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**UNIVERSITÀ  
DEL SALENTO**

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## Scientific Program - Timetable

Sun day 22	Time	Monday 23	Tuesday 24	Wednesday 25	Thursday 26	Friday 27
	9:15 30 45		Contributed sessions (15 in parallel)	Plenary Lecture Moritz Diehl	Contributed sessions (15 in parallel)	Contributed sessions (14 in parallel)
	10:15 30 45	Registration		von Mises prize lecture		
	11:15 30 45		Coffee Break	Coffee Break	Coffee Break	Coffee Break
	12:15 30 45		Plenary Lecture Thomas Böhlke	General Assembly	Plenary Lecture Ferdinando Auricchio	Contributed sessions (11 in parallel)
	13:15 30 45		Lunch	Lunch	Lunch	
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		Univ. Chorus Performance				Closing
	14:15 30 45	Prandtl Lecture Keith Moffatt	Plenary Lecture Enrique Zuazua	Contributed sessions (15 in parallel)	Plenary Lecture Daniel Kressner	
	15:15 30 45	Plenary Lecture Giovanni Galdi	Plenary Lecture Nikolaus Adams		Plenary Lecture Stanislaw Stupkiewicz	
Registration pre-opening	16:15 30 45	Coffee Break	Coffee Break Poster session	Coffee Break	Coffee Break Poster session	
	17:15 30 45	Minisymposia & Young Reseachers' Minisymposia (10 in parallel)	Contributed sessions (14 in parallel)	Contributed sessions (15 in parallel)	Contributed sessions (15 in parallel)	
	18:15 30 45		Public lecture Francesco D'Andria			
	19:15 30 45	Opening reception at Castle of Charles V				
	20:15 30 45			Conference dinner at Hotel Tiziano		
	21:15 30 45					

# GAMM 2015

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## **S19: Optimization of differential equations**

In this session novel developments devoted to optimization and optimal control problems governed by ordinary or partial differential equations will be discussed. The focus is on theoretical investigations, numerical analysis, algorithmic issues as well as on application.

# Two Types of Globally Convergent Numerical Methods for Coefficient Inverse Problems

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The goal of this talk is to present two existing types of globally convergent numerical methods for Coefficient Inverse Problems (CIPs). CIPs are nonlinear. Conventional least squares Tikhonov functionals for CIPs suffer from the phenomenon of multiple local minima and ravines. This means that any optimization method should have its starting point in a sufficiently small neighborhood of the exact solution. Therefore, conventional Tikhonov functional for a CIP inevitably leads to a locally convergent numerical method. However, such a neighborhood is rarely known in applications. Although there are many publications devoted to numerical solutions of CIPs, almost all of them still have the same fundamental drawback: local convergence. Naturally, there are counter examples showing that locally convergent numerical methods for CIPs are inherently unstable, since their results heavily depend on the starting points of iterations, see, e.g. [3, 10, 13].

Thus, both the most challenging and the most important question in a numerical treatment of a CIP is “How to rigorously obtain at least one point in a small neighborhood of the exact solution without any advanced knowledge of this neighborhood?” We call a numerical method, which positively addresses this question, *globally convergent*.

There are currently two types of globally convergent numerical methods for CIPs with single measurement data. The first type is the Beilina-Klibanov method, which was initiated in their work [2]. Results of many publications up to 2012 were summarized in the book [3]. The global convergence theory was fully developed [3, 4]. Besides, the method is completely tested on both transmitted [3, 5, 10] and backscattering [6, 7, 8, 14, 15] experimental data.

The second type is based on constructions of globally strictly convex cost functionals for CIPs. The key element of such a functional, which makes it globally strictly convex, is the presence of a Carleman Weight Function (CWF), i.e. the function involved in the Carleman estimate for a corresponding Partial Differential Operator. The development of this type of method was started by Klibanov in 1997 [11, 12]. Now is a renewed interest in it [9, 13]. First numerical results can be found in the work of Klibanov and Th  nh [13]. Besides, another close idea, which was developed recently is the one of Baudoin, de Buhan and Ervedosa [1].

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# A Riemannian SQP method for PDE constrained shape optimization

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Shape optimization problems arise frequently in technological processes which are modeled in the form of partial differential equations. In many practical circumstances, the shape under investigation is parameterized by finitely many parameters, which on the one hand allows the application of standard optimization approaches, but on the other hand limits the space of reachable shapes unnecessarily. Shape calculus, which has been the subject of several monographs [1, 3, 7] presents a way out of that dilemma. However, so far it is mainly applied in the form of gradient descent methods, which can be shown to converge. The major difference between shape optimization and the standard PDE constrained optimization framework is the lack of the linear space structure in shape spaces. If one cannot use a linear space structure, then the next best structure is the Riemannian manifold structure as discussed for shape spaces for example in [2]. The publication [4] makes a link between shape calculus and shape manifolds and thus enables the usage of optimization techniques on manifolds in the context of shape optimization. This talk presents a vector bundle framework [5] based on the Riemannian framework established in [4], which enables the discussion of Lagrange–Newton methods within the shape calculus framework for PDE constrained shape optimization. This novel Riemannian vector bundle framework will be discussed for a specific academic example. Like in [6] the representation of the shape derivative expressed as a boundary integral which is needed for a numerical implementation is deduced from its representation as a domain integral.

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# A second order convergent trial method for free boundary problems in three dimensions

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This talk is concerned with the solution of a generalized Bernoulli free boundary problem by means of a trial method. At the free boundary, we prescribe the Neumann boundary condition and update the free boundary with the help of the remaining Dirichlet boundary condition. An inexact Newton update is used which results in a second order convergent iterative method. Numerical examples show the feasibility of the present approach.

# Primal-Dual Active Set Strategy for Singular Optimal Control Problems

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Our focus is on singular optimal control problems including partial differential equations which are not described by a control-to-state operator. In such case it is not justified to consider a reduced problem with a single optimization variable. Despite not having a control-to-state operator the proving of existence of optima, the derivation of first order optimality conditions as well as the numerical solving of these problems is possible. The existence of solutions for optimal control problems including singular systems with multiple states and the derivation of first order optimality conditions by a penalization method is shown in [2].

Using Lagrangian techniques in [1] the existence of Lagrangian multipliers satisfying an unqualified optimality system is shown. For some cases the validity of the qualified form is proven.

We prove that the regularity condition of Robinson resp. Kurcyusz-Zowe holds and obtain a qualified system of optimality conditions for a broad class of linear PDEs.

Some specifics of the coupled optimality system are presented. Applicability and efficiency of the primal-dual active set strategy for this class of problems is investigated. We apply results of [3] and propose assumptions which guarantee superlinear local convergence known from classical problems.

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# Adaptive Optimal Control of the Obstacle Problem

Christian Meyer<sup>1</sup>, Andreas Rademacher<sup>1</sup>, Winnifried Wollner<sup>2</sup>

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The talk is concerned with the adaptive optimal control of the obstacle problem, as described in [1]. To this end, a posteriori error estimates for optimization problems subject to an obstacle problem are derived. To circumvent the nondifferentiability inherent to this type of problem, a sequence of penalized but differentiable problems is introduced. Differentiability of the central path is shown and separate a posteriori dual weighted residual estimates for the errors due to penalization, discretization, and iterative solution of the discrete problems are provided. The effectivity of the derived estimates is demonstrated on two numerical examples.

## References

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# Optimal Control of a linear unsteady Fluid-Structure Interaction Problem

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Fluid-Structure Interaction (FSI) problems have been extensively studied from theoretical and numerical point of view in the last decade. More and more applications for shape- and parameter- estimation of FSI are regarded recently, for example in [3] and [4]. But especially about gradient based algorithms for optimal control of the unsteady FSI problem with a distributed control, little is known. If the control is distributed in space and time it is necessary to compute the gradient of the reduced cost functional accurately to obtain a fast and converging algorithm. Thereby the difficulty in Fluid-Structure Interaction occurs due to the coupling conditions. Only if the adjoint coupling conditions are fulfilled accurately in the numerical simulation, a correct transport of information across the interface can be guaranteed.

To analyze the coupling conditions in the adjoint equation we consider a minimization problem subjected to a linear Fluid-Structure interaction problem. The linear FSI problem was already analyzed in [1] and [2]. We proof the existence of a minimizer for the optimal control problem and we derive systematically necessary optimality conditions using a novel symmetric monolithic formulation. The presented formulation enables an easy numerical implementation as the resulting equations can be solved using methods already developed for FSI. We analyze the properties of the resulting optimality system and present results on higher regularity for the optimal control.

## References

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# Parabolic optimal control problems with pointwise controls

Boris Vexler, Dmitriy Leykekhman

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We consider a parabolic optimal control problem:

$$\min_{q,u} J(q,u) := \frac{1}{2} \int_0^T \|u(t) - \widehat{u}(t)\|_{L^2(\Omega)}^2 dt + \frac{\alpha}{2} \int_0^T |q(t)|^2 dt \quad (1)$$

subject to the second order parabolic equation

$$u_t(t,x) - \Delta u(t,x) = q(t)\delta_{x_0}, \quad (t,x) \in I \times \Omega, \quad (2a)$$

$$u(t,x) = 0, \quad (t,x) \in I \times \partial\Omega, \quad (2b)$$

$$u(0,x) = 0, \quad x \in \Omega \quad (2c)$$

and subject to pointwise control constraints

$$q_a \leq q(t) \leq q_b \quad \text{a.e. in } I. \quad (3)$$

Here  $I = [0, T]$ ,  $\Omega$  is a convex polygonal or polyhedral domain,  $x_0 \in \Omega$  fixed, and  $\delta_{x_0}$  is the Dirac delta function. The parameter  $\alpha$  is assumed to be positive and the desired state  $\widehat{u}$  fulfills  $\widehat{u} \in L^2(I; L^\infty(\Omega))$ . The control bounds  $q_a, q_b \in \mathbb{R} \cup \{\pm\infty\}$  fulfill  $q_a < q_b$ .

This problem can be classified as optimal control problem with a pointwise control. To approximate the problem numerically we use the standard continuous piecewise linear approximation in space and the first order discontinuous Galerkin method in time. Despite low regularity of the state equation, we establish almost optimal  $h^2 + k$  convergence rate in 2D and  $h + \sqrt{k}$  in 3D for the control in  $L^2$  norm. I will explain the key regularity estimate and new a priori fully discrete global and local error estimates in  $L^2([0, T]; L^\infty(\Omega))$  norms for parabolic problems. These new error estimates are essential in our analysis and using we improve almost twice the previously obtained error estimates in [1]. The 2D result were published in [2], but 3D results are new and still a work in progress.

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# Optimal Control of Signorini Contact Problems

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The talk is concerned with an optimal control problem governed by the Signorini contact problem, which is modelled by a variational inequality (VI) of the first kind. The solution operator associated with this VI is known to be not Gâteaux-differentiable. However, based on a technique introduced in [1], one can prove that it is directionally differentiable with a directional derivative, which is a VI of first kind itself. This allows to derive strong stationarity conditions as necessary conditions for local optimality under rather restrictive assumptions. Moreover, we employ this directional derivative for the design of an efficient trust-region optimization algorithm.

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# Frequency-sparse Control of Bilinear Quantum Systems

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An interesting phenomenon in bilinear quantum control is the oscillatory nature of the one dimensional control field. Those oscillations pose serious problems for the interpretation and experimental realization of the field. To overcome these difficulties we propose the use of time-frequency controls in a space of function-valued measures. This leads to an optimization problem of the form

$$\min_{\psi, u} \frac{1}{2} \langle \psi, \mathcal{O} \psi \rangle + \alpha \|u\|_{\mathcal{M}(\mathbf{R}; H_0^1(0, T))}$$

$$i\psi(t) = (H_0 + (Bu)(t)H_1)\psi(t)$$

where  $u$  is an element of the space  $\mathcal{M}(\mathbf{R}; H_0^1(0, T))$  of  $H_0^1$ -valued measures on the real line and the control operator  $B$  reconstructs the control field from the time-frequency information. The operators  $H_0$  and  $H_1$  are determined by the quantum system at hand and the control objective is to minimize the expectation value of the observable  $\mathcal{O}$ . This optimal control problem is non-convex and non-smooth. Optimal control with function-valued measures was already studied for a convex parabolic problem [1].

Previous attempts to deal with the oscillatory structure of control fields in quantum control are mostly based on frequency representations [2]. However, additional frequency localization comes at the cost of less time structure. Time-frequency representations were used only in combination with derivative free algorithms [3]. Our proposed systematic optimal control approach is based on sparsity enhancing functionals and time-frequency representations. We do not control the field itself but use a time-frequency control space that promotes sparsity in the frequency component and smoothness in time. In numerical experiments this leads to control fields which consist of a small number of pure frequencies each modulated with a smooth envelope function. The frequencies as well as the envelopes are obtained automatically without prior knowledge of the quantum system.

In this talk we will present a general framework for sparse quantum control, analyze the resulting optimality conditions and study different numerical examples.

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## Looking for strictly positive solutions of elliptic PDEs

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Consider, under the usual assumptions, an elliptic PDE in weak form:

$$\int_{\Omega} \nabla v \cdot A(x) \nabla u + c(x) uv \, dx + \int_{\Gamma} r(x) vu \, ds = \int_{\Omega} f v \, dx + \int_{\Gamma} g v \, ds \quad \forall v \in V.$$

It is easy to prove that for non-negative right-hand sides  $g$  and  $f$  we obtain non-negative solutions. Moreover, it is easy to believe that  $f$  and  $g$  can be chosen in a way that  $y$  is strictly positive (even if one of  $f$  and  $g$  is required to be 0). This and similar issues are of interest in optimal control, when it comes to verifying Slater conditions for a class of concrete problems. However, a rigorous proof of this conjecture is much harder to obtain, in particular, if one wants keep the regularity assumptions on the domain and the data as weak as possible. The aim of this talk is to give an account on achieved and possible solutions to this surprisingly deep issue.

# Time optimal control for the monodomain equations – a monolithic approach

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In this talk we present and analyze a time optimal control formulation for a reaction diffusion system arising in cardiac electrophysiology. Specifically, we consider the monodomain equations, which consist of a parabolic equation coupled to an ordinary differential equation (in each point in space), and provide a simplified model describing the electric activity of the heart. They allow for challenging wave phenomena (e.g., reentry waves), which physiologically correspond to undesired arrhythmia. Since the required time frame for a successful termination of such waves depends heavily on the data, we propose an optimal control formulation with a free final time. We show that, under certain conditions on the parameters, the optimal solutions of this problem steer the system into an appropriate stable neighborhood of the resting state. To this end, we derive some new regularity results and asymptotic properties for the monodomain equations in combination with the Rogers-McCulloch gating model.

For the numerical realization we consider a monolithic optimization approach, which simultaneously optimizes for the optimal times and optimal controls. Its practical realization is based on a semismooth Newton method. We prove local superlinear convergence in function space (under a second order condition) and present a globalization strategy. We present numerical examples which show the efficiency of the proposed approach and underline the theoretical results.

# The optimal shape of a pipe

Andreas Schulz

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A recent question in fluid dynamical shape optimization is, whether or not one can optimize the shape of a pipe to reduce frictional losses in fluid transportation compared to a cylindrical shape. Under reasonable assumptions on the model, including a non-slip condition on the shell, an incompressible and stationary fluid flow, and a volume constraint, an optimality proof for the cylindrical shape will be presented. The topic was addressed in [1], whereas the presented optimality proof can be found in [2].

## References

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# Topological derivative for nonlinear magnetostatics

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In topology optimization we are looking for the optimal distribution of material in a design domain in order to minimize a given domain-dependent objective function. One way to find such optimal designs is to use topological sensitivity information. The topological derivative of a domain-dependent functional  $\mathcal{J} = \mathcal{J}(\Omega)$  represents its sensitivity with respect to a perturbation of the domain. At a spatial point  $x_0$ , the topological derivative is defined as the quantity  $G(x_0)$  satisfying a topological asymptotic expansion of the form

$$\mathcal{J}(\Omega_\varepsilon) - \mathcal{J}(\Omega) = \rho(\varepsilon) G(x_0) + o(\rho(\varepsilon)).$$

Here  $\Omega_\varepsilon$  denotes the perturbed configuration where a hole of radius  $\varepsilon$  around the point  $x_0$  has been introduced in the domain  $\Omega$ , and  $\rho(\varepsilon)$  is a positive function with  $\lim_{\varepsilon \rightarrow 0} \rho(\varepsilon) = 0$ . The sign of  $G(x_0)$  indicates whether introducing a hole around  $x_0$  would increase or decrease the objective function.

Topological derivatives for optimization problems constrained by linear partial differential equations (PDEs) are well-understood. However, little is known about topological derivatives in combination with nonlinear PDE constraints. We will derive the formula of the topological derivative for the topology optimization of an electric motor where the state equation is the nonlinear equation of two-dimensional magnetostatics. Furthermore, we will address implementational issues and present numerical results for the optimization of an electric motor.

# Multiple state optimal design problems with random perturbation

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A multiple state optimal design problem with presence of uncertainty on the right-hand side is considered, in context of stationary diffusion with two isotropic phases. Perturbation term is given by a random function on a probability space. Similar problem with one state equation is considered in [2]. We shall address the question of relaxation by the homogenization method and necessary conditions of optimality. The case of discrete probability space leads to another multiple state problem (possibly with infinite number of states), which could be treated by similar techniques to those presented in [1, 3]. Relaxation can be expressed in a simpler form for problems with spherical symmetry in case of minimization (or maximization) of convex combination of compliances.

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# Robust methods and adaptivity for the numerical solution of variational inequalities for phase-field-based fracture problems

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In this presentation, we consider phase-field-based fracture propagation in elastic media. The main purpose is the development of a robust and efficient numerical scheme. To enforce crack irreversibility as a constraint, we use a primal-dual active set strategy, which can be identified as a semi-smooth Newton's method. The active set iteration is merged with the Newton iteration for solving the fully-coupled nonlinear partial differential equation discretized using finite elements, resulting in a single, rapidly converging nonlinear scheme. It is well-known that phase-field models ask for the resolution of a length-scale regularization parameter in terms of the local mesh size parameter. To achieve this, a predictor-corrector scheme for local mesh adaptivity is presented. Finally, steps towards a posteriori error estimation and convergence results are undertaken. Numerical examples are consulted to illustrate our findings.

# A Bridge from State-constrained ODE Optimal Control to State-constrained elliptic PDE Optimal Control: New Necessary Conditions, New Optimization Problems, and New Numerical Methods

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Based on different reformulations of state-constrained elliptic optimal control problems with distributed control and a hypothesis on the structure of the active set, new necessary conditions are obtained which exhibit higher regularity of the multiplier associated with the state constraint. Moreover, we obtain also new jump and sign conditions. Measures are no longer an issue, so that regularization techniques become superfluous. Finally, the method can be fully described in function spaces which is an essential element to obtain a mesh-independent numerical method.

The new approach mimics the well-known Bryson-Denham-Dreyfus indirect adjoining method which is the preferred ansatz in solving state-constrained optimal control problems with ordinary differential equations numerically. However, in the context of PDE constrained optimization this approach turns out to be extremely involved.

Mathematically the reformulations lead to a new kind of set optimal control problem, where the active set of the state constraint, resp. the interface between the inactive and the active set are to be determined as part of the solution as the switching points in multipoint boundary value problems based on first-order necessary conditions for ODE constrained optimal control problems. Various formulations of this type of PDE optimization problem as shape and/or topology as well as bilevel optimization problem or, concerning the numerical solution, as free boundary value problem are discussed.

Moreover, parallels can be drawn to optimization on vector bundles which seems to be essential for the design of an appropriate Newton-type method, since the optimization over sets of admissible active sets have a nonlinear structure. This requires an answer to the question how does a Newton method look on a nonlinear manifold where no Banach space structure is present.

Numerical results will demonstrate the performance of the new method.

This presentation will open new research directions in PDE constrained optimal control as indicated in the final outlook.



# Optimal control for lithium-ion batteries

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The decreasing of fossil energy sources makes energy storage systems to one of the central components of electric systems, particularly, for purely battery-operated vehicles. A central challenge is the development of efficient battery management systems for the storage, delivery and recovery of electric energy. Nowadays, lithium-ion batteries are very common for portable electronics and furthermore, of growing importance for electric vehicles.

Modelling the electro-chemical phenomena occurring in re- and discharging batteries leads to very complicated systems of nonlinearly coupled partial differential, algebraic and integral equations for the ion concentrations, fluxes and potentials. If further thermal and mechanical processes or the coupling of multiple batteries are considered, the models become even more complex. Numerical simulation and, in particular, (optimal) control of such systems can therefore be a very difficult and time-consuming issue.

In this talk we will discuss a specific model for a lithium-ion battery. The model involves ionic concentrations, ionic currents and potentials in and between the positive and negative electrode together with the battery temperature as state variables. The resulting system is a nonlinear PDAE system with 10 partial and 4 algebraic equations involving the famous nonlinear Butler-Volmer kinetics for describing the interaction of ionic currents and potentials. The numerical simulation is implemented based on a finite difference approach.

Optimal control tasks for charging the system subject to control and state constraints are discussed. For the numerical treatment of the optimal control problems, a first-discretize-then-optimize approach is firstly chosen. This leads to a high-dimensional nonlinear optimization problem which is solved by an efficient nonlinear optimization solver. Necessary optimality conditions can be derived and numerically verified.

Further numerical techniques to solve the optimal control problems are presented. For the occurring state constraint of order 1, a feedback control law is computed to formulate and solve the corresponding so-called induced optimization problem. This method provides not only the state and control variables in an efficient way but also the values of switching times with high accuracy. Furthermore, the method can be used to investigate second order sufficient conditions and sensitivity analysis.

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# Numerical approximation of a quasistatic evolution problem in cohesive fracture

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Given two Euclidean spaces  $\mathcal{E}^n$  and  $\mathcal{E}^m$  of dimension  $n$  and  $m$ , respectively, with  $n > m$ , a (nonconvex, nonsmooth) energy functional  $J : \mathcal{E}^n \rightarrow [0, +\infty)$ , a linear operator  $A : \mathcal{E}^n \rightarrow \mathcal{E}^m$ , and a time dependent forcing  $f : [0, T] \rightarrow \mathcal{E}^m$ , we discuss under very general assumptions on  $J$  and  $A$  the convergence of a simple numerical procedure providing a discrete *quasistatic evolution* relative to the energy function  $J$  and the linear constraint pair  $(A, f)$ . This one is defined as a measurable mapping  $u : [0, T] \rightarrow \mathcal{E}^n$  satisfying the stationarity condition

$$u(t) \text{ is a critical point of } J \text{ on the affine space } \{Av = f(t)\} \text{ for almost every } t \in [0, T], \quad (1)$$

as well as the following energy inequality: there exists a bounded measurable function  $q : [0, T] \rightarrow \mathcal{E}^m$  such that  $A^*q(t) \in \partial J(u(t))$  (the subdifferential of  $J$  at  $u(t)$ ) and

$$J(u(t)) \leq J(u(0)) + \int_0^t \langle q(s), \dot{f}(s) \rangle ds, \text{ for almost every } t \in [0, T], \quad (2)$$

where the scalar product  $\langle \cdot, \cdot \rangle$  is the Euclidean one. The requiring of an energy inequality to be satisfied is motivated by the applications in continuum mechanics.

As a detailed case study, we indeed consider the functional  $J$  coming from the finite element discretization in space, with mesh size  $h > 0$ , of the cohesive fracture energy analysed in [2]

$$\frac{1}{2} \int_{\Omega \setminus \Gamma} |\nabla u|^2 dx + \int_{\Gamma} g(|u^+ - u^-|) d\mathcal{H}^{d-1}, \quad (3)$$

with  $\Gamma$  being a prescribed crack path,  $u$  the displacement,  $u^+$  and  $u^-$  the traces of  $u$  on the two sides of  $\Gamma$ , and  $g : [0, \infty) \rightarrow [0, \infty)$  is, in general, a  $C^1$ , nondecreasing, bounded, concave function with  $g(0) = 0$  and  $\sigma := g'(0^+) \in (0, +\infty)$ . This energy is usually coupled with a linear constraint in the form of a time-dependent *Dirichlet datum*. In a simplified situation, that is when  $d = 2$  and  $\Gamma$  is a rectilinear crack, we also show that the discrete evolution given by our *constructive* numerical procedure converges, for a mesh size  $h \rightarrow 0$ , to a continuum quasistatic evolution in the sense of [2], where existence had instead been shown by means of a *vanishing viscosity* approach.

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# Sparse optimal control of the KDV equation

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We focus in this work on optimal control problems of the following form

$$\min_{q \in \mathcal{M}(\Omega, L^2(I))} J(y) = \frac{1}{2} \|y - y_d\|_{L^2(\Omega, L^2(I))}^2 + \alpha \|q\|_{\mathcal{M}_I} \quad (1)$$

where  $y$  is the solution of the nonlinear Burgers-Korteweg de Vries equation with a time dependent measure valued source term acting as control

$$\begin{cases} \partial_t y + \partial_x y + \partial_{xxx} y - \gamma \partial_{xx} y + y \partial_x y = q & \text{in } \Omega, \\ y(\cdot, 0) = y(\cdot, L) = \partial_x y(\cdot, L) = 0 & \text{in } \Gamma, \\ y(0, \cdot) = 0 & \text{on } \Omega. \end{cases} \quad (2)$$

which is known to have traveling wave solutions. The control space  $\mathcal{M}_I$  is either the Bochner space  $L^2(I, \mathcal{M}(\Omega))$  or the space of vector measures  $\mathcal{M}(\Omega, L^2(I))$  with values in  $L^2(I)$ . For both choices the controls are sparse in space and distributed in time. But the first space allows for moving dirac measures and the second not. We will tackle the following theoretical questions: well posedness of the KdV equation with a non-smooth source term, existence and characterization of an optimal control, algorithmic treatment of the problem by a semi-smooth Newton method in function space. In the end, we present some numerical examples that motivate our work: sparse stabilization of the KDV equation and sparse inverse source problems for the KDV equation (reconstruction of the topography and/or topography changes).

# Traffic flow control: avoiding shocks via variable speed limit

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In this contribution, we propose a control strategy for a traffic flow problem. We concentrate on the variable speed limit (VSL) problem. This means that the control variable, i.e. the maximal velocity for the VSL problem, varies in space and can be used to control traffic flow in order to reduce traffic congestion. From a mathematical point of view, this leads to conservation laws, i.e. hyperbolic partial differential equations, with space-dependent flux, [4].

This kind of problems have been considered usually in a discrete setting due to the difficulties of applying optimal control theory in a continuous setting. We propose to actuate a control strategy that could be used in the continuous setting at least for the scalar conservation law. In fact, for many applications, not only the numerical simulation of the nonlinear dynamics is of interest but also optimization or control issues.

We consider the classical Lighthill-Whitham-Richards (LWR) model for traffic flow on a single infinite road [2, 3], with a space dependent flux function:

$$\begin{cases} \partial_t \rho(t, x) + \partial_x f(x, \rho(t, x)) = 0 & (t, x) \in \mathbb{R}^+ \times \mathbb{R}, \\ \rho(0, x) = \rho_0(x), \end{cases} \quad (1)$$

where  $\rho \in [0, \rho_{\max}]$  is the mean traffic density and  $\rho_{\max}$  the maximal density allowed on the road. We suppose that the flux function is space-dependent and it is given by  $f(x, \rho) = v(x, \rho)\rho$  where  $v(x, \rho) = V^{\max}(x)\rho\left(1 - \frac{\rho}{\rho_{\max}}\right)$  is the mean traffic speed.

The maximal speed  $V^{\max}(x)$  is the control parameter. We propose a theoretical approach and a numerical one to show how to reduce traffic congestion, i.e., avoiding shocks formation by modifying the maximal speed in space. In particular, we will show numerical simulations obtained with the Runge-Kutta discontinuous Galerkin method in the spirit of [1].

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# Luré dynamical systems – existence and stability results

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In this contribution we study multivalued Luré dynamical systems that can be formulated as

$$\begin{cases} \dot{x}(t) = Ax(t) + Bu(t) + f(t); x(0) = x_0 \\ u(t) \in \mathcal{M}[Cx(t) + Du(t)], \end{cases}$$

where  $\mathcal{M}$  is the subdifferential of a convex closed and proper function or more general monotone operator. Such dynamical systems were treated in finite dimensions in [1] with applications in nonsmooth electronics. Moreover, they arise in feedback control [2]. Here we extend recent existence and stability results [3, 4] to this class of dynamical systems.

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# A smooth and localized version of the Hughes model for pedestrian flow

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In the classical model of Hughes for crowd motion [1] pedestrians seek to minimize their travel time to a-priori known destinations/exits, but try to avoid regions of high density. This is achieved by coupling the continuity equation of the density  $\rho(x, t)$  to an Eikonal equation, which determines the optimal walking paths. One of the basic assumptions is that the overall density of the crowd is known to every agent at every point in time. We present results on a modification that includes localizing effects such as limited vision to a Hughes-type equation. The basic mechanism permits agents to perceive information on the current crowd density only in a local neighborhood, while taking assumptions on the density outside that region. Furthermore, we suggest a smoothing operator for the velocity field and discuss detailed boundary conditions. The model is presented on both a microscopic and macroscopic perspective. Our main object of study is the effect of localised path optimisation on the overall performance of the crowd in e. g. an evacuation scenario. We first analyse the domain of dependence for the planning problem of each pedestrians, and then quantify and illustrate the ability of the crowd to evacuate effectively with numerical experiments. Surprisingly, it will turn out that evacuation times can even improve in some situations. The question we investigate is hence complementary to mean-field game approaches [2] to crowd dynamics, where pedestrians anticipate future crowd states and therefore are *more* capable than in the original Hughes' model.

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# On Modelling, Simulation and Optimisation of Solar Updraft Towers with Sloped Collectors

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This contribution is concerned with the modelling, simulation and optimization of so called solar updraft towers, a special form of a solar thermal power plant. The classical solar updraft towers have flat collectors [1, 2, 3]. Here we focus on a generalization of this idea including sloped collectors, designed in particular for higher latitudes on earth [4].

The main idea is to study how the reduction of the solar power (per aerea) at higher latitudes on earth can be compensated by a special non-planar collector of the power plant. Our model is again a generalization of a model proposed for flat collectors [5]. We focus mainly on gas dynamic issues and use a simple model for the energy transfer. Using an appropriate one dimensional model combined with asymptotic low Mach number techniques we are able to derive a simplified model which allows fast simulations and therefore optimization with respect to system parameters. We show simulations and optimize with respect to various parameters which are important when planning such a power plant.

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# The identifiability approach for time-dependent full waveform inversion

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Full-waveform inversion (FWI) has long been considered the next logical step in deriving detailed velocity models. Despite recent advances in high-performance computing which make three dimensional acoustic FWI feasible today, it still remains a computationally very demanding inverse problem due to the huge number of geological parameters that need to be identified. A mathematically sound method is described for selecting the part of the parameter space that is best identifiable from the seismic acquisition geometry. This is combined with either interior-point or sequential quadratic programming methods for performing FWI for the subset of parameters that have been characterized as identifiable. The suggested approach results in a significant reduction of the parameter space. Local minima inherent to the original larger optimization space are avoided and the computational complexity of the inversion process, especially if second-order gradient information are desired, is therefore significantly decreased.

# Local minimization algorithms for dynamic programming equations

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To solve Hamilton-Jacobi Bellman (HJB) equations numerically often for evaluating the Hamiltonian the minimum over a set of admissible controls has to be determined. In particular, when considering control problems with nonsmooth cost functionals this is a challenging subject. In this talk we demonstrate the importance of redoing these minimization problems accurately and propose algorithms by which this can be achieved effectively. We focus the presentation on semi-Lagrangian (SL) schemes for first order HJB equations. The considered class of equations includes control problems with  $L^1$ -control term.

Starting with an infinite horizon control problem we introduce a SL-scheme and consider a first-order primal-dual method (also known as Chambolle-Pock algorithm [1]) and semi-smooth Newton methods (see, e.g., [2]) for the minimization within the SL-scheme. In contrast to the broadly used approach, to compare the values for a finite subset of controls and to compute the minimum over this set by comparison, the proposed algorithms lead for the same cpu time to more accurate solutions and for specific settings convergence can be shown. For nonsmooth optimal control problems with  $L^1$ -control term sparse controls are observed.

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# Optimization of Multirate Partial Differential Algebraic Equations

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The mathematical modeling of electric circuits yields systems of differential algebraic equations (DAEs). We consider systems of the form

$$\frac{d\mathbf{q}(\mathbf{x})}{dt} = \mathbf{f}(\mathbf{b}(t), \mathbf{x}(t)) \quad (1)$$

with the solution  $\mathbf{x} : [t_0, t_{\text{end}}] \rightarrow \mathbb{R}^k$  and predetermined input signals  $\mathbf{b} : [t_0, t_{\text{end}}] \rightarrow \mathbb{R}^\ell$ . It holds that  $\mathbf{q} : \mathbb{R}^k \rightarrow \mathbb{R}^k$  and  $\mathbf{f} : \mathbb{R}^\ell \times \mathbb{R}^k \rightarrow \mathbb{R}^k$ . We assume that the solution represents a high-frequency oscillation, whose amplitude as well as frequency changes slowly in time due to the input signals. It follows that a time integration of the system (1) becomes costly, since each fast oscillation has to be resolved. Alternatively, a multidimensional signal model changes the system of DAEs (1) into a system of multirate partial differential algebraic equations (MPDAEs), see [1, 2]. We obtain the system

$$\frac{\partial \mathbf{q}(\hat{\mathbf{x}})}{\partial t_1} + u(t_1) \frac{\partial \mathbf{q}(\hat{\mathbf{x}})}{\partial t_2} = \mathbf{f}(\mathbf{b}(t_1), \hat{\mathbf{x}}(t_1, t_2)) \quad (2)$$

with the solution  $\hat{\mathbf{x}} : [0, T_1] \times [0, T_2] \rightarrow \mathbb{R}^k$  and a local frequency function  $u : [0, T_1] \rightarrow \mathbb{R}$ . Both initial-boundary value problems (IBVPs) and bi-periodic boundary value problems (BBVPs) are considered for the system (2).

The local frequency function represents a degree of freedom in the multidimensional model. The aim is to identify appropriate solutions  $\hat{\mathbf{x}}$ , which exhibit a low amount of variation such that the solution can be resolved on a relatively coarse grid. For this purpose, we investigate minimization problems based on either the functional

$$J(\hat{\mathbf{x}}) := \int_0^{T_1} \int_0^{T_2} \left\| \frac{\partial \hat{\mathbf{x}}}{\partial t_1} \right\|_2^2 dt_2 dt_1 \quad \text{or} \quad I(t_1, \hat{\mathbf{x}}) := \int_0^{T_2} \left\| \frac{\partial \hat{\mathbf{x}}}{\partial t_1} \right\|_2^2 dt_2 \quad \text{for each } t_1 \in [0, T_1]. \quad (3)$$

The functional  $J$  is defined for the global solution, whereas the functional  $I$  is specified pointwise. Necessary conditions for optimality were derived for IBVPs in [3] and for BBVPs in [4] by assuming the existence and uniqueness of an optimal solution. Numerical methods including these necessary conditions yield the optimal solution.

In our contribution, we prove the existence and uniqueness of optimal solutions with respect to each functional in (3), which satisfy either IBVPs or BBVPs of the MPDAE system (2). Moreover, it can be shown that the pointwise minimization based on the functional  $I$  is equivalent to the global minimization using the functional  $J$ . This property allows for solving IBVPs by a method of lines, where the pointwise minimization is done successively. Furthermore, we interpret the minimization problems in the context of optimal control. It follows that the direct approach in optimal control is inefficient for this problem class, whereas the indirect approach in optimal control represents the method of choice. The numerical solution of BBVPs can be done by a method of characteristics including the necessary conditions for an optimal solution, since the MPDAEs (2) exhibit a hyperbolic structure. We present the numerical simulation of a test example modeling an electric circuit, whose solution features both amplitude modulation and frequency modulation.

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# A priori error estimates for nonstationary optimal control problems with gradient state constraints

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This talk deals with error estimates for space-time finite element discretization of semilinear parabolic optimal control problems subject to inequality constraints on the gradient of the state variable.

In particular, we will focus on pointwise in time and averaged in space gradient state constraints of the form

$$\int_{\Omega} |\nabla u(x, t)|^2 \omega(x) dx, \forall t \in [0, T],$$

where  $u$  denotes the state variable and  $\omega(x)$  is a weighting function.

Consideration of these constraints is motivated by industrial applications in the steel and glass production, where stress averages are often considered in order to avoid material failure.

Making use of the discontinuous Galerkin method for the time discretization and of standard conforming finite elements for the space discretization, we derive convergence rates as temporal and spatial mesh size tends to zero.

# Direct and indirect multiple shooting for parabolic optimal control problems

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In the context of ordinary differential equations, shooting techniques have become a state-of-the-art solver component, whereas their application with partial differential equations (PDE) is still in an early phase of development. We present two multiple shooting approaches for optimal control problems governed by parabolic PDE. We derive both direct and indirect shooting for PDE optimal control from the same extended problem formulation. This approach shows that they are algebraically equivalent on an abstract function space level. However, discussing their algorithmic realizations, we underline the differences between direct and indirect multiple shooting. In the presented numerical examples we cover both linear and nonlinear parabolic side conditions.

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# Functional a posteriori estimates for cost functionals of elliptic optimal control problems

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In this talk, new results on functional type a posteriori estimates for elliptic optimal control problems with control constraints are presented, see [1]. More precisely, we derive new, sharp, guaranteed and fully computable lower bounds for the cost functional in addition to the already existing upper bounds, see [2]. Using both, the lower and the upper bounds, we arrive at two-sided estimates for the cost functional. These bounds finally lead to sharp, guaranteed and fully computable upper estimates for the discretization error in the state and the control of the optimal control problem.

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# Multiobjective Optimization of the Flow Around a Cylinder Using Model Order Reduction

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In many applications the optimization of multiple, potentially conflicting objectives is desired. In this case, one is interested in calculating the set of optimal compromises between these goals, the so-called Pareto set [1], instead of searching for one specific optimum. This is expressed as a multiobjective optimization problem:

$$\min_{x \in \mathbb{R}^n} \{F(x)\}, \quad (\text{MOP})$$

$$F : \mathbb{R}^n \rightarrow \mathbb{R}^k, F(x) = (f_1(x), \dots, f_k(x)).$$

There exist various approaches to address (MOP) such as scalarization techniques (weighted sum) [2], continuation methods [2] or evolutionary algorithms [3]. Additionally, set oriented algorithms have proven to be very efficient for the computation of Pareto sets, e.g. the subdivision algorithm presented in [4], where the set is approximated by a nested sequence of increasingly fine box coverings. This method is capable of calculating the entire, globally optimal Pareto set, also in the situation where the set is disconnected.

All algorithms computing a set of optima have in common a high number of function evaluations. Consequently, when the evaluation of the system under consideration is costly, as is the case for dynamical systems described by partial differential equations, the computation quickly becomes infeasible. To avoid this problem, model order reduction such as Proper Orthogonal Decomposition (POD) [5] or Dynamic Mode Decomposition (DMD) [6] can be a useful tool to reduce the computational effort.

In this presentation, we apply the subdivision algorithm described above to the two-dimensional flow around a rotating cylinder in order to calculate the Pareto set for the competing objectives lift ( $C_L$ ) and drag ( $C_D$ ):

$$\min_{u \in U} J(y(u)) = \min_{u \in U} \begin{pmatrix} -C_L(y(u)) \\ C_D(y(u)) \end{pmatrix} \quad \text{s.t. } e(y(u), u) = 0, \quad (\text{P1})$$

where the state  $y = (v_x, v_y, p)^T$  consists of the velocity and pressure field of the fluid,  $u = (v_{\partial\Omega_{in}}, \omega_{cyl})^T \in U$  is the control vector consisting of the inflow velocity and the angular velocity of the cylinder and  $e$  is an equality constraint induced by the 2D incompressible Navier-Stokes equations. We then approximate the dynamical system by a reduced order model using DMD and a Galerkin Projection and solve (P1) based on the reduced model. Finally, we analyze the tradeoff between computational effort and quality of the approximation given by this method.

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# A Certified Reduced Basis Approach for Parametrized Linear-Quadratic Optimal Control Problems with Control Constraints

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Many problems in science and engineering can be modeled in terms of optimal control problems governed by parametrized partial differential equations (PDEs). While the PDE describes the underlying system or component behavior, the parameters often serve to identify a particular configuration of the component — such as boundary and initial conditions, material properties, and geometry. In such cases — in addition to solving the optimal control problem itself — one is often interested in exploring many different parameter configurations and thus in speeding up the solution of the optimal control problem. However, using classical discretization techniques such as finite elements or finite volumes even a single solution is often computationally expensive and time-consuming, a parameter-space exploration thus prohibitive. One way to decrease the computational burden is the surrogate model approach, where the original high-dimensional model is replaced by a reduced order approximation. These ideas have received a lot of attention in the past and various model order reduction techniques have been used in this context. However, the solution of the reduced order optimal control problem is generally sub-optimal and reliable error estimation is thus crucial. Besides serving as a certificate of fidelity for the sub-optimal solution, our *a posteriori* error bounds are also a crucial ingredient in generating the reduced basis with greedy algorithms.

A new approach for efficient computation of error bounds for unconstrained distributed control problems was proposed in [2]. This approach, however, and all other existing approaches in the literature, see e.g. [3, 4, 5], are not directly applicable to the important case with additional constraints on the control.

In this work we extend the methodology presented in [6] to consider PDE-constrained optimal control problems. The authors in [6] develop a certified Reduced Basis (RB) method that provides sharp *and* inexpensive *a posteriori* error bounds for variational inequalities. In particular, the approach has advantages compared to prior work on variational inequalities with the RB method [1]. The methodology in [6] not only (i) provides sharper error bounds that mimic the convergence rate of the RB approximation, but also (ii) does so at an online cost that is independent of the high dimension of the original problem.

In particular we use the approach presented in [6] (i) to construct a feasible RB approximation of the control and (ii) to derive efficiently computable *a posteriori* error bounds. The main idea is to generate two RB-systems. The first one is “standard” and is used to construct low dimensional approximations for the state and the Lagrange multiplier. In the second one we construct nonnegative slack variables for the control and so can generate feasible low dimensional surrogates for the control. Finally, we extend the proof of the *a posteriori* error bounds from [2] to derive efficient *a posteriori* bounds for the control error in the constraint case.

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# Wavelet-based lossy trajectory compression for optimal control of parabolic PDEs

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For the solution of optimal control problems governed by parabolic PDEs, methods working on the reduced objective functional are often employed to avoid a full spatio-temporal discretization of the problem. The evaluation of the reduced gradient requires one solve of the state equation forward in time, and one backward solve of the adjoint equation. As the state enters into the adjoint equation, the storage of a full 4D data set is needed. If Newton-CG methods are used, two additional trajectories have to be stored. To get accurate numerical results, in many cases very fine discretizations in time and space are necessary, which leads to a significant amount of data to be stored and transmitted to mass storage.

To overcome these storage problems, we developed and analyzed a lossy compression method, using the hierarchic basis representation of the finite element solution combined with quantization of coefficients. Due to a pointwise control of the compression error, the error transport of the adjoint equation is not taken into account [1, 2, 3].

In this talk, we present a more advanced compression scheme, based on a lifted wavelet transform, which allows to control the error in the  $L^2$ - and  $H^{-1}$ -norm instead of  $L^\infty$ . We discuss the adaptive choice of quantization tolerances and give numerical examples.

**Keywords:** optimal control, parabolic PDEs, trajectory storage, adaptive lossy compression

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