

- $Bu^{\mu} \in W^{1,s}(\Omega)$ for all $s \in (1, \frac{d}{d-1})$ uniformly:

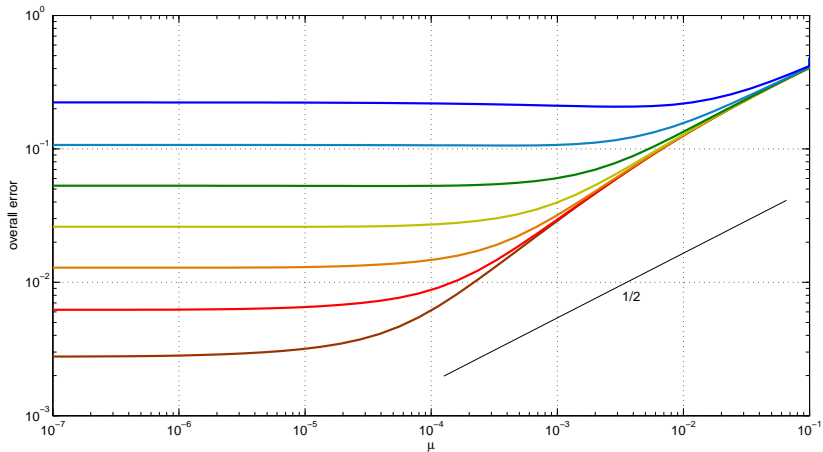
$$\|u - u_h^{\mu}\| \sim \|u - u^{\mu}\| + \|u^{\mu} - u_h^{\mu}\| \sim \sqrt{\mu} + h^{2-d/2-\epsilon},$$

- $Bu^{\mu} \in L^{\infty}(\Omega), Bu_h^{\mu} \in L^{\infty}(\Omega)$ uniformly:

$$\|u - u_h^{\mu}\| \sim \|u - u^{\mu}\| + \|u^{\mu} - u_h^{\mu}\| \sim \sqrt{\mu} + h|\log h|.$$

This is work in progress with Anton Schiela.

Relaxing constraints – barriers, numerical results



Consequence: Grid size h and parameters (λ, γ, μ) should be coupled;

Lavrentiev: $\sqrt{\lambda} \sim h^{2-d/2},$

Barriers: $\sqrt{\mu} \sim h^{2-d/2},$

Penalization ($p = \infty$): $\frac{1}{\sqrt{\gamma}} \sim h^{1+d/2}.$

Constraints on the gradient

Consider

$$\min_{u \in U_{\text{ad}}} J(u) = \frac{1}{2} \int_{\Omega} |y - z|^2 + \frac{\alpha}{r} \int_{\Omega} |u|^r \left(+ \frac{\alpha}{2} \int_{\Omega} |u|^2 \right)$$

where $y = \mathcal{G}(u)$, i.e. solves the pde, and $\nabla y \in Y_{\text{ad}}$.

Here

$$Y_{\text{ad}} = \{z \in C^0(\bar{\Omega})^d \mid |z(x)| \leq \delta, x \in \bar{\Omega}\},$$

and

$$\begin{aligned} r = 2 : & \quad U_{\text{ad}} = \{u \in L^2(\Omega) \mid a \leq u \leq b \text{ a.e. in } \Omega\} (a, b \in L^\infty), \\ r > d : & \quad U_{\text{ad}} = L^r(\Omega). \end{aligned}$$

Then $U_{\text{ad}} \subset L^r(\Omega)$ for $r > d \Rightarrow \nabla y \in C^0(\bar{\Omega})^d$.

Slater condition:

$$\exists \hat{u} \in U_{\text{ad}} \mid |\nabla \hat{y}(x)| < \delta, x \in \bar{\Omega}, \text{ where } \hat{y} \text{ solves the pde with } u = \hat{u}.$$

Optimality conditions (Casas & Fernandez)

An element $u \in U_{\text{ad}}$ is a solution if and only if there exist $\vec{\mu} \in \mathcal{M}(\bar{\Omega})^d$ and $p \in L^t(\Omega)$ ($t < \frac{d}{d-1}$) such that

$$\begin{aligned} \int_{\Omega} p \mathcal{A}z - \int_{\Omega} (y - z)z &= \int_{\bar{\Omega}} \nabla z \cdot d\vec{\mu} & \forall z \in W^{2,t'}(\Omega) \cap W_0^{1,t'}(\Omega) \\ \int_{\bar{\Omega}} (z - \nabla y) \cdot d\vec{\mu} &\leq 0 & \forall z \in Y_{\text{ad}}, \end{aligned}$$

$$\begin{aligned} \int_{\Omega} (p + \alpha u)(\tilde{u} - u) &\geq 0 & \forall \tilde{u} \in U_{\text{ad}} \text{ for } r = 2, \text{ or} \\ p + \alpha((u+)|u|^{r-2}u) &= 0 & \text{in } \Omega \text{ for } r > d. \end{aligned}$$

Structure of multiplier: $\vec{\mu} = \frac{1}{\delta} \nabla y \mu$, where $\mu \in \mathcal{M}(\bar{\Omega}) \geq 0$ is concentrated on $\{x \in \bar{\Omega} \mid |\nabla y(x)| = \delta\}$.

FE discretization, conventional

Piecewise linear, continuous Ansatz for the state $y_h = \mathcal{G}_h(u) \in X_h$.

The discrete control problem reads

$$\begin{aligned} \min_{u \in U_{\text{ad}}} J_h(u) &:= \frac{1}{2} \int_{\Omega} |y_h - z|^2 + \frac{\alpha}{r} \int_{\Omega} |u|^r \left(+ \frac{\alpha}{2} \int_{\Omega} |u|^2 \right) \\ \text{subject to } y_h &= \mathcal{G}_h(u) \text{ and } \left(\frac{1}{|T|} \int_T \nabla y_h \right)_{T \in \mathcal{T}_h} \in Y_{\text{ad}}^h, \end{aligned}$$

where

$$Y_{\text{ad}}^h := \{c_h : \bar{\Omega} \rightarrow \mathbb{R}^d \mid c_h|_T \text{ is constant and } |c_h|_T| \leq \delta, T \in \mathcal{T}_h\}.$$

FE discretization, conventional, optimality conditions

The variational discrete problem has a unique solution $u_h \in U_{\text{ad}}$. There exist $\mu_T \in \mathbb{R}^d$, $T \in \mathcal{T}_{h,X}$ and $p_h \in X_h$ such that with $y_h = \mathcal{G}_h(u_h)$ we have

$$a(v_h, p_h) = \int_{\Omega} (y_h - z) v_h + \sum_{T \in \mathcal{T}_{h,X}} |T| \nabla v_h|_T \cdot \mu_T \quad \forall v_h \in X_h,$$

$$\sum_{T \in \mathcal{T}_{h,X}} |T| (c_{hT} - \nabla y_h|_T) \cdot \mu_T \leq 0 \quad \forall c_h \in C_h,$$

$$p_h + \alpha((u_h +)|u_h|^{r-2}u_h) = 0 \quad \text{in } \Omega.$$

Structure of the multiplier: $\vec{\mu}_T = \mu_T \frac{1}{\delta} \nabla y_{hT}$, where $\mu_T \in \mathbb{R}$. Furthermore, $\mu_T \geq 0$ and $\mu_T > 0$ only if $|\nabla y_{hT}| = \delta$.

Results

Deckelnick, Günther, H. (Oberwolfach Report 2008): Let $u_h \in U_{\text{ad}}$ be the variational discrete optimal solution with corresponding state $y_h \in X_h$ and adjoint variables $p_h \in X_h$, $\vec{\mu}_T (T \in \mathcal{T}_h)$.

Then for h small enough

- $\|y_h\|, \|u_h\|_{L^r}, \|p_h\|_{L^{\frac{r}{r-1}}}, \sum_{T \in \mathcal{T}_{h,X}} |T| |\mu_T| \leq C,$

- $\|y - y_h\| \leq Ch^{\frac{1}{2}(1-\frac{d}{r})}, \|u - u_h\|_{L^r} \leq Ch^{\frac{1}{r}(1-\frac{d}{r})}, \text{ and}$
 $\|u - u_h\|_{L^2} \leq Ch^{\frac{1}{2}(1-\frac{d}{r})}.$

These results are also valid for a piecewise constant Ansatz of the control.

FE discretization, Raviart Thomas

Mixed fe approximation of the state with lowest order Raviart–Thomas element, i.e.

$$(y_h, \mathbf{v}_h) = \mathcal{G}_h(u) \in Y_h \times V_h$$

denotes the solution of

$$\begin{aligned}
 \int_{\Omega} \mathbf{A}^{-1} \mathbf{v}_h \cdot \mathbf{w}_h + \int_{\Omega} y_h \operatorname{div} \mathbf{w}_h &= 0 \quad \forall \mathbf{w}_h \in V_h \\
 \int_{\Omega} z_h \operatorname{div} \mathbf{v}_h - \int_{\Omega} a_0 y_h z_h + \int_{\Omega} u z_h &= 0 \quad \forall z_h \in Y_h.
 \end{aligned}$$

FE discretization, cont.

The discrete control problem reads

$$\begin{aligned} \min_{u \in U_{\text{ad}}} J_h(u) &:= \frac{1}{2} \int_{\Omega} |y_h - z|^2 + \frac{\alpha}{2} \int_{\Omega} |u|^2 \\ \text{subject to } (y_h, v_h) &= \mathcal{G}_h(u) \text{ and } \left(\frac{1}{|T|} \int_T A^{-1} v_h \right)_{T \in \mathcal{T}_h} \in Y_{\text{ad}}^h, \end{aligned}$$

where

$$Y_{\text{ad}}^h := \{c_h : \bar{\Omega} \rightarrow \mathbb{R}^d \mid c_h|_T \text{ is constant and } |c_h|_T| \leq \delta, T \in \mathcal{T}_h\}.$$

FE discretization, optimality conditions

The discrete problem has a unique solution $u_h \in U_{\text{ad}}$. Furthermore, there are $\vec{\mu}_T \in \mathbb{R}^d$ and $(p_h, \chi_h) \in Y_h \times V_h$ such that with $(y_h, v_h) = \mathcal{G}_h(u_h)$ we have

$$\int_{\Omega} A^{-1} \chi_h \cdot w_h + \int_{\Omega} p_h \operatorname{div} w_h + \sum_{T \in \mathcal{T}_h} \vec{\mu}_T \cdot \oint_T A^{-1} w_h = 0 \quad \forall w_h \in V_h$$

$$\int_{\Omega} z_h \operatorname{div} \chi_h - \int_{\Omega} a_0 p_h z_h + \int_{\Omega} (y_h - z) z_h = 0 \quad \forall z_h \in Y_h.$$

$$\int_{\Omega} (p_h + \alpha u_h)(\tilde{u} - u_h) \geq 0 \quad \forall \tilde{u} \in U_{\text{ad}}$$

$$\sum_{T \in \mathcal{T}_h} \vec{\mu}_T \cdot (c_h|_T - \oint_T A^{-1} v_h) \leq 0 \quad \forall c_h \in Y_{\text{ad}}^h.$$

Structure of the multiplier: $\vec{\mu}_T = \mu_T \frac{1}{\delta} \oint_T A^{-1} v_h$, where $\mu_T \in \mathbb{R}$. Furthermore, $\mu_T \geq 0$ and $\mu_T > 0$ only if $|\oint_T A^{-1} v_h| = \delta$.

Results

Deckelnick, Günther, H. (Numer. Math 2008): Let $u_h \in U_{\text{ad}}$ be the optimal solution of the discrete problem with corresponding state $(y_h, v_h) \in Y_h \times V_h$ and adjoint variables $(p_h, \chi_h) \in Y_h \times V_h$, $\vec{\mu}_T, T \in \mathcal{T}_h$.

Then for h small enough

- $\|y_h\|, \sum_{T \in \mathcal{T}_h} |\vec{\mu}_T| \leq C$, and
- $\|u - u_h\| + \|y - y_h\| \leq Ch^{\frac{1}{2}} |\log h|^{\frac{1}{2}}.$

Constraints on the gradient, example

We take $\Omega = B_2(0)$ and consider

$$\min J(u) = \frac{1}{2} \|y - z\|_{L^2(\Omega)}^2 + \frac{1}{2} \|u\|_{L^2(\Omega)}^2$$

with pointwise bounds on the constraints, i.e. $\{a \leq u \leq b\}$, where $a, b \in L^\infty(\Omega)$, and pointwise bounds on the gradient, i.e. $|\nabla y(x)| \leq \delta := 1/2$. State and control satisfy

$$-\Delta y = f + u \text{ in } \Omega, \quad y = 0 \text{ on } \partial\Omega.$$

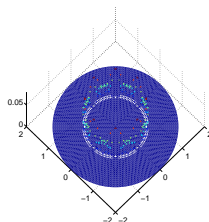
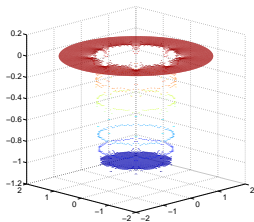
Data:

$$z(x) := \begin{cases} \frac{1}{4} + \frac{1}{2} \ln 2 - \frac{1}{4} |x|^2 & , 0 \leq |x| \leq 1 \\ \frac{1}{2} \ln 2 - \frac{1}{2} \ln |x| & , 1 < |x| \leq 2 \end{cases} \quad f(x) := \begin{cases} 2 & , 0 \leq |x| \leq 1 \\ 0 & , 1 < |x| \leq 2 \end{cases}$$

Solution:

$$y(x) \equiv z(x) \text{ and } u(x) = \begin{cases} -1 & , 0 \leq |x| \leq 1 \\ 0 & , 1 < |x| \leq 2 \end{cases}$$

Numerical experiment, piecewise constant control Ansatz

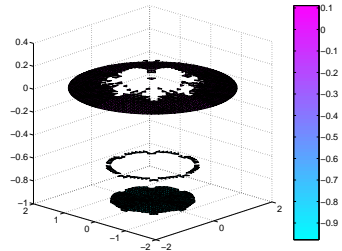
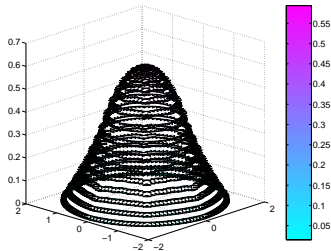


Experimental order of convergence

<i>RL</i>	$\ u - u_h\ _{L^4}$	$\ u - u_h\ $	$\ y - y_h\ $
1	0.76678	0.72339	1.90217
2	0.33044	0.64248	1.25741
3	0.27542	0.54054	1.23233
4	0.28570	0.53442	1.16576

Results show the predicted behaviour, since $r = \infty$.

Numerical solution, mixed finite elements



Experimental order of convergence

<i>RL</i>	$\ u - u_h\ $	$\ y - y_h\ $	$\ y^P - y_h^P\ $
1	0.98576	1.06726	1.08949
2	0.51814	1.02547	1.09918
3	0.50034	1.01442	1.08141

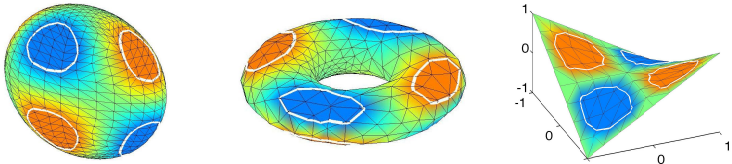
Superscript P denotes post-processed piecewise linear state. It attains the same order of convergence but yields significantly smaller approximation error.

Details can be found in

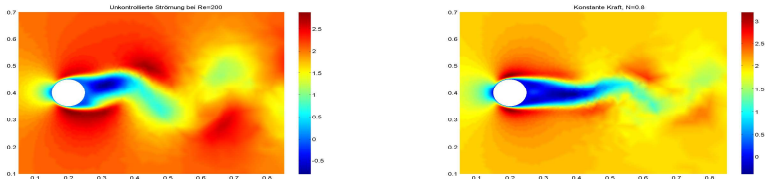


Further aspects and applications

• Optimal control of PDEs on surfaces



• Applications to flow control



PDE constrained optimization on surfaces

Formulation of optimal control problems on surfaces is along the lines of the planar case. Concerning discretization, the approximation of the surface has to be considered;

- **Elliptic case**

- Use Dziuk's finite element concept for the Laplace Beltrami operator of 1988 for the discretization of the state equation;
- Use variational discretization (H. COAP 2005) for the discretization of the control problem;
- Use a semismooth Newton method of Hintermüller, Ito and Kunisch; Michael Ulbrich (SIOPT 2003) to solve the resulting nonlinear systems.

- **Parabolic case**

- Use ESFEM from Dziuk and Elliott (Acta Numerica 2013) for the discretization of the parabolic PDE on the evolving surface;
- Use variational discretization (H. COAP 2005) for the discretization of the control problem.
- Use a semismooth Newton method of Hintermüller et al. (SIOPT 2003) to solve the resulting nonlinear systems.

→ more details on demand.

Application: control of Navier Stokes systems

The classical instationary NS system: steer y to \bar{y} , where

$$\begin{aligned}
 y_t - \nu \Delta y + (y \cdot \nabla) y + \nabla p &= \mathcal{B}u & \text{in } \Omega^T, \\
 -\operatorname{div} y &= 0 & \text{in } \Omega^T, \\
 +IC + BC.
 \end{aligned}$$

The Boussinesq approximation: steer y to \bar{y} and/or τ to $\bar{\tau}$

$$\begin{aligned}
 y_t + (y \cdot \nabla) y - \nu \Delta y + \nabla p + \beta \tau \vec{g} &= \mathcal{B}_y u & \text{in } \Omega^T, \\
 -\operatorname{div} y &= 0 & \text{in } \Omega^T, \\
 \tau_t + (y \cdot \nabla) \tau - \chi \Delta \tau - f &= \mathcal{B}_\tau u & \text{in } \Omega^T, \\
 +IC + BC.
 \end{aligned}$$

The Cahn-Hilliard Navier-Stokes system: steer c to \bar{c}

$$\begin{aligned}
 y_t - \frac{1}{Re} \Delta y + y \cdot \nabla y + \nabla p + Kc \nabla w &= \mathcal{B}u & \text{in } \Omega^T, \\
 -\operatorname{div} y &= 0 & \text{in } \Omega^T, \\
 c_t - \frac{1}{Pe} \Delta w + \nabla c \cdot y &= 0 & \text{in } \Omega^T, \\
 -\gamma^2 \Delta c + \Phi'(c) - w &= 0 & \text{in } \Omega^T, \\
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Decay, distributed control of classical NSE, H. SICON 2005

$A := -\nu \Delta$, $b(y) := P[(y \nabla) y]$, solenoidal setting. Let ρ denote stepsize in steepest descent, h time stepping.

$\rho < 2$ positive, h small(ρ), b and \bar{y} smooth and bounded in appropriate norms.

Theorem 1: The iterates $\{y^j\}$ of instantaneous control strategy satisfy

$$|y^j - \bar{y}(t_j)| \leq c \kappa^j$$

with some positive $\kappa < 1$.

Theorem 2: For the unique solution y of the continuous control law

$$\begin{aligned} \dot{y} + Ay &= b(y) - \\ &\quad - \frac{\rho}{h} B^* B(y - \bar{y}) - \rho B^* B(b(y) - b(\bar{y})) + \dot{\bar{y}} + A\bar{y} - b(\bar{y}) \\ y(0) &= y_0, \end{aligned}$$

$|y - \bar{y}|$ decays exponentially to zero with order $-\frac{\rho}{h}$, i.e.

$$|y(t) - \bar{y}(t)| \leq C \exp(-\frac{\rho}{h} t) |y(0) - \bar{y}(0)|$$

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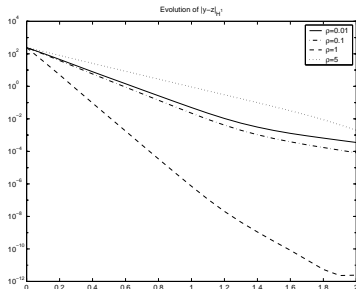
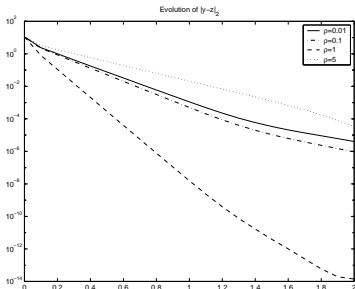
Theorem 2: For the unique solution y of the continuous control law

$$\begin{aligned} \dot{y} + Ay &= b(y) - \\ &- \frac{\rho}{h} B^* B(y - \bar{y}) - \rho B^* B(b(y) - b(\bar{y})) + \dot{\bar{y}} + A\bar{y} - b(\bar{y}) \\ y(0) &= y_0, \end{aligned}$$

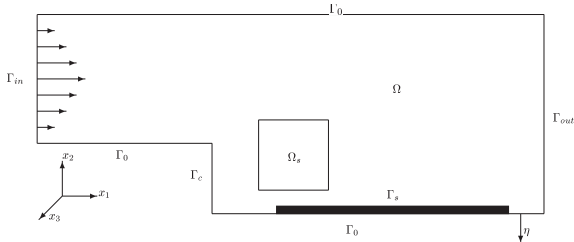
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Exponential decay, laminar cavity flow, Stokes tracking



BFS flow, domain



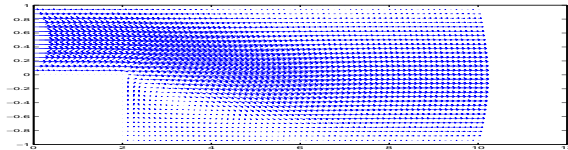
Cost functionals:

$$J(y, u) = \frac{1}{2} \int_0^T \left[\int_{\Omega_s} |y - y_{st}|^2 dx + \gamma \int_{\Gamma_c} u^2 d\Gamma_c \right] dt,$$

$$J(y, u) = \int_0^T \left[\int_{\Gamma_s} \frac{1}{2} \frac{\partial y_1}{\partial x_2} \left(\frac{\partial y_1}{\partial x_2} - \left| \frac{\partial y_1}{\partial x_2} \right| \right) d\Gamma_s + \frac{\gamma}{2} \int_{\Gamma_c} g^2 d\Gamma_c \right] dt.$$

BFS feedback control, movies

Boundary control with backflow observation in volume after the step.

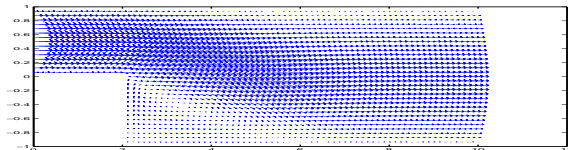


Inst. control

1-step MPC

3-step MPC

Boundary control with backflow observation at the bottom boundary.



Inst. control [2,9]

Inst. control [4,9]

Inst. control [6,9]

MPC for Boussinesq approximation in the cavity

$$A := \begin{bmatrix} -P\Delta & -Gr\vec{g} \\ 0 & -\Delta \end{bmatrix}, \quad b(x, t) = b(y, \tau) := \begin{bmatrix} P[(v\nabla)v] \\ (v\nabla)\tau \end{bmatrix}$$

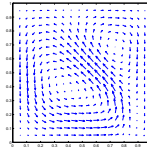
$$\begin{aligned}
 \min J(y, \tau, u, u_F, u_Q) &= \sum_{j=i+1}^{i+M} \left(\frac{c_0}{2} \int_{\Omega} (y^j - z^j)^2 dx + \frac{c_1}{2} \int_{\Omega} (\tau^j - S^j)^2 dx \right. \\
 &\quad \left. + \frac{c_2}{2} \int_{\Gamma} u^j{}^2 dx + \frac{c_3}{2} \int_{\Omega} u_F^j{}^2 dx + \frac{c_4}{2} \int_{\Omega} u_Q^j{}^2 dx \right) \quad \text{s.t. transition constraints}
 \end{aligned}$$

$$\begin{aligned}
 \frac{1}{dt}\tau^{j+1} - a\Delta\tau^{j+1} &= c_Q u_Q^{j+1} + \frac{1}{dt}\tau^j - (y^j\nabla)\tau^j \\
 a\partial_{\eta}\tau^{j+1} &= \alpha(u^{j+1} - \tau^{j+1}|_{\Gamma}) \\
 \frac{1}{dt}y^{j+1} - \nu\Delta y^{j+1} + \nabla p^{j+1} &= c_F u_F^{j+1} + \frac{1}{dt}y^j - (y^j\nabla)y^j - \frac{1}{dt}\tau^{j+1}\vec{g} \\
 -\operatorname{div} y^{j+1} &= 0 \\
 y^{j+1}|_{\Gamma} &= 0
 \end{aligned}$$

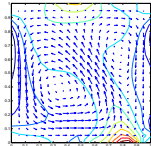
for $j = i, \dots, i + M - 1$.

MPC Results

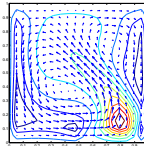
Control target



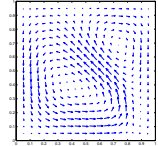
Boundary heating



Distributed heating

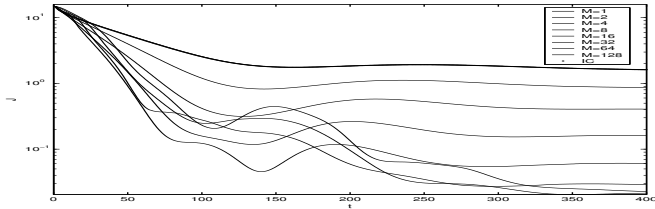


distributed force

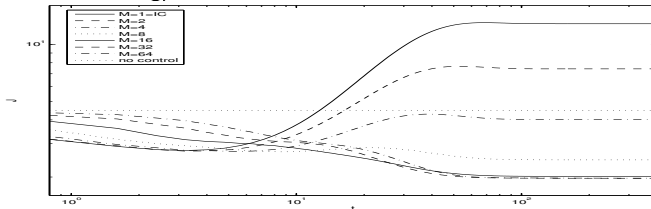


As expected: distributed force is more effective than distributed heating, which is more effective than boundary heating.

MPC results - control horizon

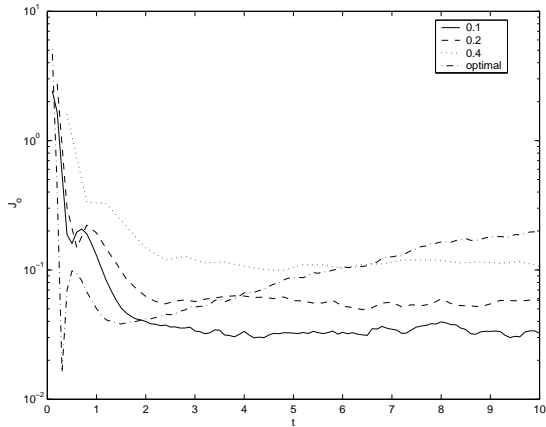


Cost decreases with increasing the length of the control horizon M (distributed heating)



MPC with boundary heating only works for sufficiently large control horizons.

Tracking perturbed optimal trajectories



Instantaneous control with distributed heating tracks perturbed trajectory, the optimal open loop strategy fails.

Instantaneous control of CHNS

At each time instance t_k solve approximately the minimization problem

$$\min_{u \in U} J^k(c, u) = \frac{1}{2} \int_{\Omega} (c - c_d^k)^2 dx + \frac{\alpha}{2} \int_{\Omega} |u|^2 dx \quad (P^k)$$

s.t.

$$y - \frac{\tau}{Re} \Delta y = u + f \quad (0.20)$$

$$c - \frac{\tau}{Pe} \Delta w = c_{old} - \tau \nabla c_{old} y \quad (0.21)$$

$$-\gamma^2 \Delta c + \lambda_s(c) - w = c_{old} \quad (0.22)$$

Here

$$\begin{aligned}
 f(c_{old}, w_{old}, y_{old}) &= y_{old} - \tau c_{old} \nabla w_{old} - \tau (y_{old} \nabla) y_{old} \\
 \lambda_s(c) &= s(\max(0, c - 1) + \min(0, c + 1))
 \end{aligned}$$

Note: scheme (0.20)-(0.22) is not recommended to integrate the CHNS. It only serves the purpose of controller construction.

The gradient of J^k

Here we have

$$\nabla J^k(u_0^k) = \alpha u_0^k + p_3,$$

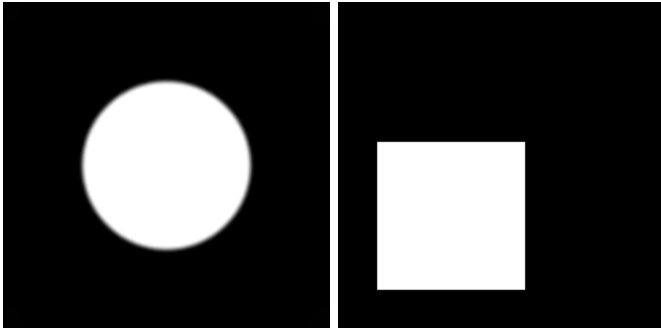
where p_3 stems from the solution to the adjoint system

$$-\gamma^2 \Delta p_2 + \lambda'_s(c) p_2 - \tau \nabla p_1 \cdot y + p_1 = c - c_d \quad (0.23)$$

$$p_2 = -\frac{\tau}{p_e} \Delta p_1 \quad (0.24)$$

$$p_3 - \frac{\tau}{Re} \Delta p_3 = \tau c \nabla p_1. \quad (0.25)$$

Example: Circle2Square



Initial state (circle) and desired state (square)

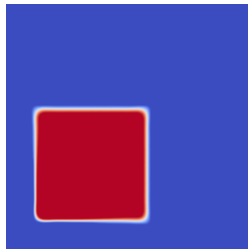
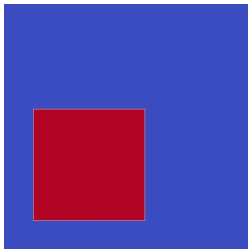
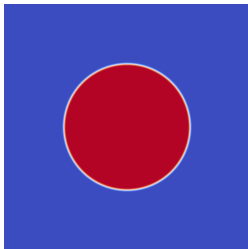
Morphing: Circle2Square

Circle2Square

Circle2Square: snapshot of controlled states



Circle to Square



MPC: Circle to Square

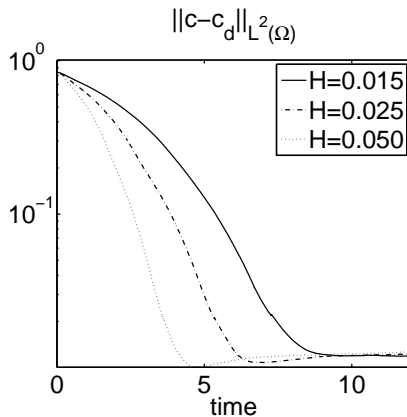


Figure: Deviation of stabilized square from desired square for several prediction horizons.

Dirichlet boundary control of rising bubble: bottom and side walls

Dirichlet boundary control of rising bubble: 20 controls at side walls

RisingBubbleControl

Instantaneous control: decay

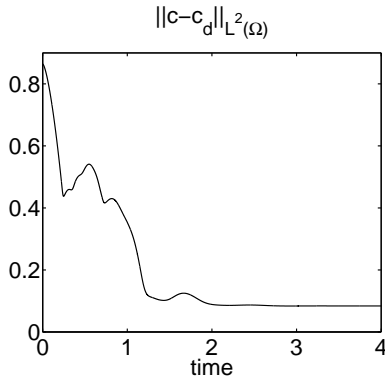


Figure: Deviation of controlled bubble from desired bubble.

Dirichlet boundary control of rising bubble: 5 controls at side walls

RisingBubbleControl

Instantaneous control: decay

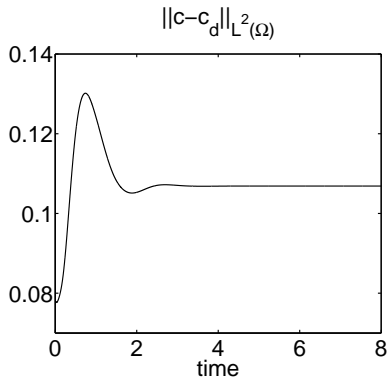
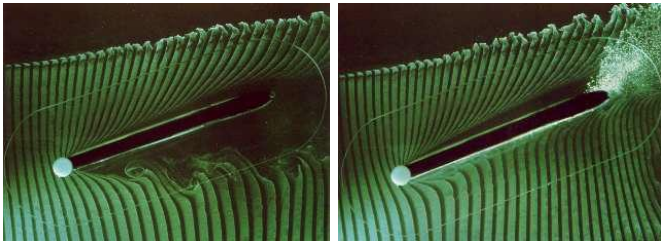


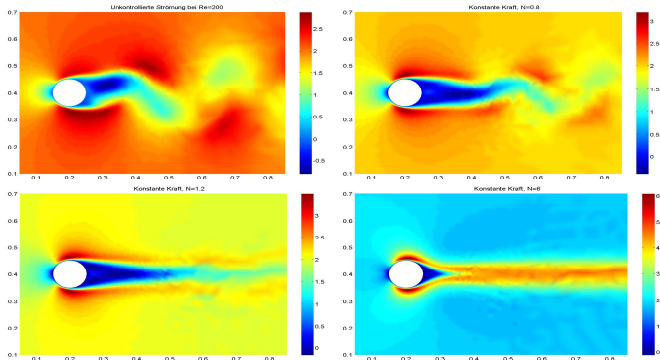
Figure: Deviation of controlled bubble from desired bubble.

Control of weakly conducting fluids (Sfb 609)

Thanks to Tom Weier, FZR Rossendorf



Develop methods for circular cylinder



Control target: Re-attach flow utilizing near wall Lorentz forces movie **Desired:**
 Open- or closed-loop control strategy

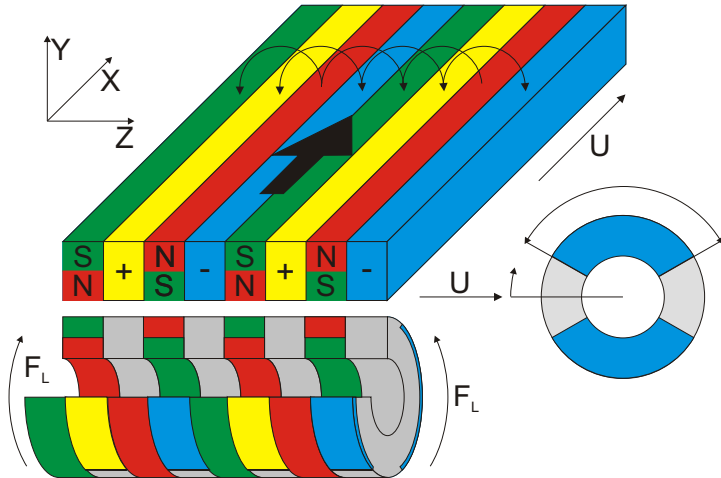
Generation of the Lorentz Force

On the surface of the cylinder a Lorentz force is generated with actuators. It decays exponentially in the flow (T. Berger et al., Phys. Fluids 2000). The Lorentz force has the form

$$F_L(x, y) := e_\phi g(\phi) e^{-\frac{\pi}{a} \cdot \text{dist}[(x, y), \text{cylinder}]},$$
$$g(\phi) = \begin{cases} 1, & \phi_0 \leq \phi \leq \phi_1 \\ -1, & 180^\circ + \phi_0 \leq \phi \leq 180^\circ + \phi_1 \\ 0, & \text{else} \end{cases}.$$

a electrode-/magnet-spacing. The direction of the Lorentz Force is defined by the arrangement of the magnets/electrodes.

Schematic



Mathematical Model: NSEs

$$u_t + (u \cdot \nabla)u + \nabla p - \frac{1}{\text{Re}} \nabla^2 u = NF_L$$
$$\nabla \cdot u = 0$$

plus initial and boundary conditions.

The Interaction parameter N describes the ratio of the electromagnetic and the inertial forces of the flow,

$$N = \frac{J_0 B_0 D}{\rho U_\infty^2} \quad ,$$

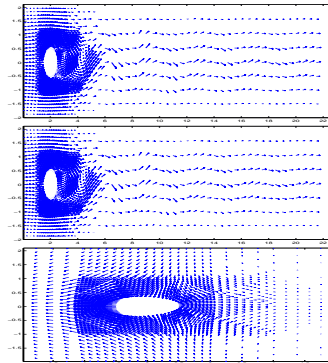
with J_0 the current density and B_0 magnetic induction.

The numerics are validated against the computations of R. Grundmann/O. Posdziech (TUD). Comparison with experiments by G. Gerbeth/T. Weier et al. (FZR) to be addressed.

Control with near wall Lorentz force

Control: $u(t, x) = \sum_{i=1}^n u_i(t) f_i(x)$, $f_i(x) = e^{-|x-x_i|^2}$.

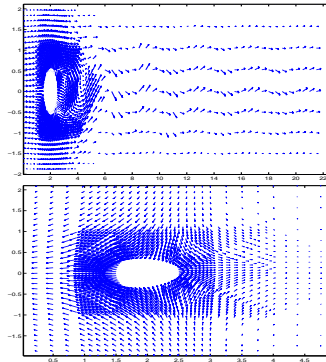
Desired flow \bar{x} : Stokes flow.



Control with near wall Lorentz force

Control: $u(t, x) = \sum_{i=1}^2 u_i(t) e_{\phi} f_i(x)$, $f_i(x) = g(\phi) e^{-\frac{\pi}{a} \cdot \text{dist}[(x,y), \text{cylinder}]}$

Desired flow \bar{x} with $x_1 = 1$.



CPU time needed to compute the instantaneous control strategy = **2,5 times**
CPU time needed for one forward solve.

This amounts to **1-2 %** of the CPU time needed to compute the optimal control trajectory.

Related research (only PDE control)

- Ito & Kunisch 2002-2006: MPC framework for abstract infinite dimensional dynamical systems (ESAIM: Control Optim. Calc. Var., 8:741–760, 2002, SIAM J. Cont. Optim., 45(1):207–225, 2006).
- Altmüller, Grüne & Worthmann 2012-2013: MPC for semilinear parabolic PDEs (GAMM Mitteilungen 35(2):131–145, 2012).
- Benner & Hein 2006-2009: Model predictive control for nonlinear parabolic differential equations based on a linear quadratic Gaussian design (PAMM 2009, PhD thesis Hein 2009).
- Bänsch & Benner 2007-2013: Riccati-based feedback control of flows (SPP 1253).
- Krstic & Smyshlyaev 2008-2010: Boundary control of parabolic PDEs using backstepping techniques (SIAM, Philadelphia, 2008; Princeton University Press, Princeton, NJ, 2010).
- Choi, Temam, Moin & Kim 1993: Feedback control for unsteady flow and its application to the stochastic Burgers equation (J. Fluid Mech. 253:509–543, 1993).
- Fursikov 2001-2004: Stabilizability of Navier-Stokes equations with boundary feedback control in 2 and 3d (J. Math. Fluid Mech., 3 (2001), pp. 259–301, Discrete Contin. Dyn. Syst., 10 (2004), pp. 289–314).
- Raymond, Raymond & Dharmatti 2006-2011: Feedback boundary stabilization of the Navier-Stokes equations (SIAM J. Cont. Optim., 45(3):790–828, 2006, SIAM J. Cont. Optim., 49(6):2318–2348, 2011).
- Hinze & Volkwein, Hinze 2002-2005: Analysis of instantaneous control (Nonlinear Anal. 50:1–26, 2002, SIAM J. Control Optim., 44(2):564–583, 2005).

That's all! Thank's for the attention!

