Mathematisches Forschungsinstitut Oberwolfach

Report No. 13/2023

DOI: 10.4171/OWR/2023/13

Optimization Problems for PDEs in Weak Space-Time Form

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5 March – 10 March 2023

Abstract. Optimization problems constrained by *time-dependent* Partial Differential Equations (PDEs) are challenging from a computational point of view: even in the simplest case, one needs to solve a system of PDEs coupled globally in time and space for the unknown solutions (the state, the costate and the control of the system). Typical and practically relevant examples are the control of nonlinear heat equations as they appear in laser hardening or the thermic control of flow problems (Boussinesq equations). Specifically for PDEs with a long time horizon, conventional time-stepping methods require an enormous amount of computer memory allocations for the respective other variables. In contrast, adaptive-in-time-and-space methods aim at distributing the available degrees of freedom in an a-posteriori fashion to capture singularities and are, therefore, most promising. Recently, well-posed weak variational formulations have been introduced for time-dependent PDEs such as the heat equation, linear transport and the wave equation. Those formulations also allow for a sharp relation between the approximation error and the residual, which is particularly relevant for model reduction. Moreover, for those tensor-basis formulations, advanced algebraic solvers designed to take into account these multiarray (tensorial) formulations appear to be particularly competitive with respect to time-marching schemes, especially in higher dimensions. We plan to discuss whether these techniques can be extended to nonlinear PDEs like Hamilton–Jacobi–Bellman equations, or stochastic PDEs and variational inequalities. Another topic will be adaptive schemes which, when properly designed, inherit the stability of the continuous formulation.

The central goals of the workshop are the analysis, fast solvers and model reduction for PDE-constrained control and optimization problems based on weak formulations of the underlying PDE(s).

Mathematics Subject Classification (2020): 65xx, 49xx.

Introduction by the Organizers

The workshop *Optimization Problems for PDEs in Weak Space-Time Form*, organised by Helmut Harbrecht (Basel), Angela Kunoth (Köln), Valeria Simoncini (Bologna) and Karsten Urban (Ulm) was well attended with over 25 participants with broad geographic representation and a nice blend of researchers with various backgrounds.

The workshop was directed at control and optimization problems constrained by *evolutive PDEs*. Our main goal was to design most efficient guaranteed numerical solvers, building upon variational formulations of the underlying PDE(s). The idea was to encourage interaction between scientists from different areas (numerical analysis, optimization and optimal control, numerical linear algebra, model reduction) and thereby result in more rapid advances of new methodologies in these various domains. It was, therefore, also a bridge from theoretical foundations to applications, such as mechanical engineering, quantum chemistry, signal and image processing, complex fluid flows, or finance.

Topics that were addressed in our workshop were:

- Weak and very weak variational formulations of PDEs and inequalities; weak discontinuous Petrov-Galerkin methods, and corresponding stable discretizations; optimization and control problems constrained by these formulations
- Robust numerical linear algebra techniques for tensor linear and nonlinear equations, for reduction-based approximations and low rank problems, for structure-aware representations, and for adaptive-in-time discretizations; their discretization-dependent convergence properties
- Shape calculus and numerical solution of shape optimization problems with time-dependent PDE, especially in case of time-dependent domains
- Error estimation, convergence and complexity estimates on different grids for the different variables state, costate and control; exchange of information from different grids while maintaining accuracy
- Optimal control of parametric/random PDEs and sparse discretization thereof
- Open and closed loop control problems
- Linear and nonlinear reduced modeling for forward and inverse problems
- Optimal actor and sensor placement in control for inverse problems and their efficient solution

The different concepts and expertises are in our opinion relevant for further development of efficient solution methods for optimization problems constrained by time-dependent PDEs. Indeed, the participants of the workshop discussed synergies and possible cross-fertilization.

Workshop: Optimization Problems for PDEs in Weak Space-Time Form

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Abstracts

Introduction to Optimization Problems for PDEs in Weak Space-Time Form

Angela Kunoth
(joint work with Sarah Knoll (last part))

Optimization problems constrained by PDEs (partial differential equations) are challenging from a computational point of view: one needs to solve a *system of PDEs* coupled globally in space, and, in addition, *globally* in time if the underlying PDE is time-dependent. This global coupling is an unavoidable feature of such control problems; typically an adjoint PDE problem comes into place as specified next.

PDE-constrained control problems. We recall some general statements about constrained optimization problems. Let Y, U be Hilbert spaces over $\mathbb{R}$ which shall host the *state* y of a system and a *control* u by which the state can be influenced. Let $J : Y \times U \to \mathbb{R}$ be a functional which is twice differentiable with respect to y and u, and $K : Y \times U \to Y'$ be a (in y, u Fréchet-) differentiable function where Y' denotes the topological dual of Y. We shall be concerned with the constrained minimization problem

$$\inf_{(y,u)\in Y\times U} \quad J(y,u) \quad \text{subject to } K(y,u) = 0. \tag{1}$$

For the constraints $K(y, u) = 0$ (which will play the role of the PDE later), we assume that there exists a unique solution $y \in Y$ for the case that $u \in U$ is given. A typical way to solve (1) is to compute the zeroes of the first order Fréchet derivatives of the corresponding Lagrangian functional. These are built by introducing a new variable p, the *costate* or *adjoint state* in terms of which the constraints are appended to the functional, i.e.,

$$L(y,u,p) := J(y,u) + \langle K(y,u), p\rangle_{Y'\times Y} \tag{2}$$

with $L : Y\times U\times Y \to \mathbb{R}$. Denoting by $L_z(y,u,p) := \frac{\partial}{\partial z}L(y,u,p)$ and $L_{zz}(y,u,p) := \frac{\partial^2}{\partial z^2}L(y,u,p)$ the first and second variation, respectively, of L with respect to $z = y, u, p$, the necessary conditions for optimality read

$$\delta L(y,u,p) := \begin{pmatrix} L_y(y,u,p) \\ L_u(y,u,p) \\ L_p(y,u,p) \end{pmatrix} = \begin{pmatrix} J_y(y,u) + \langle K_y(y,u), p\rangle_{Y'\times Y} \\ J_u(y,u) + \langle K_u(y,u), p\rangle_{Y'\times Y} \\ K(y,u) \end{pmatrix} = 0. \tag{3}$$

If J is now quadratic in both y, u, and K linear in y, u, system (3) can be specified to the linear system of equations

$$\begin{pmatrix} L_{yy} & L_{yu} & K_y^* \\ L_{uy} & L_{uu} & K_u^* \\ K_y & K_u & 0 \end{pmatrix} \begin{pmatrix} y \\ u \\ p \end{pmatrix} = g \Longleftrightarrow: \begin{pmatrix} \mathcal{A} & \mathcal{B}^* \\ \mathcal{B} & 0 \end{pmatrix} \begin{pmatrix} (y,u)^\top \\ p \end{pmatrix} = g \Longleftrightarrow: \; G\,q = g \tag{4}$$

with some right hand side g and C^* denoting the dual of C. The Hessian of L or the Karush-Kuhn-Tucker (KKT) operator G has for such *linear-quadratic problems* constant entries. For linear-quadratic optimization problems, the necessary conditions are also sufficient for the infimum. Moreover, if J or K do not contain products yu, one has $L_{yu} = L_{uy} = 0$ so that $\mathcal{A}$ is a block diagonal operator. Typically, the quadratic functional (1) contains inner products so that the resulting Riesz operators L_{yy}, L_{uu} are symmetric which implies that $\mathcal{A}$ and, thus, G is *symmetric*. Moreover, in all the cases we consider, $\mathcal{A} : \mathcal{V} \to \mathcal{V}, \mathcal{B} : \mathcal{V} \to \mathcal{Q}'$ for some Hilbert spaces $\mathcal{V}$, $\mathcal{Q}$ are continuous, $\operatorname{Im} \mathcal{B} = \mathcal{Q}'$ and $\mathcal{A}$ is invertible on $\operatorname{Ker} \mathcal{B}$ so that the saddle point problem (4) has for $g \in \mathcal{V}' \times \mathcal{Q}'$ a unique solution $q \in \mathcal{V} \times \mathcal{Q}$ by the Brezzi-Fortin theory. Thus, we can consider constrained linear-quadratic minimization problems as *symmetric saddle point problems* (4) with a boundedly invertible linear mapping $G : \mathcal{V} \times \mathcal{Q} \to \mathcal{V} \times \mathcal{Q}'$ where $\mathcal{V} := Y \times U$ and $\mathcal{V} := Q$.

The most prominent example of a control problem constrained by a linear parabolic PDE in weak space-time form to which this scenario applies is the following [5].

Parabolic PDE with distributed control. We consider a linear parabolic evolution PDE in full space-time weak formulation from [7] as constraint $K(y, u) = 0$ in (1). The parabolic operator equation is formulated such that the resulting operator $B = \partial_t + A$ is boundedly invertible from $X := (L^2(I) \otimes V) \cap (H^1_T(I) \otimes V')$ to $Y := (L^2(I) \otimes V) \times L_2(\Omega)$ where $H^1_T(I)$ is the closure of the functions in $H^1(I)$ which vanish at end time T and $I := (0, T)$ denotes the time interval. Here $A : V \to V'$ is the operator expressing the weak form of the elliptic PDE.

With a corresponding objective functional, we arrive at a system of the form (4) with symmetric $\mathcal{A}$ where the corresponding operator G is a boundedly invertible mapping.

Computational challenges. For control problems subject to a linear parabolic evolution PDE, conventional time-stepping methods require an enormous storage. In contrast, adaptive methods in both space and time based on the formulation in [7] which aim at distributing the available degrees of freedom in an a-posteriori-fashion to capture singularities are most promising. Employing wavelet schemes for full weak space-time formulations of the parabolic PDEs, we can prove convergence and optimal complexity for control problems constrained by a linear parabolic PDE [3].

Yet another level of challenge are control problems constrained by evolution PDEs involving stochastic or countably many infinite parametric coefficients: for each instance of the parameters, this requires the solution of the complete control problem. Our method of attack is based on the following new theoretical paradigm. It is first shown for control problems constrained by evolution PDEs, formulated in full weak space-time form as in [7], that state, costate and control are analytic as functions depending on these parameters. We establish that these functions allow expansions in terms of sparse tensorized generalized polynomial chaos (gpc) bases. Their sparsity is quantified in terms of p-summability of the coefficient sequences for some $0 < p \leq 1$. Resulting a-priori estimates establish

the existence of an index set for concurrent approximations of state, co-state and control for which the gpc approximations attain rates of best N-term approximation. This entails corresponding sparse realizations in terms of deterministic adaptive Galerkin approximations of state, co-state and control on the entire, possibly infinite-dimensional parameter space, see [5]. We specify in [6] how to realize these Galerkin approximations.

Optimal preconditioners for elliptic PDEs. For the control problems discussed here, the fast numerical solution of the underlying parabolic PDE in weak space-time form is of central importance. A BPX-type preconditioner based on higher order B-splines as proposed in [1] for a linear elliptic PDE is investigated in the present setting in [4].

Pricing American Put Options using Black-Scholes leads to a parabolic variational inequality including a non-symmetric, non-coercive bilinear form

$$a^B(u,v) = \int_I \frac{\sigma^2}{2} S^2 \frac{\partial u}{\partial S}\frac{\partial v}{\partial S} + ruv + (\sigma^2 + D_0 - r)\frac{\partial u}{\partial S} v \, \mathrm{d}S \tag{5}$$

where σ, r, D_0 are constants and $u, v \in \mathcal{V} := \{u \in L_2(I) \ : \ S\frac{\partial u}{\partial S} \in L_2(I)\}$. As shown in [2], (5) satisfies a Garding inequality

$$a^B(u,u) \geq \alpha \|u\|^2_{\mathcal{V}} - \beta \|u\|^2_{L_2(I)} \text{ with } \alpha \geq 0 \text{ and } \beta := \tfrac{|\sigma^2 + D_0 - r|}{2}. \tag{6}$$

Discretization of (5) using higher order B-splines and coinciding knots at the strike price as developed in [2] results in a (slightly) non-symmetric matrix A, whose spectral condition number is approximated by $\kappa_2(A) \approx \sqrt{\kappa_2(A^T A)}$. Shifting the matrix A by the constant β in (6), we were able to apply the BPX-type preconditioner with an SSOR-decomposition as in [1] resulting in the following spectral condition numbers on discretization level J for B-splines of order $k = 4$.

J	without preconditioner	with BPX-type preconditioner
4	3652	3.21
5	18966	3.50
6	100662	3.75
7	540558	4.11
8	2.92e6	4.86
9	1.58e7	5.96
10	8.66e7	7.35

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Introduction to the Workshop from my Perspective

Karsten Urban

My point of departure is Model Order Reduction using the Reduced Basis Method (RBM) for Parametrized Partial Differential Equations (PDEs). Originally, RBMs have been constructed, analysed and realized for coercive (stationary) problems and it was partly thought that an extension to evolutionary problems would be out of reach due to the exponential behaviour over time. However, variational space-time methods combined with uniformly stable discretizations and efficient tensorproduct solvers offered the path towards efficient RBM for parabolic problems. In turn, optimization and optimal control problems using model reduction was then possible.

These advances make it now possible to consider many other interesting question concerning weak variational formulations of PDE-constrained optimization problems such as transport, wave-type, Schrödinger equations, problems beyond optimal-Kolmogorov reduction, fast solvers, inclusion of data and nonlinear techniques including ML and AI. The workshop is designed to collect recent advances in these fields.

Chances and Challenges in PDE Constrained Optimization

Arnd Rösch
(joint work with Eduardo Casas, Mariano Mateos)

In this talk we discuss non-standard formulations of optimization problems. There are at least five reasons for designing a different optimization problem:

(1) desired properties of the control (or state): sparsity, smoothness, ...
(2) the PDE does not have the desired properties (existence and uniqueness of solutions, differentiability,...)
(3) the optimal control problem does not have the desired properties (for instance the existence of an optimal control cannot be guaranteed)
(4) the properties of the optimality system differ significantly from that one of the state equation.
(5) the PDE has not the properties expected from the physics (artificial viscosity was introduced to obtain a well-posed PDE)

We start with an example from a paper of Casas and Chrysafinos [1]. We aim to minimize

$$J(y,u) = \frac{1}{8}\int_0^T \|y - y_d\|^8_{L^4(\Omega)}\,dx + \frac{\gamma}{2}\|y(T) - y_\Omega\|^2_{L^2(\Omega)} + \frac{\lambda}{2}\|u\|^2_{L^2(Q)}$$

subject to the instationary Navier-Stokes equations

$$\begin{aligned} y_t - \nu\Delta y + (y\cdot\nabla)y + \nabla p &= f + u \quad \text{in } Q \\ \operatorname{div} y &= 0 \quad \text{in } Q \\ y(0) &= y_0 \quad \text{in } \Omega \\ y &= 0 \quad \text{on } \Sigma \end{aligned}$$

and additional box constraints for the control.

The used norms overcomes a fundamental problem of the Navier-Stokes equations. We have the existence of a weak solution. Due to the objective, the solution belongs to the space $L^8(0,T;L^4(\Omega)^3)$. Each weak solution belonging to the space $L^8(0,T;L^4(\Omega)^3)$ is a strong solution. Strong solutions are unique.

In the main part of the talk, we discuss a parabolic problem with a functional promoting directional sparsity, see [2, 3]. We want to minimize the functional

$$\min_{u\in L^\infty(Q)} J(u),$$

where $J(u) = F(u) + \mu j(u)$ with $\mu > 0$,

$$F(u) = \frac{1}{2}\int_Q (y_u - y_d)^2\,dx\,dt + \frac{\nu}{2}\int_Q u^2\,dx\,dt, \quad (\nu > 0)$$

and

$$j(u) = \|u\|_{L^1(\Omega;L^2(0,T))} = \int_\Omega \|u(x)\|_{L^2(0,T)}\,dx = \int_\Omega \Big(\int_0^T u^2(x,t)\,dt\Big)^{1/2} dx$$

subject to the semilinear parabolic equation

$$\begin{cases} \partial_t y + Ay + a(x,t,y) = u \ \text{ in } \ Q, \\ y = 0 \ \text{ on } \ \Sigma, \\ y(0) = y_0 \ \text{ in } \ \Omega. \end{cases}$$

As a first result we establish the first-order necessary optimality condition. If $\bar u$ is a local solution, then there exist $\bar y, \bar\varphi \in Y$, $\bar\lambda \in \partial j(\bar u)$ such that

$$\bar\varphi + \nu\bar u + \mu\bar\lambda = 0.$$

Moreover, $\bar u \in C(\bar Q)\cap H^1(Q)$ and the following relations hold

$$\|\bar u(x)\|_{L^2(0,T)} = 0 \Leftrightarrow \|\bar\varphi(x)\|_{L^2(0,T)} \le \mu \text{ (directional sparsity)}$$

$$\bar\lambda(x,t) = \begin{cases} -\dfrac{1}{\mu}\bar\varphi(x,t) & \text{if } x\in\Omega^0_{\bar u}, \\ \dfrac{\bar u(x,t)}{\|\bar u(x)\|_{L^2(0,T)}} & \text{if } x\in\Omega_{\bar u}. \end{cases}$$

Furthermore, $\bar\lambda$ is unique.

For the discretization we use a Discontionuous Galerkin method in time.

$$Y_h = \{z_h \in C_0(\bar{\Omega}) : \ z_{h|K} \in P_1(K) \ \forall K \in \mathcal{K}_h\},$$

$$\mathcal{Y}_\sigma = \{y_\sigma \in L^2(0,T;Y_h) : y_{\sigma|I_k} \in Y_h \ \forall k = 1,\dots,N_\tau\}.$$

We use the same space for the controls, i.e.,

$$U_\sigma = \mathcal{Y}_\sigma.$$

To get sparse controls for the discretized problem, we study the minimization problem

$$J_\sigma(u_\sigma) = \frac{1}{2}\int_Q |y_\sigma(u_\sigma) - y_d|^2 \, dx\, dt + \frac{\nu}{2}\|u-\sigma\|_\sigma^2 + \mu|u_\sigma|_\sigma,$$

where

$$\|u_\sigma\|_\sigma^2 = \sum_{j=1}^{N_h}\sum_{k=1}^{N_\tau} u_{jk}^2 \tau_k \int_\Omega e_j \, dx.$$

and

$$|u_\sigma|_\sigma = \sum_{j=1}^{N_h} \int_\Omega e_j \, dx \Big[\sum_{k=1}^{N_\tau} \tau_k u_{jk}^2\Big]^{1/2}.$$

The discrete problem is defined by

$$\min_{u_\sigma \in U_\sigma} J_\sigma(u_\sigma).$$

The sparsity of the discrete controls follows again from the optimality condition. Let $\bar{u}_\sigma$ be a local minimum of modified discrete problem, then $j \in I_\sigma^0$ if and only if

$$\Big(\int_0^T \Big[\frac{1}{\int_\Omega e_j \, dx}\int_\Omega \bar{\varphi}_\sigma e_j \, dx\Big]^2 dt\Big)^{1/2} \le \mu.$$

Moreover, we derive a priori error estimates of the form

$$\frac{\delta}{2}\|\bar{u}_\sigma - \bar{u}\|_{L^2(Q)}^2 \le c(\tau + h^2).$$

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Space-Time Finite Element Methods for Optimal Control Problems

Olaf Steinbach

(joint work with U. Langer, R. Löscher, F. Tröltzsch, H. Yang, M. Zank)

We consider the minimization of tracking type functionals

$$\mathcal{J}(u_\varrho, z_\varrho) = \frac{1}{2}\,\|u_\varrho - \overline{u}\|^2_{L^2(\mathcal{D})} + \frac{1}{2}\,\varrho\,\|z_\varrho\|^2_{Y^*}$$

subject to an abstract operator equation $Bu_\varrho = z_\varrho$. We assume that X and Y are Hilbert spaces satisfying $X \subset L^2(\mathcal{D}) \subset X^*$ and $Y \subset L^2(\mathcal{D}) \subset Y^*$, respectively, where $\mathcal{D} = \Omega \subset \mathcal{R}^n$, or $\mathcal{D} = Q = \Omega \times (0,T) \subset \mathcal{R}^{n+1}$. We assume that the linear operator $B : X \to Y^*$ is an isomorphism, satisfying

$$\|Bv\|_{Y^*} \le c_2^B\,\|v\|_X, \quad c_1^B\,\|v\|_X \le \sup_{0\neq q\in Y} \frac{\langle Bv, q\rangle_{\mathcal{D}}}{\|q\|_Y} \quad \text{for all } v \in X.$$

In addition, let $A : Y \to Y^*$ be linear, bounded, self-adjoint, and elliptic, such that $\|\cdot\|_{A^{-1}}$ defines an equivalent norm in Y^*. Hence we can consider the reduced minimization problem

$$\widetilde{J}(u_\varrho) = \frac{1}{2}\,\|u_\varrho - \overline{u}\|^2_{L^2(\mathcal{D})} + \frac{1}{2}\,\varrho\,\|Bu_\varrho\|^2_{A^{-1}} \to \min_{u_\varrho\in X}.$$

In the case of neither state nor control constraints the minimizer of the reduced cost functional is given as the unique solution of the gradient equation

$$u_\varrho + \varrho\,Su_\varrho = \overline{u} \quad \text{in } X^*,$$

where $S := B^*A^{-1}B : X \to X^*$ is self-adjoint and elliptic. Depending on the regularity of the target $\overline{u}$ we have the following estimates for the regularization error

$$\|u_\varrho - \overline{u}\|_{L^2(\mathcal{D})} \le \|\overline{u}\|_{L^2(\mathcal{D})}, \quad \|u_\varrho - \overline{u}\|_{L^2(\mathcal{D})} \le \varrho\,\|S\overline{u}\|_{L^2(\mathcal{D})}.$$

When introducing a conforming finite-dimensional ansatz space $X_h \subset X$ we can compute a (space-time) finite element approximation $u_{\varrho h} \in X_h$ satisfying

$$\langle u_{\varrho h}, v_h\rangle_{L^2(\mathcal{D})} + \varrho\,\langle Su_{\varrho h}, v_h\rangle_{L^2(\mathcal{D})} = \langle \overline{u}, v_h\rangle_{L^2(\mathcal{D})} \quad \text{for all } v_h \in X_h.$$

Since the operator $S = B^*A^{-1}B$ does not allow a direct evaluation in general, we introduce a second finite element space $Y_h \subset Y$ for its discretization. It is worth mentioning that the finite element spaces X_h and Y_h can be chosen independently of each other, we only assume some approximation properties of $X_h \subset X$, and $Y_h \subset Y$, respectively. Unique solvability and related error estimates follow due to the regularization term involved. When relating the error $\|u_\varrho - u_{\varrho h}\|_{L^2(\mathcal{D})}$ of the finite element discretization with the regularization error $\|u_\varrho - \overline{u}\|_{L^2(\mathcal{D})}$, we conclude an optimal choice for $\varrho = h^2$ independently of the regularity of $\overline{u}$.

As a first model problem we consider a distributed control problem subject to the Dirichlet problem for the Poisson equation in a bounded Lipschitz domain $\mathcal{D} = \Omega \subset \mathbb{R}^n$, where we have $X = Y = H^1_0(\Omega)$, $A = B = -\Delta : H^1_0(\Omega) \to H^{-1}(\Omega)$. In this case, the regularization error estimates as obtained in [10] were combined with finite element error estimates in [6]. Instead of a constant regularization

parameter $\varrho = h^2$ we may also use a mesh dependent function $\varrho(x) = h_\ell^2$ of local finite element mesh widths h_ℓ, see [2]. For a comparison with the more common approach of a control $z_\varrho \in L^2(\Omega)$, see [3]. However, for $Y = L^2(\Omega)$ the Laplace operator $B = -\Delta$ being an isomorphism implies $X = \{u \in H_0^1(\Omega) : \Delta u \in L^2(\Omega)\}$.

Based on the space-time finite element method as analyzed in [11] we have considered the numerical solution of distributed optimal control problems subject to the heat equation with homogeneous Dirichlet and initial conditions in the space-time domain $\mathcal{D} = Q = \Omega \times (0,T)$, see [4] for the control in $L^2(Q)$, and [5] for the energy regularization. Within the general setting we have the function spaces $Y = L^2(0,T;H_0^1(\Omega))$, $X = \{u \in Y : \partial_t u \in Y^*, u(x,0) = 0, x \in \Omega\}$, and $B = \partial_t - \Delta_x : X \to Y^*$, $A = -\Delta_x : Y \to Y^*$, see [7]. As an alternative, we can also consider a variational formulation of the heat equation in anisotropic Sobolev spaces [12], i.e., find $u_\varrho \in H_{0;0,}^{1,1/2}(Q)$ such that

$$\langle \partial_t u_\varrho, v\rangle_Q + \langle \nabla_x u_\varrho, \nabla_x v\rangle_{L^2(\Omega)} = \langle z_\varrho, v\rangle_Q \quad \text{for all } v \in H_{0;,0}^{1,1/2}(Q).$$

While the test and ansatz spaces differ in the zero initial and terminal conditions at $t = 0$ and $t = T$, respectively, we can introduce a modified Hilbert transformation $\mathcal{H}_T : H_{0;0,}^{1,1/2}(Q) \to H_{0;,0}^{1,1/2}(Q)$ to overcome this, see [12], i.e., $X = Y = H_{0;0,}^{1,1/2}(Q)$. Note that the space-time finite element discretization of such an approach results in a symmetric and positive definite stiffness matrix approximating the first-order time derivative, and a non-symmetric but positive definite approximation of the spatial Laplacian. Hence we conclude unique solvability for any conforming choice of the finite element space $X_h \subset X$.

As a last example we consider a distributed optimal control problem subject to the wave equation with homogeneous Dirichlet and initial conditions. The space-time variational formulation of the primal problem reads to find $u_\varrho \in H_{0;0,}^{1,1}(Q)$ such that

$$-\langle \partial_t u_\varrho, \partial_t v\rangle_{L^2(\Omega)} + \langle \nabla_x u_\varrho, \nabla_x v\rangle_{L^2(Q)} = \langle z_\varrho, v\rangle_{L^2(Q)} \quad \text{for all } v \in H_{0;,0}^{1,1}(Q).$$

Although unique solvability follows for $z_\varrho \in L^2(Q)$ this setting does not define an isomorphism onto $H_{0;0,}^{1,1}(Q)$. Moreover, a space-time finite element discretization using tensor-product ansatz spaces requires a CFL condition for the spatial and temporal mesh sizes to be satisfied, see [12]. However, when using the modified Hilbert transformation $\mathcal{H}_T : H_{0;0,}^{1,1}(Q) \to H_{0;,0}^{1,1}(Q)$ we end up with a variational formulation which is unconditionally stable for any choice of the space-time finite space $X_h \subset X$, see [9].

When considering the wave operator $\Box := \partial_{tt} - \Delta_x$ with homogeneous Dirichlet and initial conditions and setting $Y = H_{0;,0}^{1,1}(Q)$ we need to define X appropriately such that $B : X \to Y^*$ is an isomorphism. Following [13], we define the enlarged space-time domain $Q_- := \Omega \times (-T,T)$ as well as

$$\mathcal{H}(Q) := \Big\{ u = \widetilde{u}_{|Q} : \widetilde{u} \in L^2(Q_-),\ \widetilde{u}_{|\Omega\times(-T,0)} = 0,\ \Box\widetilde{u} \in [H_0^1(Q_-)]^* \Big\},$$

with the graph norm $\|u\|_{\mathcal{H}(Q)} := \sqrt{\|u\|^2_{L^2(Q)} + \|\Box\widetilde{u}\|^2_{[H^1_0(Q_-)]^*}}$. Then we define

$$X = \mathcal{H}_{0;0,}(Q) := \overline{H^{1,1}_{0;0,}(Q)}^{\|\cdot\|_{\mathcal{H}(Q)}}, \quad \|u\|_{\mathcal{H}_{0;0,}(Q)} = \|\Box\widetilde{u}\|_{[H^1_0(Q_-)]^*},$$

for which we can apply the general framework, see [8] for a detailed discussion.

Finally, we can also include state and control constraints, see [1] in the case of a distributed control problem for the Poisson equation with homogeneous Dirichlet conditions. This general setting also applies to boundary control problems as well as to problems with partial observation and partial control. Of interest is also the formulation and analysis of preconditioned iterative solution strategies which are robust with respect to adaptive mesh refinement, and an adaptive choice of the regularization parameter.

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Low-Rank Solution of Optimal Control Problems in Fluid Dynamics

Sergey Dolgov
(joint work with Peter Benner, Martin Stoll, Akwum Onwunta)

Low-rank tensor decompositions have become a valuable tool for compressed approximation and fast computation of high-dimensional tensors, including expansion coefficients of multivariate functions. The efficiency of tensor approximations hinges on the rate of convergence of an approximation with tensor ranks (which for hierarchical tensor decompositions are ranks of certain matrix reshapes of the tensor). It is now known that highly smooth or weakly correlated functions exhibit rapidly converging hierarchical tensor approximations. However, it used to be unclear whether this applies to functions arising in fluid dynamics (such as solutions to the Navier-Stokes equations), since in the most interesting regimes of turbulence, the solutions seem neither smooth nor locally correlated. We demonstrate that certain optimal control problems constrained by the Navier-Stokes equations do lend themselves to efficient tensor approximations, even at high Reynolds numbers. The key difference compared to the uncontrolled problem is that it is natural to optimize the flow such that the desired solution exhibits some regularity, for example, minimal vorticity. However, resolution of the optimality conditions requires the solution of a saddle-point coupled space-time problem, which is not amenable to standard tensor approximation algorithms such as Alternating Least Squares. We show a block version of this algorithm which preserves the well-posedness of the optimality conditions, and can solve a stochastic time-dependent problem with the asymptotic complexity of the deterministic problem, or a deterministic time-dependent problem with the asymptotic complexity of the stationary problem.

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Solution Concepts for Optimal Feedback Control of Nonlinear Differential Equations

Karl Kunisch

(joint work with Behzad Azmi, Dante Kalise, Donato Vasquez, and Daniel Walter)

Consider the optimal control problem:

$$\text{(OC)} \qquad \begin{cases} \min\limits_{u(\cdot)\in U_{ad}} & J(y,u) = \int\limits_0^\infty \ell(y(t)) + \frac{\gamma}{2}|u(t)|^2\, dt \\ \text{subject to} & \dot y(t) = f(y(t)) + Bu(t)\,, \quad y(0) = x \end{cases}$$

with $f(0) = \ell(0) = 0$, so that (OC) becomes an optimal stabilisation problem. The associated optimal value function is given by

$$V(x) := \min_{u(\cdot)\in U_{ad}} J(u(\cdot), x).$$

If V is a C^1 function, then it satisfies the Hamilton-Jacobi-Bellman (HJB) equation

$$\min_{u\in U_{ad}} \{\nabla V(x)^\top (f(x) + Bu) + \ell(x) + \frac{\gamma}{2}|u|^2\} = 0\,, \quad V(0) = 0, \nabla V(0) = 0. \tag{1}$$

If moreover U_{ad} is unconstrained then the optimal control in feedback form is given by

$$u^*(x) = -\frac{1}{\gamma} B^\top \nabla V(x)\,, \tag{2}$$

and the HJB eqation is of the form

$$\nabla V(x)^\top f(x) - \frac{1}{2\gamma}\nabla V(x)^\top BB^\top \nabla V(x) + \ell(x) = 0\,.$$

The resulting closed loop equation is given by:

$$\dot y(t) = Ay(t) - \frac{1}{\gamma} BB^\top \nabla V(y(t))\,, \quad y(0) = x.$$

We observe that (1) is a first order hyperbolic in a dimension which is determined by the state-space dimension of the dynamical system appearing in (OC). In particular if the dynamical system arises from a grid-based discretisation of a partial differential equation, resulting in an ordinary differential equation of dimension d and (OC) is discretized over a grid of N nodes in each dimension, we arrive at a nonlinear system of order N^d unknowns, a severe case of a curse of dimensionality. Consequently, the development of techniques which allow to obtain approximations to the solution of the HJB equation is of fundamental importance. We subsequently address two such techniques.

Data driven approach

We assume the availability of a gradient enriched data set: $\{\mathbf{x_j}, V(\mathbf{x_j}), \nabla V(\mathbf{x_j})\}_{j=1}^{N_D}$, where $\{\mathbf{x_j}\}_{i=1}^{N_D}$ denotes a sampled data set of initial conditions in state space. The values of $V(\mathbf{x_j}), \nabla V(\mathbf{x_j})\}_{j=1}^{N_D}$ are obtained in the course of open loop solves of the optimal control problem. It is of importance to recall that in the process of each

open loop solve for the generation of $V(\mathbf{x_j})$, the gradient $\nabla V(\mathbf{x_j})$ is computed as a by-product via the adjoint state. Next we choose a polynomial model for the value function

$$V_\theta(\mathbf{x}) = \sum_{i=1}^{q} \theta_i \Phi_i(\mathbf{x}),$$

where $\Phi_i(\mathbf{x})$ are ansatz-functions, for example chosen in separable form with $\Phi_\mathbf{i}(\mathbf{x}) := \Pi_{j=1}^d \phi_{i_j}(x_j)$ with $\phi_{i_j}(\cdot)$ monomials. Denoting the data by $V = (V_j)_{i=1}^{N_D}$, and setting $V_j = V(\mathbf{x_j})$, and abbreviating $\Phi_{j,i} = \Phi_i(\mathbf{x_j})$ we consider the LASSO regression problem for the unknown coefficients θ_i, given by

$$\min_{\theta \in \mathbb{R}^q} \|(\Phi, \nabla\Phi)^\top \theta - (V(x_\bullet), \nabla V(x_\bullet))^\top\|_2^2 + \lambda \|\theta\|_1. \tag{3}$$

The $\|\theta\|_1-$ penalty term is introduced to enhance sparsity of the coefficients and to speed up interpolation procedures. Once (3) is solved the optimal feedback control can be determined through:

$$u^*(\mathbf{x}) = \operatorname*{argmin}_u \ \{\langle f(\mathbf{x}) + B(u), \nabla V_\theta(\mathbf{x})\rangle + \ell(\mathbf{x}) + \frac{1}{2}|u|^2 .$$

In numerical practice for the approximation of the value function and its gradient, and ultimately for the optimal control in feedback form, this procedure has proved to be effective and reliable. More details and examples are reported on in [1].

Learning based technique

In the learning approach we search for a feedback function F which minimizes the original cost-functional J that appeared in (OC) along an ensemble of trajectories with initial conditions in a compact set Y_0. Note that as a consequence of the Bellman principle the training does not only occur for the samples in Y_0 but additionally for each state $y(t; y_0)$ visited by a trajectory originating from $y_0 \in Y_0$.

$$(\mathcal{P}) \qquad \begin{cases} \min\limits_{\substack{F\in\mathcal{H},\\ \mathbf{y}\in L^\infty_\mu(Y_0,W_\infty)}} j(\mathbf{y}, F) = \displaystyle\int_{Y_0} J(\mathbf{y}(y_0), F(\mathbf{y}(y_0)))\, d\mu(y_0), \\ \dfrac{d}{dt}\mathbf{y}(y_0) = f(\mathbf{y}(y_0)) + BF(\mathbf{y}(y_0)), \quad \text{for } \mu\text{-a.e. } y_0 \in Y_0, \\ |y|_{L^\infty_\mu(Y_0,W_\infty)} \le M_0 \end{cases}$$

where $W_\infty = \{\, y \in L^2(0,\infty;\mathbb{R}^n) \mid \dot{y} \in L^2(0,\infty;\mathbb{R}^n) \,\}$, $B \in \mathbb{R}^{n\times m}$, $(Y_0, \mathcal{A}, \mu)$ is a complete probability space. Here $\mathcal{H}$ denotes a Banach space of at least Lipschitz continuous feedback function. Since the value function is Lipschitz continuous under mild conditions on f and ℓ, existence to $(\mathcal{P})$ is straightforward since the optimal control in feedback form is given by (2). In [2] and [4] we investigate the approximation of $(\mathcal{P})$ by means of replacing $\mathcal{H}$ by deep neural networks and polynomial functions, respectively. Convergence results are provided and numerical results illustrate the feasibility and strengths of the approach.

In [3, 5] related questions are investigated for finite horizon problems. In this case the value function depends on time and space and consequently additional

considerations are necessary concerning its approximation. In [3], the cost in the finite horizon version of $(\mathcal{P})$ is augmented by the running cost of the value function and its gradient.

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On Optimal Control Problems with State Constrained Parabolic Partial Differential Equation

Ira Neitzel

We begin this talk by reviewing results on optimal control problems governed by quasilinear parabolic partial differential equations and additional inequality constraints on the state given by

$$\begin{aligned} &\text{Minimize } J(u,q) \\ \partial_t u + A(u)u &= Bq && \text{in } I\times\Omega, \\ u|_{\Gamma_D} &= 0, && \text{in } I\times\Gamma_D, \\ u(0) &= u_0, && \text{in } \Omega \\ q_a \le q \le q_b, &\quad u\in U_{\mathrm{ad}}, \end{aligned}$$

obtained by Hoppe and the speaker in [6]. The problem features a uniformly elliptic operator $A(u)$ of the form

$$A(u) = -\nabla\cdot\xi(u)\mu\nabla,$$

and an operator B that is included to allow control functions acting either in the whole domain or on a Neumann part of the boundary, either depending on space and time or purely on time. The set U_{ad} may be given in two different ways, either by

$$U_{\mathrm{ad}} = \{u\in C(\bar I\times\bar\Omega)\colon u_a(t,x)\le u(t,x)\le u_b(t,x)\ \forall\,(t,x)\in\bar I\times\bar\Omega\},$$

or by

$$U_{\mathrm{ad}} = \{u\in L^1(I,C(\bar\Omega))\colon u_a(x)\le \int_0^T u(t,x)\,dt\le u_b(x)\ \forall\, x\in\bar\Omega\}.$$

For the precise setting, we refer to [6]. We present an overview about second order sufficient conditions for this model problem, see also the talk [10, Oberwolfach Report 9, 2021], focussing on the need of an interplay between different control structures, different constraint structures, and different regularity assumptions from either [3] or [1], that deal with quasilinear purely control constrained problems under different assumption. The latter work by Bonifacius and the speaker builds on regularity results for parabolic equations from e.g.[8]. In this talk, particular emphasis lies on the structure of the control functions, particularly on finitely many time-dependent controls

$$Bq = \sum q_i(t)e_i(x)$$

for given, fixed functions e_i, and different constraint structure displayed in the two different choices of U_{ad}, that we will exploit further in a regularization context for the model problem

$$\begin{aligned} &\text{Minimize } J(u,q) \\ \partial_t u - \Delta u &= q(t)e(x) && \text{in } I\times\Omega, \\ u|_{\Gamma_D} &= 0, && \text{in } I\times\Gamma_D, \\ u(0) &= u_0, && \text{in } \Omega \\ q_a \le q \le q_b, &\quad u \le u_b \end{aligned}$$

with tracking type objective and linear state equation. We first review some of the challenges of state constraints that are well-known since the meanwhile classical work of Casas [2]. In essence, using classical Slater type techniques to prove necessary optimality conditions leads to the appearance of measures in the first order optimality conditions, leading to lower regularity of the adjoint state, even though this can be improved in some cases, cf. e.g. [4]. These regularity issues also influence the discussion of second order sufficient conditions and further question of (numerical) analysis.

Several regularization methods are meanwhile well-established. We focus on an extension of a method originally developed for boundary control problems in [13] for elliptic problems or by Tröltzsch and the speaker in [12] for parabolic problems, i.e. we apply the adjoint S^* of the control-to-state operator S to an auxiliary control v, that is defined in the whole space-time domain, setting $q_{\mathrm{reg}} = S^*v$, thus $u = SS^*v$. The state constraints are then regularized by a standard Lavrentiev Ansatz, [9],

$$\lambda v + u \le u_b \quad \text{a. e. in } I\times\Omega$$

and can be transferred into easier control bounds. By this ansatz, however, additional pure control bounds become artificial state constraints

$$q_a \le S^*v \le q_b.$$

For purely time dependent controls, control constraints will become averaged in space and pointwise in time state constraints, i.e. an auxiliary variable z solving

an adjoint equation is restricted to the set Z_{ad} defined by

$$Z_{\text{ad}} = \{z \in C([0,T], L^1(\Omega)) \colon \int_\Omega z(t,x)e(x)\,dx \le u_b(t)\ \forall\, t \in [0,T]\}.$$

Problems with these type of constraints and additional control constraints have been analyzed in [7] For more details regarding the application to our model problem, we refer to [11].

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High-Order Polytopic Discontinuous Galerkin Methods for Radiation Transport Problems

Paul Houston

(joint work with Matthew E. Hubbard, Thomas J. Radley, Oliver J. Sutton, and Richard S. J. Widdowson)

The linear Boltzmann transport problem describes the flow of particles through a scattering and absorbing medium, and is commonly employed within a wide range of application areas, including medical imaging, radiotherapy treatment planning,

and the design of nuclear reactors, for example. Here, we consider the numerical approximation of the stationary form of the problem, seeking a solution which is a function of up to six independent variables. The high dimensionality of this problem means that the development of efficient discretisation schemes is imperative.

To this end, we let $\Omega \subset \mathbb{R}^d$, $d \geq 2$, denote an open bounded polyhedral spatial domain with boundary $\partial\Omega$, $\mathbb{S} = \{\boldsymbol{\mu} \in \mathbb{R}^d : |\boldsymbol{\mu}|_2 = 1\}$ denote the surface of the d-dimensional unit sphere and $\mathbb{E} = \{E \in \mathbb{R} : E \geq 0\}$ the real half line. Writing $\mathcal{D} = \Omega \times \mathbb{S} \times \mathbb{E}$ we seek to find $u : \mathcal{D} \to \mathbb{R}$ such that

$$\begin{aligned} \boldsymbol{\mu} \cdot \nabla_{\mathbf{x}} u(\mathbf{x}, \boldsymbol{\mu}, E) + (\alpha(\mathbf{x}, \boldsymbol{\mu}, E) + \beta(\mathbf{x}, \boldsymbol{\mu}, E))u(\mathbf{x}, \boldsymbol{\mu}, E) &= \mathcal{S}[u](\mathbf{x}, \boldsymbol{\mu}, E) \\ &\quad + f(\mathbf{x}, \boldsymbol{\mu}, E) \text{ in } \mathcal{D}, \\ u(\mathbf{x}, \boldsymbol{\mu}, E) &= g_{\mathrm{D}}(\mathbf{x}, \boldsymbol{\mu}, E) \text{ on } \Gamma_{\mathrm{in}}, \end{aligned} \tag{1}$$

where $f, g, \alpha, \beta : \mathcal{D} \to \mathbb{R}$ are given data terms, $\nabla_{\mathbf{x}}$ is the spatial gradient operator, and $\Gamma_{\mathrm{in}} = \{(\mathbf{x}, \boldsymbol{\mu}, E) \in \bar{\mathcal{D}} : \mathbf{x} \in \partial\Omega \text{ and } \boldsymbol{\mu} \cdot \boldsymbol{n} < 0\}$ denotes the inflow boundary of $\mathcal{D}$, where $\boldsymbol{n}$ denotes the unit outward normal vector on the boundary $\partial\Omega$. The action of the *scattering operator* applied to the solution u is denoted by

$$\mathcal{S}[u](\mathbf{x}, \boldsymbol{\mu}, E) = \int_{\mathbb{E}} \int_{\mathbb{S}} \theta(\mathbf{x}, \boldsymbol{\eta} \to \boldsymbol{\mu}, E' \to E) u(\mathbf{x}, \boldsymbol{\eta}, E') \, d\boldsymbol{\eta} \, dE',$$

where θ is a specified scattering kernel, and $\beta(\mathbf{x}, \boldsymbol{\mu}, E) = \int_{\mathbb{E}} \int_{\mathbb{S}} \theta(\mathbf{x}, \boldsymbol{\mu} \to \boldsymbol{\eta}, E \to E') \, d\boldsymbol{\eta} \, dE'$.

In this talk, we consider the development of *hp*-version discontinuous Galerkin finite element methods (DGFEMs) for the numerical approximation of (1), where the spatial, angular, and energy components of the solution are approximated in a unified manner. In many applications, particularly those arising in medical physics, the spatial domain may be highly complicated; to deal with such strong complexity of the physical geometry, in an efficient manner, we admit the use of general polygonal/polyhedral (polytopic) meshes; see, for example, [1, 2, 3] and the references cited therein. The exploitation of a unified DGFEM discretisation of the linear Boltzmann problem over the entire computational domain ensures that the resulting scheme is naturally high-order. We note that historically, there has largely been a single standard approach to energy discretisation known as the multigroup approximation; see [4, Chapter 2] and the references cited therein. Here the essential idea is to approximate the solution by a piecewise constant function with respect to a finite number of nonoverlapping energy groups, which limits the accuracy of the resulting numerical method to first-order.

The stability and *hp*–version *a priori* error analysis of the proposed scheme is undertaken based on deriving suitable *hp*–approximation estimates, together with a novel inf-sup bound. By employing a judicious selection of the quadrature and local polynomial bases in the angular and energy domains, highly efficient solvers for the proposed DGFEM may be designed which are naturally parallelisable. In this way the underlying scheme may be implemented as a generalised multigroup discrete ordinates method. Numerical experiments are presented to highlight the accuracy of the proposed method, as well as to benchmark with more standard kinetic Monte Carlo simulations.

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Shape Optimization in Diffusive Optical Tomography

Johannes Tausch

(joint work with Helmut Harbrecht)

The talk is concerned with an inverse problem of the heat equation. The goal is to determine the diffusion and absorption coefficients α and β in the overdetermined boundary value problem of the heat equation

$$\begin{aligned} \partial_t u - \nabla\cdot \alpha\nabla u + \beta u = 0 \quad & \text{in } \Omega\times(0,T),\\ u = f \quad & \text{on } \Sigma\times(0,T),\\ \partial_\nu u = g \quad & \text{on } \Sigma\times(0,T),\\ u = 0 \quad & \text{in } \Omega\times\{0\}. \end{aligned}$$

Here $\Sigma=\partial\Omega$ and ν is the normal on Σ. The domain $\Omega\subset\mathbb{R}^d$ is bounded and contains a smooth and possibly time dependent subdomain $\Omega_1(t)$ with $\bar\Omega_1(t)\subset\Omega$ and boundary $\Gamma(t)=\partial\Omega_1(t)$. Here it is assumed that there is a sufficiently smooth isomorphism $\kappa:\mathbb{R}^d\times[0,T]\to\mathbb{R}^d$ and a smooth domain $\hat\Omega$ such that $\Omega_1(t)=\kappa(\hat\Omega,t)$. The coefficients are piecewise constants for a fixed time t. Specifically, if $\Omega_2(t):=\Omega\setminus\bar\Omega_1(t)$ then

$$\alpha(x,t)=\begin{cases}\alpha_1 & \text{in } \Omega_1(t),\\ \alpha_2 & \text{in } \Omega_2(t),\end{cases}\qquad \beta(x,t)=\begin{cases}\beta_1 & \text{in } \Omega_1(t),\\ \beta_2 & \text{in } \Omega_2(t).\end{cases}$$

We assume that $\alpha_1,\alpha_2,\beta_1$ and β_2 are known and determine the shape of the domain $\Omega_1(t)$.

The motivation for studying this problem arises in diffusion optical tomography, which is a medical imaging technique where an object occupied by Ω_1 is reconstructed from light transmitted and scattered through the object Ω. Here u is the photon density and the boundary conditions correspond to the measured signal and source strengths of an impinging infrared laser.

This inverse problem is formulated as a shape optimization problem. Here one solves the Dirichlet problem for an assumed $\Omega_1(t)$ and minimizes the functional

$$J(\Omega_1) = \frac{1}{2}\int_0^T \int_\Sigma (\partial_\nu u - g)^2 \, d\sigma dt.$$

For a time independent Ω_1 the uniqueness of the inverse problem and the existence of a shape derivative was established in [1]. In addition, techniques for a time dependent Ω_1 in the context of the inclusion problem (i.e., Dirichlet conditions instead of transmission conditions on $\Gamma(t)$) have been developed in [2].

In light of this previous work, it is possible to derive the shape derivative and the adjoint equation for the present problem. Specifically, consider the perturbation of the inner domain by the vector field

$$\psi_\epsilon(x,t) = x + \epsilon V(x,t)$$

where V is $C_0^2(\bar{\Omega})$ and $V = 0$ in a neighborhood of Σ. Then for $\epsilon > 0$ sufficiently small ψ_ϵ maps Ω to Ω one-to-one and onto. Moreover, the perturbed coefficients are $\alpha_\epsilon = \alpha \circ \psi_\epsilon^{-1}$ and $\beta_\epsilon = \beta \circ \psi_\epsilon^{-1}$. With the bilinear form

$$a_\epsilon(w,v) = \int_0^T \int_\Omega \partial w_t v + \alpha_\epsilon \nabla w \nabla v + \beta_\epsilon w v \, dxdt$$

where $(w,v) \in \check{H}_0^{1,\frac{1}{2}}(\Omega \times (0,T)) \times \hat{H}_0^{1,\frac{1}{2}}(\Omega \times (0,T))$, the variational form of the Dirichlet problem with the perturbed coefficients is: Find $u_\epsilon \in \check{H}_0^{1,\frac{1}{2}}(\Omega \times (0,T))$ such that

$$a_\epsilon(u_\epsilon, v) = f(v), \quad \forall\, v \in \hat{H}_0^{1,\frac{1}{2}}(\Omega \times (0,T)). \tag{1}$$

Here $f(v) = \int_0^T \int_\Omega f v \, dxdt$, where f is the extension of the Dirichlet data into the domain.

The shape derivative is as usual defined as $u' := \lim_{\epsilon \to 0}(u_\epsilon \circ \psi_\epsilon^{-1} - u_0)/\epsilon$. To describe the regularity of the shape derivative define the space-time tubes

$$Q_k = \{(\Omega_k(t), t) : \ t \in (0,T)\}, \quad k \in \{1,2\}.$$

Further, the Sobolev spaces $H^{r,s}(Q_k)$, $k \in \{1,2\}$ consist of the functions w such that the pullback $w \circ \kappa^{-1}$ is in $H^{r,s}(\hat{\Omega} \times (0,T))$. Then it is possible to show that $u'|_{Q_k} \in \check{H}^{1,\frac{1}{2}}(Q_k)$, $k \in \{1,2\}$ with $u' = 0$ on Σ. Moreover, assuming that the solution of (1) has additional regularity $u_\epsilon|_{Q_k} \in \check{H}_0^{2,1}(Q_k)$, $k \in \{1,2\}$, then u' satisfies

$$a_0(u', p) = -a'(u_0, p)$$

where

$$a'(u_0,p) := \int_0^T \int_{\Gamma(t)} V_\nu \Big([\partial_t u_0]_\pm p + [\alpha \nabla u_0 \cdot \nabla p]_\pm + [\beta]_\pm u_0 p \Big) d\sigma \, dt \tag{2}$$

for all $p \in \hat{H}_0^{1,\frac{1}{2}}(\Omega \times (0,T))$ and $p|_{Q_k} \in \hat{H}_0^{2,1}(Q_k)$. Here, V_ν is the normal component of the vector field V and $[\cdot]_\pm$ is the jump across the interface $\Gamma(t)$. The

derivative of the functional $J'(\Omega_1; V) = \lim_{\epsilon\to 0}(J(\psi_\epsilon\Omega_1) - J(\Omega_1))/\epsilon$ is given by

$$J(\Omega_1) = \int_0^T \int_\Sigma (\partial_\nu u - g)\, \partial_\nu u'\, d\sigma dt.$$

This suggests that the adjoint equation is

$$\begin{aligned} -\partial_t p - \nabla\cdot \alpha\nabla p + \beta p &= 0 \quad \text{in } \Omega\times(0,T),\\ p &= \partial_\nu u - g \quad \text{on } \Sigma\times(0,T),\\ p &= 0 \quad \text{in } \Omega\times\{T\}. \end{aligned} \tag{3}$$

It follows from Green's second identity, the fact that $u' = 0$ on Σ and from (3) that

$$J'(\Omega_1; V) = \int_0^T \int_\Sigma \partial_\nu u' p - \partial_\nu p u' d\sigma dt = a_0(u', p) = -a'(u_0, p)$$

Thus with the solution of the adjoint equation (3) the the dependence of $J'(\Omega_1; V)$ on the vector field V is made explicit in (2).

The remainder of the talk is focused on solving the state and adjoint equations unsing boundary integral methods.

For the domains Ω_1 and Ω_2 the Green's function is

$$G_k(x, y, t, s) = \frac{\exp(-\beta_k(t-s))}{[4\pi\alpha_k(t-s)]^{\frac{d}{2}}} \exp\left(-\frac{|x-y|^2}{4\alpha_k(t-s)}\right), \quad k = 1, 2.$$

Integral equations for the boundary data can be derived by taking traces and normal traces of the Green's representation formula. In the case of the heat equation for moving domains this formula contains additional terms that involve normal velocity of the boundary n_t, which can be expressed by the following modification of the normal trace operator, see [3]

$$\gamma_1^{\pm}\phi := \frac{\partial\phi}{\partial\nu_s} \pm \frac{1}{2} v_t \phi \tag{4}$$

With this, the weakly and strongly singular Green's integral equations are

$$\begin{aligned} \frac{1}{2} u(x,t) &= \mathcal{V}\gamma_1^- u(x,t) - \mathcal{K}u(x,t),\\ \frac{1}{2}\gamma_1^- u(x,t) &= \mathcal{K}'\gamma_1^- u(x,t) - \mathcal{D}u(x,t), \end{aligned}$$

where $x \in \partial\Omega_k(t)$. Here the thermal layer potentials also involve the modified trace operator, thus

$$\mathcal{V}\phi(x,t) = \int_0^t \int_{\partial\Omega_k(s)} G(x,y,t,s)\phi(y,s)\, d\sigma_y ds\,,$$

$$\mathcal{K}\phi(x,t) = \int_0^t \int_{\partial\Omega_k(s)} \gamma_{1,y}^+ G(x,y,t,s)\phi(y,s)\, d\sigma_y ds\,,$$

$$\mathcal{D}\phi(x,t) = \mathrm{pf}\int_0^t \int_{\partial\Omega_k(s)} \gamma_{1,x}^- \gamma_{1,y}^+ G(x,y,t,s)\phi(y,s)\, d\sigma_y ds\,.$$

The hypersingular operator $\mathcal{D}$ has to be understood as a finite-part integral. Enforcing the boundary condition on Σ and the continuity of the functions and fluxes on Γ then leads to a system of integral equations. The talk will conclude with a discussion of a Nyström discretization method to solve the state and adjoint equations which eventually leads to an efficient gradient based minimization method to compute the optimal shape Ω_1.

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Shape Optimization for Time-Dependent Domains

Helmut Harbrecht

(joint work with Rahel Brügger and Johannes Tausch)

1. Introduction

We are concerned with the solution of time-dependent shape optimization problems. Specifically, we consider the heat equation in a domain which might change over time. We develop the respective shape calculus by means of the perturbation of identity. We derive the local shape derivative and compute Hadamard's shape gradient in case of both, domain integrals and boundary integrals. As particular examples, we consider the one-phase Stefan problem and the detection of a time-dependent inclusion. We discuss the numerical solution of these problems and present respective results.

2. Shape calculus

2.1. **Space-time tubes.** We shall introduce space-time tubes. For every point of time $t \in [0,T]$, we have a time-dependent spatial domain which we denote by $\Omega_t \subset \mathbb{R}^d$, $d \geq 2$. This spatial domain has a time-dependent spatial boundary $\Gamma_t := \partial\Omega_t$. For every point of time t, we assume to have a smooth C^2-diffeomorphism $\boldsymbol{\kappa}$, which maps the reference domain Ω_{ref} onto the time-dependent domain Ω_t. We write

$$\boldsymbol{\kappa} : [0,T] \times \overline{\Omega}_{\mathrm{ref}} \to \mathbb{R}^d, \quad (t,\mathbf{x}) \mapsto \boldsymbol{\kappa}(t,\mathbf{x}) \tag{1}$$

to emphasize the dependence of the mapping $\boldsymbol{\kappa}$ on the time, where we have $\boldsymbol{\kappa}(t,\Omega_{\mathrm{ref}}) = \Omega_t$. Here, $\boldsymbol{\kappa} \in C^2([0,T]\times\overline{\Omega}_{\mathrm{ref}})$ and we assume the uniformity condition

$$\|\boldsymbol{\kappa}(t,\mathbf{x})\|_{C^2([0,T]\times\overline{\Omega}_{\mathrm{ref}};\mathbb{R}^d)}, \|\boldsymbol{\kappa}(t,\mathbf{x})^{-1}\|_{C^2([0,T]\times\overline{\Omega}_{\mathrm{ref}};\mathbb{R}^d)} \leq C_{\boldsymbol{\kappa}} \tag{2}$$

for some constant $C_{\boldsymbol{\kappa}} > 0$. To reduce the technical level of the ensuing discussion, we assume that Ω_0 has a C^2-smooth boundary which implies that the boundary of Ω_t has the same regularity. We finally define the space-times tube

$$Q_T := \bigcup_{0<t<T} \big(\{t\} \times \Omega_t\big).$$

with mantle

$$\Sigma_T := \bigcup_{0<t<T} \big(\{t\} \times \Gamma_t\big).$$

2.2. **Perturbation of identity.** In order to apply the traditional shape calculus, we would like to perturb the tube. To this end, we consider a vector field $\mathbf{Z}(t,\mathbf{x})$, which is C^2-smooth, to generate the perturbation of identity $\mathbf{I} + s\mathbf{Z}$. It yields a new tube

$$Q_T^s = \bigcup_{0<t<T} \big(\{t\} \times (\mathbf{I} + s\mathbf{Z})(\Omega_t)\big).$$

Notice that the perturbations under consideration are horizontal, meaning that we consider perturbations of $(t,\boldsymbol{\kappa})$ of the type $(0,\mathbf{Z})$. Moreover, $\mathbf{I} + s\mathbf{Z}$ should satisfy a uniformity condition as in (2). An illustration of our setting is found in Figure 1.

2.3. **Local shape derivative.** Given a sufficiently smooth function f, we shall consider the heat equation on the space-time tube

$$\begin{aligned} (\partial_t - \Delta)u &= f \quad && \text{in } Q_T, \\ u &= 0 && \text{on } \Sigma_T, \\ u(0,\cdot) &= 0 && \text{in } \Omega_0. \end{aligned} \tag{3}$$

Note that the solution theory to this initial boundary value problem has been studied in [3] by using boundary integral operators and associated integral equations.

As in the time-independent case, we can define non-cylindrical material and local shape derivatives of (3). The material derivative $\dot{u}[\mathbf{Z}]$ is defined as

$$\dot{u}[\mathbf{Z}] = \lim_{s\to 0} \frac{u_t^s \circ (\mathbf{I} + s\mathbf{Z}) - u_t}{s}, \tag{4}$$

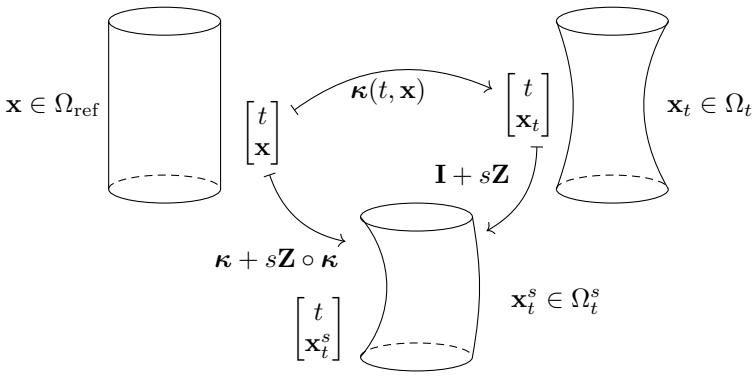

FIGURE 1. Perturbation of identity in the Lagrangian setting.

while the local shape derivative $\delta u = \delta u[\mathbf{Z}]$ in the direction $\mathbf{Z}$ is formally given by

$$\delta u[\mathbf{Z}](t, \mathbf{x}) = \lim_{s \to 0} \frac{u_t^s(t, \mathbf{x}) - u_t(t, \mathbf{x})}{s}, \quad (t, \mathbf{x}) \in Q_T^s \cap Q_T.$$

Here, u_t^s denotes the state computed on the perturbed domain Q_T^s and u_t the state computed on Q_T. These two non-cylindrical derivatives are connected by the relation

$$\delta u[\mathbf{Z}] = \dot{u}[\mathbf{Z}] - \nabla v \cdot \mathbf{Z}.$$

Theorem. *The local shape derivative of the state u from (3) in the direction $\mathbf{Z}$ is given as the solution of the partial differential equation*

$$\begin{aligned} (\partial_t - \Delta)\delta u &= 0 && \text{in } Q_T, \\ \delta u &= -\langle \mathbf{Z}, \mathbf{n} \rangle \frac{\partial v}{\partial \mathbf{n}} && \text{on } \Sigma_T, \\ \delta u(0, \cdot) &= 0 && \text{in } \Omega_0. \end{aligned}$$

2.4. **Shape functionals.** We shall next comment on the derivative of shape functionals. For the domain integral

$$J(Q_T) = \int_0^T \int_{\Omega_t} u \, \mathrm{d}\mathbf{x} \, \mathrm{d}t,$$

one finds the shape gradient

$$\delta J(Q_T)[\mathbf{Z}] = \int_0^T \int_{\Omega_t} \delta u[\mathbf{Z}] \, \mathrm{d}\mathbf{x} \, \mathrm{d}t + \int_0^T \int_{\Gamma_t} u \langle \mathbf{Z}, \mathbf{n} \rangle \, \mathrm{d}\sigma \, \mathrm{d}t.$$

Whereas, for the boundary integral

$$J(Q_T) = \int_0^T \int_{\Gamma_t} u \, \mathrm{d}\sigma \, \mathrm{d}t, \tag{5}$$

one has the shape gradient

$$\delta J(Q_T)[\mathbf{Z}] = \int_0^T \int_{\Sigma_t} \delta u[\mathbf{Z}] \, \mathrm{d}\sigma \, \mathrm{d}t + \int_0^T \int_{\Gamma_t} \left(\frac{\partial u}{\partial \mathbf{n}} + \mathcal{H}_{\mathbf{x}} u \right) \langle \mathbf{Z}, \mathbf{n} \rangle \, \mathrm{d}\sigma \, \mathrm{d}t.$$

We emphasize that the shape functional (5) of boundary integral form is different from

$$J(Q_T) = \int_{\Sigma_T} u \, \mathrm{d}\vec{\sigma},$$

whose shape gradient differs from the above one.

3. Applications

In [1], the classical Stefan problem has been reformulated as a shape optimization problem. Namely, motivated by [4] in the one-dimensional setting, we considered the heat equation (3) and enforced the Stefan condition by tracking the Neumann data correspondingly. In contrast, [2] was concerned with a time-dependent shape optimization problem for the heat equation. Namely, from the measurements of the temperature and the heat flux at the outer, fixed boundary of a body we intended to reconstruct an unknown, time-dependent void of zero temperature. We refer to the respective articles for all the details.

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Neural Operators for Partial Differential Equations: Challenges and Results

Ivan Oseledets

(joint work with V. Fanaskov, A. Rudikov, T. Yu)

In this talk I discussed two papers. The first one ist "Spectral Neural Operators". It discussed how to approximate function-to-function mapping that has discretization invariance and zero-shot superresolution. Second is a way to augment trraining data for N.D. by random variable transformations. The improvement is significant.

A Space-Time Variational Method for Linear Parabolic Optimal Control Problems –Well-Posedness, Stability and Numerical Solution

Nina Beranek

(joint work with Alexander Reinhold, Karsten Urban)

Formulation. We consider an optimal control problem with quadratic cost function constrained by a linear parabolic partial differential equation. We impose the parabolic partial differential equation in a space-time variational formulation, e.g. [4], where space and time are both treated in a variational sense. The space-time formulation of the parabolic problem takes the form

$$\text{(1)} \qquad \text{given } u \in \mathcal{U}, \text{ find } y \in \mathcal{Y}: \quad b(y,z) = f(u,z) + h(z) \quad \text{for all } z \in \mathcal{Z},$$

where $\mathcal{Y}$, $\mathcal{Z}, \mathcal{U}$ denote some appropriate Lebesgue–Bochner spaces and $b : \mathcal{Y} \times \mathcal{Z} \to \mathbb{R}$, $f : \mathcal{U} \times \mathcal{Z} \to \mathbb{R}$ and $h : \mathcal{Z} \to \mathbb{R}$ are continuous (bi)linear forms. In the optimal control framework the space $\mathcal{Y}$ arises as state space and the space $\mathcal{U}$ is the control space. The quadratic cost function can be written in the form

$$J : \mathcal{Y} \times \mathcal{U} \to \mathbb{R}, \quad J(y,u) = \frac{\omega}{2} \cdot d(y - y_d, y - y_d) + \frac{\lambda}{2} \cdot n(u,u),$$

where $\omega, \lambda > 0$ are some weighting factors, $d : \mathcal{D} \times \mathcal{D} \to \mathbb{R}$ and $n : \mathcal{U} \times \mathcal{U} \to \mathbb{R}$ are some bilinear forms and $y_d \in \mathcal{D} \supseteq \mathcal{Y}$ is the desired state.

Existence and uniqueness. The continuous left-hand side $b : \mathcal{Y} \times \mathcal{Z} \to \mathbb{R}$ of the state equation (1) satisfies an inf-sup condition of kind

$$\beta := \inf_{0 \neq y \in \mathcal{Y}} \sup_{0 \neq z \in \mathcal{Z}} \frac{|b(y,z)|}{\|y\|_{\mathcal{Y}} \, \|z\|_{\mathcal{Z}}} = \inf_{0 \neq z \in \mathcal{Z}} \sup_{0 \neq y \in \mathcal{Y}} \frac{|b(y,z)|}{\|y\|_{\mathcal{Y}} \, \|z\|_{\mathcal{Z}}} > 0,$$

which, applying the Banach–Nečas–Babuška theorem, e.g. [2], ensures the well-posedness (in the sense of Hadamard) of the state equation (1) in space-time form. In our setting one can realize that the inf-sup constant is optimal, i.e., $\beta = 1$.

The well-posedness of the state equation guarantees that the state equation assigns a unique state $y \in \mathcal{Y}$ to each control $u \in \mathcal{U}$ which allows to formulate the optimal control problem in a (on the control) reduced form. Existence and uniqueness of an optimal solution can be shown by applying a standard result from optimal control theory requiring that the reduced cost function is weakly lower semicontinuous, bounded and strictly convex.

Optimality system. Following the optimize-then-discretize approach, we set up first-order necessary optimality conditions in function space at first (which are also sufficient due to the convexity of the problem) and then discretize the arising optimality system. Formulated in Karush–Kuhn–Tucker form, the optimality system consists of the constraint itself, i.e., the state equation, the gradient equation, ensuring the optimality, and the adjoint equation, which is a helper equation in order to simplify the gradient equation. In the suggested functional analytic setting the adjoint problem directly arises from the state equation by exchanging the

roles of trial and test spaces and by another right-hand side. It takes the form

$$\text{given } y \in \mathcal{Y},\ \text{find } z \in \mathcal{Z}: \quad b(\tilde{y}, z) = \omega \cdot d(\tilde{y}, y_d - y) \quad \text{for all } \tilde{y} \in \mathcal{Y}. \tag{2}$$

A crucial question in the analysis of the optimality system is whether the adjoint problem (2) is well-posed. In the chosen functional analytic setting the well-posedness directly follows from the well-posedness of the state equation, yielding the same inf-sup constant for both problems, i.e., $\beta = 1$.

Concerning the stability analysis of the optimality system it is convenient to formulate the optimality system in a reduced form by eliminating the control,

$$L \begin{pmatrix} y \\ z \end{pmatrix} = g \quad \text{in } \mathcal{W}', \tag{3}$$

where $L : \mathcal{W} := (\mathcal{Y} \times \mathcal{Z}) \to \mathcal{W}'$ is a linear operator and $g \in \mathcal{W}'$ specifies the right-hand side of the optimality system. Due to the well-posedness of the state equation we can prove that L is boundedly invertible, ensuring well-posedness of the optimality system (3). Exploiting that $\beta = 1$ and choosing $n(u, \tilde{u}) := (u, \tilde{u})_{\mathcal{U}}$ (which is a standard choice for a quadratic cost function) the estimate boils down to

$$\|L^{-1}\|_{\mathcal{W}' \to \mathcal{W}} \leq 2 + \frac{1}{\lambda}.$$

Based upon this, we can derive some stability estimates for the optimal triple, i.e., the optimal state and the corresponding optimal adjoint state and optimal control.

Discretization. In order to discretize the optimality system we introduce a conforming finite element tensorproduct discretization, simultaneously in space and time, which amounts to construct finite-dimensional spaces $\mathcal{Y}_\delta \subset \mathcal{Y}$, $\mathcal{Z}_\delta \subset \mathcal{Z}$ and $\mathcal{U}_\delta \subset \mathcal{U}$ for the state space, the adjoint state space and the control space. Using finite elements of appropriate orders in space and time for $\mathcal{Y}$ and $\mathcal{Z}$, this setting is known to be equivalent to a Crank–Nicolson time-stepping scheme applied to (1), [3]. As we face a Petrov–Galerkin setting, i.e., $\mathcal{Y} \neq \mathcal{Z}$, the discrete spaces $\mathcal{Y}_\delta$ and $\mathcal{Z}_\delta$ need to satisfy a discrete inf-sup condition,

$$\beta_\delta := \inf_{0 \neq y_\delta \in \mathcal{Y}_\delta} \sup_{0 \neq z_\delta \in \mathcal{Z}_\delta} \frac{|b(y_\delta, z_\delta)|}{\|y_\delta\|_{\mathcal{Y}} \, \|z_\delta\|_{\mathcal{Z}}} = \inf_{0 \neq z_\delta \in \mathcal{Z}_\delta} \sup_{0 \neq y_\delta \in \mathcal{Y}_\delta} \frac{|b(y_\delta, z_\delta)|}{\|y_\delta\|_{\mathcal{Y}} \, \|z_\delta\|_{\mathcal{Z}}} > 0, \tag{4}$$

in order to guarantee well-posedness of the discrete version of (1). Following the suggestions of [1] concerning the choice of $\mathcal{Y}_\delta$ and $\mathcal{Z}_\delta$ and using suitable norms, we can realize an optimally stable discretization, i.e., $\beta_\delta = 1$. Moreover, we have $\dim(\mathcal{Y}_\delta) = \dim(\mathcal{Z}_\delta) =: \mathcal{N}$.

Applying the discretization to the reduced optimality system (3) yields an algebraic system of kind

$$\mathrm{L}_\delta \begin{pmatrix} \mathrm{y}_\delta \\ \mathrm{z}_\delta \end{pmatrix} = \mathrm{g}_\delta, \tag{5}$$

where $\mathrm{L}_\delta \in \mathbb{R}^{2\mathcal{N} \times 2\mathcal{N}}$ and $\mathrm{g}_\delta \in \mathbb{R}^{2\mathcal{N}}$ specify the discrete optimality system and $\mathrm{y}_\delta \in \mathbb{R}^{\mathcal{N}}$ and $\mathrm{z}_\delta \in \mathbb{R}^{\mathcal{N}}$ are the unknowns. As in the continuous setting we can

derive a stability estimate for (5), bounding the norm of the inverse of L_δ by

$$\|\mathrm{L}_\delta^{-1}\| \leq 2 + \frac{1}{\lambda}. \tag{6}$$

Error analysis. Recalling that $\|\mathrm{L}_\delta^{-1}\|$ is equal to the inverse of the inf-sup constant of the discrete optimality system (5), the upper bound (6) is at the same time a lower bound for the inf-sup constant. Thus, applying the Xu–Zikatanov lemma, [5], which yields a quasi-best approximation statement with multiplicative factor of the inverse of the inf-sup constant, allows us to derive the a priori estimate

$$\begin{aligned}&\|y - y_\delta\|_{\mathcal{Y}} + \|z - z_\delta\|_{\mathcal{Z}} + \|u - u_\delta\|_{\mathcal{U}} \\ &\leq \max\left\{1, \frac{1}{\lambda}\right\}\left(2 + \frac{1}{\lambda}\right)\left(\inf_{\tilde{y}_\delta \in \mathcal{Y}_\delta} \|y - \tilde{y}_\delta\|_{\mathcal{Y}} + \inf_{\tilde{z}_\delta \in \mathcal{Z}_\delta} \|z - \tilde{z}_\delta\|_{\mathcal{Z}} + \inf_{\tilde{u}_\delta \in \mathcal{U}_\delta} \|u - \tilde{u}_\delta\|_{\mathcal{U}}\right).\end{aligned}$$

for the optimal triple. Moreover, we can state a a posteriori estimate, including the bound (6) as well as the dual norm of the residual of the system (5).

Numerical results. Firstly, we compute the discrete inf-sup constant of the optimality system for different values of the regularization parameter λ and different discretizations. Comparing it with the derived lower bound $(2 + \frac{1}{\lambda})^{-1}$, we observe the same quantitative behavior. The bound seems to be almost sharp for increasing values of λ, whereas for small values of λ the bound is too pessimistic.

Secondly, we compare our space-time method with a time-stepping method based on a semi-variational formulation of the parabolic problem. We compare the value of the cost function that we obtain by solving the optimality system with the two approaches for different temporal and spatial discretizations. Both methods converge to the same value of the cost function as the number of temporal degrees of freedom increases. However, we observe that the space-time method yields the optimal value of the cost function already for very coarse temporal discretizations whereas the semi-variational method requires a sufficient fine temporal discretization in order to reach this value. Hence, the space-time method requires fewer degrees of freedom in time (and therefore a smaller number of unknowns) to reach the same accuracy. This might offer computational savings compared to the semi-variational method, and, since the CPU-times for the same number of unknowns turned out to be similar for both methods, also potential for significant speedup. This beneficial effect of the space-time method might be due to the improved stability properties compared to the semi-variational method that become visible depicting the computed control function for different temporal discretizations. For coarse temporal discretizations we can observe some stability issues for the semi-variational approach, which do not appear in the space-time context.

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Compression of Boundary Integral Equations Discretised by Anisotropic Wavelet Bases

Remo von Rickenbach
(joint work with Helmut Harbrecht)

Given a domain $\Omega \subset \mathbb{R}^3$, we are interested in the solution of a partial differential equation, such as, for example, the Laplace equation with Dirichlet boundary condition $g \in H^{\frac{1}{2}}(\Gamma)$, that is

$$\begin{cases} \Delta v &= 0, \quad \text{in } \Omega, \\ v &= g, \quad \text{on } \Gamma. \end{cases}$$

We require that $\Gamma = \partial\Omega$ can be decomposed into surface patches $\Gamma = \bigcup_{i=1}^{r} \Gamma_i$, where each surface patch Γ_i can be smoothly parametrised by a mapping $\boldsymbol{\gamma}_i : \square := [0,1]^2 \to \Gamma_i$. Moreover, Γ is required to admit overall Lipschitz continuity.

By considering the fundamental solution $G(\boldsymbol{x},\boldsymbol{y}) = \frac{1}{4\pi\|\boldsymbol{x}-\boldsymbol{y}\|}$, it is well known that

$$\Delta_{\boldsymbol{z}} \int_\Gamma G(\boldsymbol{z},\boldsymbol{y}) u(\boldsymbol{y}) \, \mathrm{d}S_{\boldsymbol{y}} = 0, \qquad \boldsymbol{z} \in \Omega,$$

for any $u \in H^{-\frac{1}{2}}(\Gamma)$. By taking the limit $\Omega \ni \boldsymbol{z} \to \boldsymbol{x} \in \Gamma$, we arrive at the boundary integral equation

$$\mathcal{A}u(\boldsymbol{x}) := \int_\Gamma G(\boldsymbol{x},\boldsymbol{y}) u(\boldsymbol{y}) \, \mathrm{d}S_{\boldsymbol{y}} = g(\boldsymbol{x}), \qquad \boldsymbol{x} \in \Gamma, \tag{1}$$

where $\mathcal{A}$ is called the *single layer operator*. This equation is known to be uniquely solvable, cf. [8, 10].

Testing (1) with $\phi \in H^{-\frac{1}{2}}(\Gamma)$ yields the variational formulation

$$\text{find } u \in H^{-\frac{1}{2}}(\Gamma) \text{ such that } \langle \mathcal{A}u, \phi\rangle_\Gamma = \langle g, \phi\rangle_\Gamma \text{ for any } \phi \in H^{-\frac{1}{2}}(\Gamma).$$

By the restriction to a finite-dimensional trial space $V_J = \operatorname{span}\{\phi_{J,1}, \dots, \phi_{J,N_J}\}$, we get a Galerkin problem, which is for $u = \sum_{k=1}^{N_J} u_{J,k}\phi_{J,k} \in V_J$ equivalent to the linear system

$$\mathbf{A}\mathbf{u} = \mathbf{g}, \quad \mathbf{A} = \big[\langle \mathcal{A}\phi_{J,\ell}, \phi_{J,k}\rangle_\Gamma\big]_{k,\ell=1}^{N_J}, \quad \mathbf{g} = \big[\langle g, \phi_{J,k}\rangle_\Gamma\big]_{k=1}^{N_J}. \tag{2}$$

Let us briefly remark that there exist other approaches for solving the Laplace equation with the boundary element method, such as, for example, the double layer ansatz or a direct formulation. Moreover, there are similar methods to solve a Neumann problem. However, all these methods encounter the same difficulty:

As the bilinear form involves a nonlocal operator $\mathcal{A} : H^q(\Gamma) \to H^{-q}(\Gamma)$, defined as the convolution with a nonlocal kernel, the system matrix is *densely populated*.

Methods were developed to deal with the dense population, among which we want to focus on the wavelet matrix compression, cf. [1, 9]. By choosing a sequence of nested trial spaces $V_0 \subset \cdots \subset V_{J-1} \subset V_J \subset V_{J+1} \subset \cdots \subset H^q(\Gamma)$, with

$$V_j = \operatorname{span}\{\phi_{j,k} : k \in \Delta_j\},$$

we can decompose $V_j = V_{j-1} \oplus W_j$, where the difference spaces W_j are given by

$$W_j = \operatorname{span}\{\psi_{j,k} : k \in \nabla_j\}, \qquad \nabla_j := \Delta_j \setminus \Delta_{j-1}.$$

Recursively, this is $V_J = V_0 \oplus W_1 \oplus \cdots \oplus W_J$. We can thus express the system (2) with respect to the multilevel wavelet basis.

The main advantage of the wavelet basis is that it admits the cancellation property: Given a sufficiently smooth function f, the integral of f against any wavelet function $\psi_{j,k}$ decays as

$$\big|\langle f, \psi_{j,k}\rangle_\Gamma\big| \lesssim 2^{-(\tilde{d}+1)j} |f|_{W^{\tilde{d},\infty}(\operatorname{supp}\psi_{j,k})}, \tag{3}$$

see e.g. [9] for the details. Note that this generalises to domains $\Omega \subset \mathbb{R}^n$, too, in which case the additional summand 1 in the exponent in (3) needs to be replaced by $\frac{n}{2}$.

By using such an isotropic wavelet basis, it was shown in [1] that for any J, there exists a compression scheme such that the solution u_J with respect to the compressed operator converges to u at the rate

$$\|u - u_J\|_{H^q(\Gamma)} \lesssim 2^{-(d-q)J} \|u\|_{H^d(\Gamma)}, \tag{4}$$

that is in line with the discretisation error, while the compressed matrix $\mathbf{A}_J$ contains at most $\mathcal{O}(N)$ nontrivial entries. We remark that the estimate (4) can even be extended to a whole range of Sobolev spaces.

Meanwhile, it was already shown that in general boundary integral operators are *$s^\star$-compressible* in these wavelet coordinates, cf. [11], apart from which adaptive methods have been developed. In [2, 4], it is shown that one can approximate the solution at the rate of the *best N-term approximation* in the sense of [3] with respect to this basis, using only $\mathcal{O}(N)$ operations. Therefore, it is crucial that the best N-term approximation admits a good convergence. This is, however, impossible in the case of geometric singularities, coming from edges for example, in which case the convergence rate deteriorates. This might be overcome by using an anisotropic tensor product wavelet basis.

Anisotropic tensor product wavelets were already used in [5] in the context of sparse tensor product spaces. As suggested by the name, on the unit square, the wavelet functions are defined by

$$\psi_{\mathbf{j},\mathbf{k}} := \psi_{j_1,k_1} \otimes \psi_{j_2,k_2}, \qquad \mathbf{k} \in \nabla_{\mathbf{j}} := \nabla_{j_1} \times \nabla_{j_2}.$$

When considering associated matrix entries $a_{(\mathbf{j},\mathbf{k}),(\mathbf{j}',\mathbf{k}')} = \langle \psi_{\mathbf{j}',\mathbf{k}'}, \mathcal{A}\psi_{\mathbf{j},\mathbf{k}}\rangle_\Gamma$, we encounter a lot of wavelet pairs which overlap. In fact, we even encounter a lot of wavelet pairs for which even the support of one wavelet overlaps with the singular

support of the other wavelet and vice versa at the same time. In the classical compression scheme, such entries cannot be compressed.

However, according to [7], if the integral under consideration is broken down to a one-dimensional integral, for example, like

$$\int_{\square}\int_{\square} \psi_{\mathbf{j}',\mathbf{k}'}(\boldsymbol{x}')G(\boldsymbol{x},\boldsymbol{x}')\psi_{\mathbf{j},\mathbf{k}}(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{x}' = \int_0^1\int_0^1 \psi_{j_1',k_1'}(x_1')k_1(x_1,x_1')\psi_{j_1,k_1}(x_1)\,\mathrm{d}x_1\,\mathrm{d}x_1',$$

with

$$k_1(x_1,x_1') := \int_0^1\int_0^1 \psi_{j_2',k_2'}(x_2')G\big((x_1,x_2),(x_1',x_2')\big)\psi_{j_2,k_2}(x_2)\,\mathrm{d}x_2\,\mathrm{d}x_2',$$

one can still make use of a generalised cancellation property similar to (3), provided that *at least in one spatial direction* the support of one wavelet is sufficiently far away from the singular support of the other. In [7], estimates for radial operators as well as for anisotropic integrodifferential operators have been derived and corresponding compression schemes have been developed, taylored to sparse tensor product spaces on the unit cube.

On the fundament of these estimates, we have developed a compression scheme on the full tensor product space, which results in a compressed system matrix containing only $\mathcal{O}(N)$ nontrivial entries whilst the solution converges with discretisation error accuracy, i.e., (4) holds in this case as well. For the details, we refer to the forthcoming paper [6]. An adaptive version of this compression scheme is work in progress.

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FOSLS for Parabolic and Instationary Stokes Equations

Rob Stevenson
(joint work with Gregor Gantner)

1. FOSLS for parabolic equations

Let $\Omega \subset \mathbb{R}^d$, $d \geq 1$, be a Lipschitz domain with boundary $\Gamma := \partial\Omega$, and $T > 0$ a given end time point with corresponding time interval $I := (0, T)$. We abbreviate the space-time cylinder $Q := I \times \Omega$ with lateral boundary $\Sigma := I \times \Gamma$. We consider the following parabolic PDE with homogeneous Dirichlet boundary conditions

$$\begin{aligned} \partial_t u - \operatorname{div}_{\mathbf{x}}(\mathbf{A}\nabla_{\mathbf{x}} u) + \mathbf{b} \cdot \nabla_{\mathbf{x}} u + cu &= f && \text{in } Q, \\ u &= 0 && \text{on } \Sigma, \\ u(0,\cdot) &= u_0 && \text{on } \Omega. \end{aligned} \tag{1}$$

where $\mathbf{A} = \mathbf{A}^\top \in L_\infty(Q)^{d\times d}$ is uniformly positive, $\mathbf{b} \in L_\infty(Q)^d$, and $c \in L_\infty(Q)$.

With $Y := L_2(I; H^1_0(\Omega))$, any $f \in Y' = L_2(I; H^{-1}(\Omega))$ can be written as

$$f = f_1 + \operatorname{div}_{\mathbf{x}} \mathbf{f}_2,$$

for some $f_1 \in L_2(Q)$ and $\mathbf{f}_2 \in L_2(Q)^d$. With such a decomposition, and $\mathbf{u} = (u_1, \mathbf{u}_2) \colon Q \to \mathbb{R} \times \mathbb{R}^d$, (1) can be written as the first-order system

$$G_P \mathbf{u} := \begin{pmatrix} \operatorname{div} \mathbf{u} + \mathbf{b} \cdot \nabla_{\mathbf{x}} u_1 + cu_1 \\ -\mathbf{u}_2 - \mathbf{A}\nabla_{\mathbf{x}} u_1 \\ u_1(0,\cdot) \end{pmatrix} = \begin{pmatrix} f_1 \\ \mathbf{f}_2 \\ u_0 \end{pmatrix} =: \mathbf{f}, \quad u_1|_\Sigma = 0, \tag{2}$$

Building on earlier work from [1], we have the following result:

Theorem ([2, Theorem 2.3 and Proposition 2.5])**.** *The operator G_P is a linear isomorphism from the space*

$$U := \{\mathbf{u} = (u_1, \mathbf{u}_2) \in L_2(I; H^1_0(\Omega)) \times L_2(Q)^d \colon \mathbf{u} \in H(\operatorname{div}; Q)\} \tag{3}$$

equipped with the corresponding graph norm, to the space

$$L := L_2(Q) \times L_2(Q)^d \times L_2(\Omega). \tag{4}$$

Consequently, for *any* closed subspace $U^\delta \subset U$, the least-squares approximation

$$\mathbf{u}^\delta := \operatorname*{argmin}_{\mathbf{w}^\delta \in U^\delta} \tfrac{1}{2}\|G_P \mathbf{w}^\delta - \mathbf{f}\|_L^2$$

is a quasi-best approximation to $\mathbf{u} \in U$ from U^δ ('Cea's lemma'). The least-squares functional provides an a posteriori estimator that is equivalent to the norm on U of the error. The squared estimator is a sum of squared local error indicators associated to the individual elements, which immediately suggests an adaptive solution method.

A potential disadvantage is that finding $\mathbf{u}^\delta$ requires the solution of a discretized PDE in the $d+1$ dimensional space-time cylinder instead of the solution of a sequence of (elliptic) PDEs in the d-dimensional spatial domain, which can be expected to be more memory consuming. In [4], three applications are discussed where the advantages of the space-time approach are in any case prevailing. First, the application of the reduced basis method to solve a parameter-dependent parabolic PDE is considered. In this case, the reduced basis methodology does not only reduce the complexity in space but equally well in time. As a second application, optimal control problems constrained by parabolic PDEs are considered. Since the optimality system consists of a parabolic PDE forward in time coupled with a parabolic PDE backward in time, it does not allow for an easy solution by time marching. The final application is the solution of a parabolic PDE on a time-dependent domain. Whilst technically involved with a time-marching scheme, it does not impose any difficulties with a space-time solver.

2. FOSLS for instationary Stokes equations

2.1. **Stokes problem with slip conditions.** In [3] we followed the same program for the instationary Stokes equations as for the parabolic equation. Given vector fields $\underset{\sim}{u}_0$ on Ω and $\underset{\sim}{f}$ on $I\times\Omega$, a function g on $I\times\Omega$, and a viscosity $\nu>0$, we consider the instationary Stokes problem with *slip boundary* conditions of finding a velocity field $\underset{\sim}{u}$ and corresponding pressure p that satisfy

$$\left\{\begin{aligned} \partial_t \underset{\sim}{u} - \nu \underset{\approx}{\Delta}_x \underset{\sim}{u} + \nabla_{\mathbf{x}}\, p &= \underset{\sim}{f} && \text{in } I\times\Omega,\\ \operatorname{div}_{\mathbf{x}} \underset{\sim}{u} &= g && \text{in } I\times\Omega,\\ \underset{\sim}{u}\cdot\underset{\sim}{n} &= 0 && \text{on } I\times\partial\Omega,\\ (\mathrm{Id}-\underset{\approx}{n}\underset{\approx}{n}^\top)\underset{\approx}{T}(\nu\underset{\sim}{u},p)\underset{\sim}{n} &= 0 && \text{on } I\times\partial\Omega,\\ \underset{\sim}{u}(0,\cdot) &= \underset{\sim}{u}_0 && \text{on } \Omega. \end{aligned}\right. \tag{5}$$

Here $(0,\underset{\sim}{n})\in\mathbb{R}^{d+1}$ denotes the outward pointing normal vector on $I\times\partial\Omega$, and for $\underset{\sim}{v}\colon I\times\Omega\to\mathbb{R}^d$ and $q\colon I\times\Omega\to\mathbb{R}$, the *symmetric gradient* and *stress tensor* are defined by $\underset{\approx}{D}(\underset{\sim}{v}) := \underset{\approx}{\nabla}_x \underset{\sim}{v} + (\underset{\approx}{\nabla}_x \underset{\sim}{v})^\top$ and $\underset{\approx}{T}(\underset{\sim}{v},q) := \underset{\approx}{D}(\underset{\sim}{v}) - q\mathrm{Id}$, respectively.

A classical solution $(\underset{\sim}{u},p)$ of (5) with $\underset{\approx}{w} := -\underset{\approx}{T}(\nu\underset{\sim}{u},p)$ satisfies

$$G_S(\underset{\sim}{u},\underset{\approx}{w},p) := (\underset{\approx}{w}+\underset{\approx}{T}(\nu\underset{\sim}{u},p), \partial_t\underset{\sim}{u}+\operatorname{div}_x\underset{\approx}{w}, \operatorname{div}_x\underset{\sim}{u}, \underset{\sim}{u}(0,\cdot)) = (0,\underset{\sim}{f}+\nu\underset{\sim}{\nabla}_x g, g, \underset{\sim}{u}_0),$$

as well as $\underset{\sim}{u}\cdot\underset{\sim}{n}=0$ on $I\times\partial\Omega$, and $(\mathrm{Id}-\underset{\approx}{n}\underset{\approx}{n}^\top)\underset{\approx}{w}\underset{\sim}{n}=0$ on $I\times\partial\Omega$.

We define the Hilbert spaces

$$\begin{aligned} L_{2,0}(\Omega) &:= \{p\in L_2(\Omega)\colon \int_\Omega p\,dx = 0\},\\ \mathbb{H}^1(\Omega) &:= \{\underset{\sim}{u}\in \underset{\sim}{H}^1(\Omega)\colon \underset{\sim}{u}\cdot\underset{\sim}{n}=0 \text{ on } \partial\Omega\} \end{aligned}$$

and

$$\begin{aligned} \mathscr{Z} := \{(\underset{\sim}{u},\underset{\approx}{w})\in L_2(I;\mathbb{H}^1(\Omega))\times L_2(I;L_2(\Omega;\underset{\approx}{\mathbb{S}}))\colon \partial_t\underset{\sim}{u}+\operatorname{div}_{\mathbf{x}}\underset{\approx}{w}\in \underset{\sim}{L}_2(I\times\Omega),\\ \operatorname{div}_{\mathbf{x}}\underset{\sim}{u}\in H^1(I;L_{2,0}(\Omega)), (\mathrm{Id}-\underset{\approx}{n}\underset{\approx}{n}^\top)\underset{\approx}{w}|_{I\times\partial\Omega}\underset{\sim}{n}=0\}, \end{aligned}$$

equipped with the corresponding graph norm

$$\|(\underset{\sim}{u},\underset{\approx}{w})\|^2_{\mathscr{Z}} := \|\underset{\sim}{u}\|^2_{L_2(I;\underset{\sim}{\mathbb{H}}^1(\Omega))} + \|\underset{\approx}{w}\|^2_{\underset{\approx}{L}_2(I\times\Omega)} + \|\partial_t \underset{\sim}{u} + \operatorname{div}_{\mathbf{x}} \underset{\approx}{w}\|^2_{\underset{\sim}{L}_2(I\times\Omega)} + \|\operatorname{div}_{\mathbf{x}} \underset{\sim}{u}\|^2_{H^1(I;L_{2,0}(\Omega))}.$$

Theorem. *Let Ω be convex or has a C^2-boundary. Then*

$$\|G_S(\underset{\sim}{u},\underset{\approx}{w},p)\|_{\underset{\approx}{L}_2(I\times\Omega)\times\underset{\sim}{L}_2(I\times\Omega)\times H^1(I;L_{2,0}(\Omega))\times\underset{\sim}{L}_2(\Omega)} \eqsim \|(\underset{\sim}{u},\underset{\approx}{w},p)\|_{\mathscr{Z}\times L_2(I;L_{2,0}(\Omega))}$$

for all $(\underset{\sim}{u},\underset{\approx}{w},p) \in \mathscr{Z} \times L_2(I;L_{2,0}(\Omega))$.

Analogously to the parabolic case, this result gives rise to computable least-squares approximations that are quasi-best approximations from the trial space that is applied.

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Stability Analysis for Electromagnetic Waveguides

Leszek Demkowicz

(joint work with Jens M. Melenk, Stefan Henneking, Jacob Badger)

The reported work is part of a continued effort to build reliable, high-fidelity Finite Element (FE) models for investigating Transverse Mode Instability (TMI) in optical amplifiers [1, 2]. The model consists of a system of two nonlinear time-harmonic Maxwell equations coupled with each other and with the transient heat equation to account for thermal effects. Modeling of a 1–10 m long fiber segment involves the solution with $\mathcal{O}$(1-10 M) wavelengths. Solving such a problem with a direct FE discretization is infeasible, even on state-of-the-art supercomputers.[1] For this reason, even simplified models typically resolve a longer length scale. In the context of TMI studies, it is common to resolve only the length scale of the *mode beat* between the fundamental mode and higher-order modes since the mode instabilities occur at that scale. In a typical weakly-guiding, large-mode-area fiber amplifier, the mode beat length is on the order of $\mathcal{O}$(1,000) wavelengths. This brought forth the idea of the *full envelope approximation* in which the solution to the Maxwell equations is sought using the ansatz including an exponential factor,

$$E(x,y,z) = e^{ikz} E_0(x,y,z)$$

[1] A sophisticated *hp* code using MPI+OpenMP parallelization and up to 512 manycore compute nodes enabled us to model fibers with up to $\mathcal{O}$(10,000) wavelengths [2].

where wavenumber k corresponds to circa one thousand wavelengths, and the new unknown, $E_0(x, y, z)$, involves only $\mathcal{O}(1{,}000\text{–}10{,}000)$ wavelengths. The presented work summarizes our efforts to investigate the stability and convergence of the Discontinuous Petrov-Galerkin (DPG) method used to solve the problem [3, 4].

DPG essentials. The *ideal* DPG method with optimal test functions reproduces automatically the stability of the continuous problem. Assume that a system of first-order differential equations is represented with a *bounded below* closed operator A,

$$A : L^2(\Omega)^N \supset D(A) \to L^2(\Omega)^N, \qquad \alpha\|u\| \leq \|Au\|, \quad \alpha > 0$$

where $\Omega \subset \mathbb{R}^3$, N is the number of equations, and $\|\cdot\|$ denotes the L^2-norm. The stability of the DPG method based on the *ultraweak* (UW) formulation:

$$\begin{cases} u \in L^2(\Omega)^N \\ (u, A^*v) = (f, v) \quad v \in D(A^*) \end{cases}$$

where the test space—domain of L^2-adjoint A^*—has been equipped with the scaled graph norm,

$$\|v\|_V^2 := \|A^*v\|^2 + \beta^2\|v\|^2, \quad \beta > 0$$

is governed by the inf–sup constant [3]:

$$\gamma \geq \left[1 + \left(\frac{\beta}{\alpha}\right)^2\right]^{-\frac{1}{2}}.$$

Hence our interest in constant α corresponding to the modified Maxwell problem resulting from the full envelope ansatz. The first, very simple result, may be a bit surprising.

Lemma 1: Let $\tilde{A}$ be the operator corresponding to the full envelope ansatz, i.e.,

$$\tilde{A}\tilde{u} := e^{ikz}A(e^{-ikz}\tilde{u}),$$

where A denotes the operator corresponding to the acoustic or EM waveguide problem. Then, the operator $\tilde{A}$ is bounded below if and only if operator A is bounded below, and the corresponding boundedness below constants are identical:

$$\|Au\| \geq \alpha\|u\| \quad \Leftrightarrow \quad \|\tilde{A}\tilde{u}\| \geq \alpha\|\tilde{u}\|.$$

Proof: We observe

$$\|\tilde{A}\tilde{u}\| = \|e^{ikz}A(e^{-ikz}\tilde{u})\| = \|A(e^{-ikz}\tilde{u})\| \geq \alpha\|e^{-ikz}\tilde{u}\| = \alpha\|\tilde{u}\|.$$

In other words, using the full envelope ansatz may help with the approximability (if the simulated phenomenon, indeed, occurs at the scale of thousands of wavelengths) but *it does not affect* the stability. This observation brought us back to the study of stability of waveguide problems. For a fixed domain, we are usually interested in the dependence of the stability constant upon frequency ω, e.g., under technical assumptions, one can show the linear dependence of α^{-1} upon ω. For optical fibers, the frequency is fixed, and we are interested in the dependence of the stability constant upon the length L of the waveguide or, in other words, the number of wavelengths.

We started our study with the acoustic waveguide. Eliminating the velocity, we obtain the standard Helmholtz equation for the pressure, accompanied by appropriate boundary conditions (BCs) and a non-local Dirichlet-to-Neumann (DtN) BC at the fiber exit. Employing the separation of variables ansatz, we obtain an eigenvalue problem involving a self-adjoint operator defined in the transversal domain D (in x, y). For each eigenvalue λ then, we obtain a 1D Helmholtz-like problem in z with a homogeneous BC at $z = 0$, and an impedance BC at $z = L$. Application of the DtN operator is then equivalent to selecting the outgoing wave. Expanding solution u in terms of the orthogonal eigenmodes (self-adjointness of the operator in the transversal domain is critical), we obtain the following result.

Theorem 1. *Let $(u, p) \in H(\mathrm{div}, \Omega) \times H^1(\Omega)$ be the solution to the acoustic waveguide problem with the right-hand side $(f, g) \in L^2(\Omega) \times L^2(\Omega)^3$ with appropriate BCs. There exists then a constant $C > 0$ depending upon the frequency and the material properties of the waveguide but independent of length L, such that*

$$\|u\|_{H(\mathrm{div},\Omega)} + \|p\|_{H^1(\Omega)} \leq CL \left[\|f\|_{L^2(\Omega)} + \|g\|_{L^2(\Omega)^3}\right] .$$

In the remaining two pages we will describe briefly the techniques that we used to arrive at the corresponding result for the Maxwell waveguide problem. First of all, to our surprise, we learned that the well-posedness result for a *non-homogeneous* Maxwell waveguide, was an open problem. To begin with, we cannot reduce the Maxwell problem to a single scalar-valued equation, so the separation of variables approach is out. But, anticipating the 1D Helmholtz problem in z, we can start with an exponential ansatz in the z direction, and seek the solution in the form $e^{i\beta z}(E_t(x, y), E_3(x, y))$, $e^{i\beta z}(H_t(x, y), H_3(x, y))$ where E_t, H_t and E_3, H_3 are the transversal and z components of the electric and magnetic field defined in the transversal domain D, respectively. We then obtain a non-standard[2] eigenvalue problem for E_t, H_t, E_3, H_3 involving first-order operators. Upon eliminating E_3, H_3 we obtain an 'EH eigenvalue problem' involving two second-order equations. However, the corresponding operator (even for the homogeneous case) is *not* self-adjoint. Finally, eliminating H_t or E_t respectively, we obtain single-equation 'E-eigenvalue' and 'H-eigenvalue' problems. For example, the E-problem is:

$$\left\{ \begin{array}{l} E_t \in H_0(\mathrm{curl}, D),\ \mathrm{curl} E_t \in H^1(D),\ \frac{1}{\epsilon}\mathrm{div}\,\epsilon E_t \in H_0^1(D) \\ \boldsymbol{\nabla} \times \mathrm{curl} E_t - \omega^2 \epsilon E_t - \boldsymbol{\nabla}(\frac{1}{\epsilon}\mathrm{div}\epsilon E_t) = -\beta^2 E_t\,. \end{array} \right. \tag{1}$$

The regularity assumptions are *inherited* from the previous eigenvalue problems involving more unknowns. The operator in (1) is self-adjoint for the homogeneous case (with dielectric constant $\epsilon = 1$) but, for a variable ϵ, the operator is still *not* self-adjoint. We then began with a study of the homogeneous waveguide problem.

Lemma 2: Let (λ_i, ϕ_i) and (μ_j, ψ_j) denote the Dirichlet and Neumann eigenpairs of the Laplacian in the domain D. The eigenvalues β_i^2 for (1) are classified into the following three families.

[2]Mass terms for E_3, H_3 are missing.

(a) $\beta^2 = \omega^2 - \mu_j$ with μ_j distinct from all λ_i. The corresponding eigenvectors are curls:

$$E = \boldsymbol{\nabla} \times \psi_j \,,$$

with multiplicity of β^2 equal to the multiplicity of μ_j.

(b) $\beta^2 = \omega^2 - \lambda_i$ with λ_i distinct from all μ_j. The corresponding eigenvectors are gradients:

$$E = \boldsymbol{\nabla} \phi_i \,,$$

with multiplicity of β^2 equal to the multiplicity of λ_i.

(c) $\beta^2 = \omega^2 - \mu_j = \omega^2 - \lambda_i$ for $\mu_j = \lambda_i$. The corresponding eigenvectors are linear combinations of curls and gradients:

$$E = A\boldsymbol{\nabla} \times \psi_j + B\boldsymbol{\nabla}\phi_i \,, \quad A, B \in \mathbb{C} \,,$$

with multiplicity of β^2 equal to the sum of multiplicities of μ_j and λ_i.

With a similar result for the H-eigenvalue problem, we were now able to guess the ansatz for the 3D E, H fields:

$$\begin{aligned} E &= \textstyle\sum_i \boldsymbol{\nabla} \times \psi_i \alpha_i(z) + \sum_j \boldsymbol{\nabla}\phi_j \beta_j(z) + \sum_j e_z \phi_j \gamma_j(z) \\ H &= \textstyle\sum_i \boldsymbol{\nabla}\psi_i \delta_i(z) + \sum_j \boldsymbol{\nabla} \times \phi_j \eta_j(z) + \sum_i e_z \psi_i \zeta_i(z) \end{aligned} \tag{2}$$

where $e_z = (0, 0, 1)$ is the z unit vector.

After substituting ansatz (2) into the Maxwell equations, we were able to obtain a similar effect as for the acoustics waveguide. For each mode, we obtained a system of six ODEs for coefficients $\alpha_i(z), \beta_j(z), \gamma_j(z), \delta_i(z), \eta_j(z), \zeta_i(z)$ which decouples into two subsystems consisting of two first-order ODEs and one algebraic equation. Eventually, each subsystem reduces to a single second-order equation identical with that for the acoustic waveguide. Furthermore, the orthogonality of the modes in (2) leads to the final result.

Theorem 2. *There is $C > 0$ independent of L such that the solution (E, H) of the Maxwell homogeneous*[3] *waveguide problem with right-hand side (f, g) satisfies*

$$\|(E, H)\|_{L^2(\Omega)^3 \times L^2(\Omega)^3} \leq CL \|(f, g)\|_{L^2(\Omega)^3 \times L^2(\Omega)^3} .$$

For details on the discussed results for the acoustic and homogeneous Maxwell waveguide problems, see [3]. In [4] we tackled the non-homogeneous Maxwell problem. A simple perturbation argument shows that the well-posedness of the homogeneous Maxwell problem implies the well-posedness of the non-homogeneous case for a sufficiently small perturbation $\epsilon = 1 + \delta\epsilon$. However, the 'smallness' of $\delta\epsilon$ depends on length L; the longer the waveguide, the smaller perturbation $\delta\epsilon$ must be. The linear dependence of the stability constant upon length L is thus lost. Instead, the analysis in [4] is based on classical perturbation theory of self-adjoint operators applied to E-, H-eigenvalue problems and corresponding adjoint operators. By a judicious argument, we were again able to reduce the problem to independent systems of six ODEs in z, and reduce the stability analysis to analysis of a single second-order ODE in z. The lack of orthogonality of the (perturbed)

[3] In the non-dimensional setting, both permeability μ and permittivity ϵ equal one.

eigenvectors led to the need of analyzing the (linearized) mass matrices. In the end, we were able to obtain the same result as for the homogeneous waveguide under the assumption of $\delta\epsilon$ being sufficiently small in the L^∞-norm only.[4] However, the analysis is based on a formal perturbation technique and is not a full proof yet.

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Recent Advances in Low Rank Matrix Equations Solvers

Valeria Simoncini

Linear matrix equations such as the Lyapunov and Sylvester equations and their generalizations have classically played an important role in the analysis of dynamical systems, in control theory and in eigenvalue computation. More recently, matrix equations have emerged as a natural linear algebra framework for the discretized version of (systems of) deterministic and stochastic partial differential equations, and new challenges have arisen. Growing attention starts to be given to multiterm linear matrix equations, that allow for the numerical treatment of computationally expensive discretization techniques addressing advanced problems.

In this talk we will review some of the key methodologies for numerically solving large scale linear matrix equations, and how they arise in various settings. In particular, we will focus on application problems associated with space-time discretizations, which pose insurmountable difficulties to classical numerical linear algebra solution strategies.

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Deep Barron Classes

Reinhold Schneider
(joint work with Angela Kunoth and Mathias Oster)

Barron spaces characterize approximation rates of shallow neural networks (NN), formally without curse of dimensions. However the concepts are applicable also to Gaussian mixture models and Gaussian wave packets with minor changes. Functions in Barron spaces are supposed to have a continuous representation formula

$$h(x) = \int_U a\,\sigma(Ax+b)\,d\mu_1(a,A,b)$$

with a random measure μ_1. The discrete versions are based on approximations of the measure by Dirac delta's (i.e., in the weak-* sense)

$$\mu_1 = \frac{1}{N}\sum_{i=1}^N \delta_{a^i,A^i,b^i}, \quad (a^i,A^i,b^i)\in U \qquad \Longrightarrow \qquad h(x) = \frac{1}{N}\sum_{i=1}^N a^i\,\sigma(A^i x + b^i)\,,$$

where the a^i, A^i, b^i are sampled from the random measure μ_1. Convergence can be deduced from error estimates of Monte Carlo quadrature. More details can be found, e.g., in [2].

In order to consider deep neural networks, we recall that a large family of deep neural networks, e.g., ResNets, can be viewed as an Euler discretization of an ODE $\dot{x}(t) = v(t,x)\ ,\ x(0) := x$, with driving field v given as a shallow NN.

This leads to the following feedback optimal control problem. We seek to learn a function f by deep neural networks with activation function σ. An abstract feedback optimal control problem with measure-valued controls $\mu_2(t)$ is of the form

$$\min_{\mu_1,\mu_2} \mathcal{J}(\mu_1,\mu_2), \quad \mathcal{J}(\mu_1,\mu_2) := \int_{\mathbb{R}^d} \|f(x) - \int a\,\sigma(A\ z(T,x)+b)\ d\mu_1(t;a,A,b)\|^2 dx$$
$$\text{such that} \quad \frac{d}{dt}z(t,x) = \int a\,\sigma(Az(t,x)+b)\,d\mu_2(t;a,A,b), \quad z(0,x) = x.$$

This perspective provides an interesting mathematical framework to analyse the expressivity and optimization of such networks from a continuous point of view. It also has a strong relationship to Hamilton Jacobi Bellmann equations and Potential Mean Field Games. The above control problem can be interpreted as an infinite deep neural network where the last layer is of a particular form. We exploit the ideas of Barron spaces and the corresponding representation as continuous

interpretation of wide shallow networks and neural ODEs as infinite deep residual network architectures.

We discuss the issue of existence and the employment of gradient schemes. We observe that the parametrisations of the functions under consideration with respect to the sought measures μ_1, μ_2 are *linear*. However, the set of random measures is NOT a linear space. In particular, the definition of gradient flow requires sophisticated analytical tools, see, e.g., [1]. Details are deferred to the talk of Matthias Oster. He has shown the existence of minimizers to the optimal control problem by using Prokhorov's theorem on tight measures and some regularity assumptions on the activation function [4].

We became aware of a recent paper with similar content we would like to mention [3].

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Optimization Based Formulation and Regularization of Inverse Problems

Barbara Kaltenbacher

(joint work with Kha Van Huynh, William Rundell)

The conventional way of formulating inverse problems such as identification of a (possibly infinite dimensional) parameter, is via some forward operator, which is the concatenation of the observation operator with the parameter-to-state-map for the underlying model.

Recently, all-at-once formulations have been considered as an alternative to this reduced formulation, avoiding the use of a parameter-to-state map, which would sometimes lead to too restrictive conditions. Here the model and the observation are considered simultaneously as one large system with the state and the parameter as unknowns.

A still more general formulation of inverse problems, containing both the reduced and the all-at-once formulation, but also the well-known and highly versatile so-called variational approach (not to be mistaken with variational regularization) as special cases, is to formulate the inverse problem as a minimization problem

(instead of an equation) for the state and parameter. Regularization can be incorporated via imposing constraints and/or adding regularization terms to the objective.

A classical example of a nonstandard variational formulation of an inverse problem is *electrical impedance tomography* EIT in two space dimensions, as derived in the seminal 1987 paper by Kohn and Vogelius [1]

$$\begin{aligned}&\min_{\sigma,\underline{\phi},\underline{\psi}} \sum_{i=1}^{I} \tfrac{1}{2} \int_\Omega \Big(\sigma|\nabla\phi_i|^2 + \frac{1}{\sigma}|\nabla^\perp\psi_i|^2\Big)\, dx \\ &\text{s.t. } \psi_i = \gamma_i\,,\ \phi_i = \upsilon_i \ \text{ on } \partial\Omega\,, \quad i = 1,\dots,I\end{aligned}$$

where ϕ and ψ are potentials for the electric field and the current density, respectively $J_i = -\nabla^\perp\psi_i\,, \quad E_i = -\nabla\phi_i\,, \quad i = 1,\dots,I\,,$ and I is the number of measured current-voltage observation pairs (γ_i, υ_i). It can be regularized, e.g., by adding constraints on the searched for conductivity σ and relaxing the data misfit constraint:

$$\begin{aligned}&\min_{\sigma,\Phi,\Psi} \sum_{i=1}^{I} \left\{ \tfrac{1}{2} \int_\Omega \sum_{i=1}^{I} \tfrac{1}{2} \int_\Omega \Big(\sigma|\nabla\phi_i|^2 + \frac{1}{\sigma}|\nabla^\perp\psi_i|^2\Big)\, dx + \tfrac{\alpha}{2}\|(\phi_i,\psi)\|^2_{H^{1+\epsilon}(\Omega)^2} \right\} \\ &\text{s.t.} \quad \underline{\sigma} \le \sigma \le \overline{\sigma} \text{ on } \Omega\,, \\ &\qquad \left.\begin{aligned} \upsilon_i^\delta - \tau\delta \le \phi_i \le \upsilon_i^\delta + \tau\delta\,, \\ \gamma_i^\delta - \tau\delta \le \psi_i \le \gamma_i^\delta + \tau\delta\,, \end{aligned}\right\} \quad \text{on } \partial\Omega\,, \quad i = 1,\dots,I\,.\end{aligned}$$

with the noise level $\delta \ge \|y - y^\delta\|$ and a safetly factor $\tau > 1$ Some crucial features of the resulting problem are the following.

- The problem is formulated in Hilbert spaces X, V for design variables q, u (easier applicability of iterative minimization methods).
- The cost function J^δ is differentiable;
- The constraints are pointwise bounds, which can be efficiently implemented and are practically relevant in view of known a prior bounds on σ;
- The model takes the form of a first order least squares formulation of the PDE model;
- The Euler-Lagrange equation for unregularized problem yields the well-known second order PDE model $\nabla\cdot(\sigma\nabla\phi_i) = 0$ for EIT;

These properties are shared by a formulation of the inverse problem of *localizing sound sources* f from observation of the pressure at sensor positions x_ℓ by minimizing the sum of the norms of the residuals in the balance and observation equations

$$\begin{aligned}&\varrho_0 v_t + \nabla p = f && \text{in } \Omega\times(0,T) && \varrho_0 v\cdot\nu + \kappa p = 0 && \text{on } \Gamma_a\times(0,T) \\ &\tfrac{1}{c_0^2} p_t + \varrho_0 \nabla\cdot v = 0 && \text{in } \Omega\times(0,T) && v\cdot\nu = 0 && \text{on } \Gamma_r\times(0,T) \\ &y_\ell = p(x_\ell)\,,\ \ell\in\{1,\dots,L\}.\end{aligned}$$

Moving into nonlinear acoustics, the model equations become, e.g.,

$$
\begin{aligned}
&\varrho_0 \vec{v}_t + \nabla p_\sim + \varrho_0 \nabla \vec{v} \cdot \vec{v} - \mu \Delta \vec{v} + \nabla p_0 - \vec{f} \\
&\tfrac{1}{c^2} p_{\sim t} + \nabla \cdot (\varrho_0 \vec{v}) + \nabla \cdot (\tfrac{1}{c^2} p_\sim \vec{v}) - \kappa \, (p_\sim)_t^2 \\
&y = \mathrm{tr}_{\Sigma_T}(p_\sim + p_0)
\end{aligned}
\tag{1}
$$

(equipped with initial and boundary conditions) and the inverse problem under consideration is identification of the space-dependent coefficient $\kappa(x)$, which appears as the crucial quantity in *nonlinearity parameter tomography*. The formulation (1) also opens up the possibility to apply space-tine addaptivity for a numerically efficient solution of the inverse problem.

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Parameter Estimation for ODEs

Roland Becker

We consider least-squares problems for parameter estimation, with an ordinary differential equation as state equation. Let $I =]0, T[$ be the time interval. For the initial value problem

$$u_t = f(p, u), \quad u(0) = u_0(p)$$

with parameter dependent right-hand side and initial data, we use the variational formulation

$$u \in X : \int_0^T u_t \cdot v + u(0) \cdot v_0 = \int_0^T f(p, u) \cdot v + u_0(p) \cdot v_0 \quad \forall (v, v_0) \in Y,$$

where $X = H^1(I, \mathbb{R}^n)$ and $Y = L^2(I, \mathbb{R}^n) \times \mathbb{R}^n$, see [1, 2, 3].

The equation is discretized by a space-time Petrov-Galerkin formulation with discontinuous test functions and continuous trial functions on a time mesh δ. The idea is to use a global adaptive algorithm in the spirit of adaptive methods for elliptic equations.

We derive error estimators in a more general framework. Let Q, X and Y be Hilbert spaces and $a : Q \times X \times Y \to \mathbb{R}$ smooth and linear with respect to the last argument. We assume

$$a'_u(p,u)(w,v) \le C_{a'} \|w\|_X \|v\|_Y \quad \forall p \in P, u, w \in X, v \in Y, \tag{1}$$

and the following Lipschitz condition: for all $p \in P, u_1, u_2, w \in X, v \in Y$

$$|a'_u(p,u_1)(w,v) - a'_u(p,u_2)(w,v)| \le C_{a''} \|u_1 - u_2\|_X \|w\|_X \|v\|_Y . \tag{2}$$

The continuous and discrete problems, depending on $p \in Q$, read

$$u \in X : \quad a(p,u)(v) = l(p,v) \quad \forall v \in Y \quad \text{and} \tag{3}$$

$$u_\delta \in X_\delta : \quad a(p,u_\delta)(v) = l(p,v) \quad \forall v \in Y_\delta \tag{4}$$

with finite-dimensional subspaces $X_\delta \subset X$ and $Y_\delta \subset Y$. We suppose that for $p \in P$, (3) and (4) define unique solutions $u(p)$ and $u_\delta(p)$, respectively. Then the least-squares problem minimizes the cost functional

$$\widehat{J}(p) = J(u(p)) = \frac{1}{2} \|R(p)\|_Z^2 + \alpha_{\mathrm{LM}} \|p - \overline{p}\|_Q^2 , \quad R(p) = C(u(p)) - \overline{C},$$

where $C : X \to Z$ is a bounded linear observation operator, Z being a Hilbert space, and $\overline{C} \in Z$ and $\overline{p} \in P$ are given. The discrete analogues are denoted $R_\delta(p)$ and $\widehat{J}_\delta$.

Following [4], where an adaptive finite element method for elliptic problems has been analyzed, our goal is to derive error estimators for the parameter error. At the same time we obtain estimators for the cost functional as well as the gradient, which can be used to guide the optimization algorithm.

First we note that for any $p \in P$

$$\begin{aligned}
\widehat{J}(p) - \widehat{J}_\delta(p) =& \frac{1}{2} \|R(p)\|_Z^2 - \frac{1}{2} \|R_\delta(p)\|_Z^2 \\
=& \frac{1}{2} \|R(p) - R_\delta(p)\|_Z^2 + \langle R(p) - R_\delta(p), R_\delta(p) \rangle_Z \\
\le& \frac{1}{2} \|C(u(p)) - C(u_\delta(p))\|_Z^2 + \|C(u(p)) - C(u_\delta(p))\|_Z \|R_\delta(p)\| .
\end{aligned}$$

Similarly, we obtain for any $p \in P$

$$\begin{aligned}
\left\| \nabla \widehat{J}(p) - \nabla \widehat{J}_\delta(p) \right\| \le& \|C(u(p)) - C(u_\delta(p))\|_Z \|C(u'(p)) - C(u'_\delta(p))\|_Z \\
&+ \|C(u(p)) - C(u_\delta(p))\|_Z \|C(u'_\delta(p))\|_Z \\
&+ \|C(u'(p)) - C(u'_\delta(p))\|_Z \|R_\delta(p)\|_Z ,
\end{aligned}$$

where $u'(p)$ and $u'_\delta(p)$ are solutions to the tangent problems

$$\begin{aligned}
u' \in X : \quad & a'_u(p,u)(u',v) = l'(p,v) - a'_p(p,u)(v) \quad \forall v \in Y \quad \text{and} \\
u'_\delta \in X_\delta : \quad & a'_u(p,u_\delta)(u'_\delta,v) = l'(p,v) - a'_p(p,u_\delta)(v) \quad \forall v \in Y_\delta .
\end{aligned}$$

In order to bound the errors, we consider the adjoint problems

$$\begin{aligned} z \in Y: \quad a'_u(p,u)(w,z) =& C(w) \quad \forall w \in X \quad \text{and} \\ z_\delta \in Y_\delta: \quad a'_u(p,u_\delta)(w,z_\delta) =& C(w) \quad \forall w \in X_\delta. \end{aligned}$$

Thanks to conformity, we have for any $v \in Y_\delta$

$$\int_0^1 a'_u(p,(1-s)u_\delta + su)(u-u_\delta,v)\,ds = a(p,u)(v) - a(p,u_\delta)(v) = 0,$$

such that with (2)

$$\begin{aligned} a'_u(p,u)(u-u_\delta,v) =& \int_0^1 \left(a'_u(p,u)(u-u_\delta,v) - a'_u(p,(1-s)u_\delta+su)(u-u_\delta,v)\right) ds \\ \leq& \frac{C_{a''}}{2} \left\|u-u_\delta\right\|_X^2 \left\|v\right\|_Y \end{aligned}$$

and with (1)

$$\begin{aligned} C(u(p)-u_\delta(p)) =& a'_u(p,u)(u-u_\delta,z) \\ =& a'_u(p,u)(u-u_\delta,z-z_\delta) + a'_u(p,u)(u-u_\delta,z_\delta) \\ \leq& C_{a'} \left\|u-u_\delta\right\|_X \left\|z-z_\delta\right\|_Y + \frac{C_{a''}}{2} \left\|u-u_\delta\right\|_X^2 \left\|z_\delta\right\|_Y. \end{aligned}$$

We summarize the obtained bounds.

Theorem 1. *Let*

$$\begin{aligned} E_\delta(p) :=& C_{a'} \left\|u(p)-u_\delta(p)\right\|_X \left\|z(p)-z_\delta(p)\right\|_Y + \frac{C_{a''}}{2} \left\|u(p)-u_\delta(p)\right\|_X^2 \left\|z_\delta(p)\right\|_Y, \\ F_\delta(p) :=& C_{a'} \left\|u'(p)-u'_\delta(p)\right\|_X \left\|z(p)-z_\delta(p)\right\|_Y + \frac{C_{a''}}{2} \left\|u'(p)-u'_\delta(p)\right\|_X^2 \left\|z_\delta(p)\right\|. \end{aligned}$$

Then we have

$$|\widehat{J}(p) - \widehat{J}_\delta(p)| \leq E_\delta^2(p) + E_\delta(p) \left\|R_\delta(p)\right\|_Z \tag{5}$$

and

$$\left\|\nabla \widehat{J}(p) - \nabla \widehat{J}_\delta(p)\right\| \leq E_\delta(p)F_\delta(p) + F_\delta(p) \left\|R_\delta(p)\right\|_Z + E_\delta(p) \left\|C(u'_\delta)\right\|_Z.$$

Under the strict convexity assumption $\nabla^2 \widehat{J}(p) \succeq \mu > 0$ for all $p \in [p^*, p^*_\delta]$, we have

$$\mu^{\frac{1}{2}} \left\|p^* - p^*_\delta\right\|_P \leq E_\delta(p^*_\delta)F_\delta(p^*_\delta) + F_\delta(p^*_\delta) \left\|R_\delta(p^*_\delta)\right\|_Z + E_\delta(p^*_\delta) \left\|C(u'_\delta(p^*_\delta))\right\|_Z. \tag{6}$$

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Symplectic Model Reduction of Hamiltonian Systems

Silke Glas
(joint work with Patrick Buchfink, Bernard Haasdonk)

Classical model reduction methods based on linear approximation schemes for parameter-dependent partial differential equations (PDEs) or ordinary differential equations are known to work very well for certain classes of problems, e.g., elliptic PDEs. For other types of problems, e.g., for transport-dominated problems, the decay of the Kolmogorov N-width, which describes the best-possible error of a reduced model constructed with linear approximation schemes, can admit a slow decay, see e.g., [7, 4].

In this contribution, which has been published in [2], we are interested to obtain a reduced model via nonlinear approximation methods, that can overcome the Kolmogorov N-width barrier, while at the same time preserving the symplectic structure in the reduced model, i.e., having that the reduced model is again a Hamiltonian system. See e.g., [6, 8, 2] for symplectic model reduction with linear approximation methods. To this end, we first introduce the high-dimensional Hamiltonian system: let $I := (0, T]$ with $0 < T < \infty$ be a finite time interval and let $\boldsymbol{\mu} \in \mathcal{P} \subset \mathbb{R}^p$ be the parameters the equation depends on. Then, we define a smooth function $\mathcal{H} : \mathbb{R}^{2N} \times \mathcal{P} \to \mathbb{R}$, which is the so-called *Hamiltonian function*. We seek a solution to the following problem: for given parameter $\boldsymbol{\mu} \in \mathcal{P}$, given parameter-dependent initial condition $\boldsymbol{x}_0(\boldsymbol{\mu}) \in \mathbb{R}^{2N}$, find $\boldsymbol{x}(\cdot; \boldsymbol{\mu}) \in C^1(I, \mathbb{R}^{2N})$ such that

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{x}(t; \boldsymbol{\mu}) = \mathbb{J}_{2N} \nabla_{\boldsymbol{x}} \mathcal{H}(\boldsymbol{x}(t; \boldsymbol{\mu}); \boldsymbol{\mu}), \quad \boldsymbol{x}(0; \boldsymbol{\mu}) = \boldsymbol{x}_0(\boldsymbol{\mu}),$$

where $C^1(I, \mathbb{R}^{2N})$ are the at least once continuously differentiable functions with values in $\mathbb{R}^{2N}$ and the matrix $\mathbb{J}_{2N} \in \mathbb{R}^{2N \times 2N}$ is the so-called canonical Poisson matrix given by

$$\mathbb{J}_{2N} := \begin{pmatrix} \mathbf{0}_{N \times N} & \mathbb{I}_N \\ -\mathbb{I}_N & \mathbf{0}_{N \times N} \end{pmatrix} \in \mathbb{R}^{2N \times 2N},$$

where $\mathbb{I}_N$ denotes the unity matrix of size N and $\mathbf{0}_{N \times N}$ denotes the matrix of size $N \times N$ where all entries equal to zero.

The goal ofs the nonlinear approximation methods is to approximate the detailed solution manifold

$$\mathcal{M} := \left\{ \boldsymbol{x}(t; \boldsymbol{\mu}) \in \mathbb{R}^{2N} \;\middle|\; t \in [0, T], \boldsymbol{\mu} \in \mathcal{P} \right\},$$

with a nonlinear symplectic trail manifold. To achieve this approximation, we extend the classical linear subspace model reduction methods to nonlinear approximations methods of the form

$$\widetilde{\boldsymbol{x}}(t;\boldsymbol{\mu}) := d(\boldsymbol{x}_r(t;\boldsymbol{\mu})) \approx \boldsymbol{x}(t;\boldsymbol{\mu}),$$

which is an ansatz that is also known as *model reduction on manifolds*. In the aforementioned definition, the function $d : \mathbb{R}^{2n} \to \mathbb{R}^{2N}$ is the *reconstruction function*, $\boldsymbol{x}_r(t;\boldsymbol{\mu}) \in \mathbb{R}^{2n}$ are the *reduced coordinates* with $n \ll N$ and $\widetilde{\boldsymbol{x}}(t;\boldsymbol{\mu}) \in \mathbb{R}^{2N}$ is the *reconstructed solution*. Moreover, we require d to be a *symplectic map*, which means that the Jacobian $\boldsymbol{D}_{\boldsymbol{x}} d(\boldsymbol{x}) \in \mathbb{R}^{2N\times 2n}$ of d is a symplectic matrix for every $\boldsymbol{x} \in \mathbb{R}^{2n}$, i.e.,

$$\left(\boldsymbol{D}_{\boldsymbol{x}} d(\boldsymbol{x})\right)^{\mathsf{T}} \mathbb{J}_{2N} \boldsymbol{D}_{\boldsymbol{x}} d(\boldsymbol{x}) = \mathbb{J}_{2n},$$

in order to guarantee that the resulting reduced systems is again Hamiltonian. Note that in the latter equation, $\mathbb{J}_{2n} \in \mathbb{R}^{2n\times 2n}$ is the canonical Poisson matrix of size $2n$ and that due to the definition of d being a symplectic map, the Jacobian $\boldsymbol{D}_{\boldsymbol{x}} d(\boldsymbol{x})$ has full column rank.

In order to construct the reduced order model, we introduce the time-continuous residual of the high-dimensional model

$$r\left(t;\boldsymbol{\mu}\right) := \frac{\mathrm{d}}{\mathrm{d}t}\widetilde{\boldsymbol{x}}(t;\boldsymbol{\mu}) - \mathbb{J}_{2N}\nabla_{\boldsymbol{x}}\mathcal{H}(\widetilde{\boldsymbol{x}}(t;\boldsymbol{\mu});\boldsymbol{\mu}),$$

with respect to the reconstructed solution $\widetilde{\boldsymbol{x}}(t;\boldsymbol{\mu})$. We assume that the symplectic projection

$$\left(\boldsymbol{D}_{\boldsymbol{x}_r} d(\boldsymbol{x}_r(t;\boldsymbol{\mu}))\right)^{+} r\left(t;\boldsymbol{\mu}\right) \stackrel{!}{=} \mathbf{0}_{2n}, \tag{1}$$

of the residual, i.e., projection with the symplectic inverse

$$\left(\boldsymbol{D}_{\boldsymbol{x}} d(\boldsymbol{x})\right)^{+} := \mathbb{J}_{2n}^{\mathsf{T}} \left(\boldsymbol{D}_{\boldsymbol{x}} d(\boldsymbol{x})\right)^{\mathsf{T}} \mathbb{J}_{2N},$$

vanishes. Equation 1 can be reformulated to

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{x}_r(t;\boldsymbol{\mu}) &= \left(\boldsymbol{D}_{\boldsymbol{x}_r} d(\boldsymbol{x}_r(t;\boldsymbol{\mu}))\right)^{+} \mathbb{J}_{2N}\nabla_{\boldsymbol{x}}\mathcal{H}(d(\boldsymbol{x}_r(t;\boldsymbol{\mu}));\boldsymbol{\mu}) \\ &= \mathbb{J}_{2n} \underbrace{\left(\boldsymbol{D}_{\boldsymbol{x}_r} d(\boldsymbol{x}_r(t;\boldsymbol{\mu}))\right)^{\mathsf{T}} \nabla_{\boldsymbol{x}}\mathcal{H}(d(\boldsymbol{x}_r(t;\boldsymbol{\mu}));\boldsymbol{\mu})}_{=\nabla_{\boldsymbol{x}_r}\mathcal{H}_r(\boldsymbol{x}_r(t;\boldsymbol{\mu});\boldsymbol{\mu})},\end{aligned}$$

and we arrive at the reduced problem: for given parameter $\boldsymbol{\mu} \in \mathcal{P}$, given reduced initial condition $\mathrm{s}\boldsymbol{x}_{r,0}(\boldsymbol{\mu}) \in \mathbb{R}^{2n}$, find $\boldsymbol{x}_r(\cdot;\boldsymbol{\mu}) \in C^1(I, \mathbb{R}^{2n})$ such that

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{x}_r(t;\boldsymbol{\mu}) = \mathbb{J}_{2n}\nabla_{\boldsymbol{x}_r}\mathcal{H}_r(\boldsymbol{x}_r(t;\boldsymbol{\mu});\boldsymbol{\mu}), \qquad \boldsymbol{x}_r(0;\boldsymbol{\mu}) = \boldsymbol{x}_{r,0}(\boldsymbol{\mu}), \tag{2}$$

with reduced Hamiltonian $\mathcal{H}_r(\cdot;\boldsymbol{\mu}) : \mathbb{R}^{2n} \to \mathbb{R}, \boldsymbol{x}_r \mapsto \mathcal{H}(d(\boldsymbol{x}_r);\boldsymbol{\mu})$.

For the reduced model in (2) it can be shown that for any $\boldsymbol{\mu} \in \mathcal{P}$ the error in the Hamiltonian is constant for all $t \in I$

$$\Delta\mathcal{H}(t;\boldsymbol{\mu}) := |\mathcal{H}(\boldsymbol{x}(t;\boldsymbol{\mu});\boldsymbol{\mu}) - \mathcal{H}(\widetilde{\boldsymbol{x}}(t;\boldsymbol{\mu});\boldsymbol{\mu})|,$$

which is due to the property that the Hamiltonian is preserved over time for the high-dimensional model as well as for the reduced model. Additionally, we are able

to provide stability results in the sense of Lyapunov, as well as derive a rigorous error bound, see [1].

For the numerical experiments, we provide results for a linear wave equation for which a slow decay of the Kolmogorov-n-width can be observed, see e.g. [3, 4]. The map d is constructed via a weakly symplectic deep convolutional autoencoder, which is an extension of the deep convolutional autoencoder provided in [5]. For the detailed description of the weakly symplectic deep convolutional autoencoder and further numerical results, we refer to [1].

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Deep Barron Classes — Continued

Mathias Oster

(joint work with Angela Kunoth and Reinhold Schneider)

We seek to learn a function f by deep neural networks with activation function σ. An abstract optimal control problem with measure-valued controls $\mu(t)$ of the form

$$\min_{\mu(\cdot)} \mathcal{J}(\mu(\cdot)), \quad \mathcal{J}(\mu(\cdot)) := \int_{\mathbb{R}^d} \|f(x) - \int a\sigma(A\ z(T,x) + b)\ d\mu(t;a,A,b)\|^2 dx$$

$$\text{such that} \quad \frac{d}{dt} z(t,x) = \int a\sigma(Az(t,x) + b)\, d\mu(t;a,A,b), \quad z(0,x) = x$$

provides an interesting mathematical framework to analyse the expressivity and optimization of such networks from a continuous point of view. This control problem can be seen as an infinite deep neural network where the last layer is of a special form. We exploit the ideas of Barron spaces as continuous interpretation of infinite wide shallow networks and neural ODEs as infinite deep residual network architectures.

We show the existence of minimizers to the optimal control problem by using Prokhorov's theorem on tight measures and some regularity assumptions on the activation function [3].

Secondly, we analyse corresponding gradient flows in the space of probability measures [1]. To this end, we introduce the Wasserstein metric on probability measures with bounded second moment and define the notion of absolute continuous curves. We define a notion of Wasserstein gradient and exemplify it on the example of a potential functional $\mathcal{E}(\mu) = \int V(u)d\mu(u)$ for some twice continuously differentiable function V. By using the equivalence of absolute continuous curves and solutions to the continuity equation, we can state the gradient flow equations for the optimal control problem. We sketch the proof of existence of gradient flows based on the so-called generalized minimizing movement [3].

It was shown in [2] that, if a gradient point has a limit point within support of all of $\mathbb{R}^M$, it is a global minimizer. It is not clear whether this statement holds true in the above context.

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Computing Certain Invariants of Topological Spaces of Dimension Three

Marc Dambrine

(joint work with F. Caubet, G. Gargantini, B. Puig, S. Zerrouq)

The optimisation of structures under different types of constraints is a core problem in mechanical engineering. In the last decades, topological and shape optimisation techniques have provided engineers with alternative tools for designing better performing structures. One of the main aspects that engineers have to consider when designing a mechanical structure is the treatment of uncertainties, both in the shape itself and in the applied loads. This paper deals with the optimisation of elastic structures in this context of taking into account uncertainties in the definition of the criterion to be optimised.

In a first step, I presented a worst case approach to solve the inverse homogenization problem taking into account geometrical uncertainties. Additive manufacturing allows to produce parts with a structure typical of porous media and one may then want to produce materials with a given Hooke tensor and a given density. Unfortunately, the manufacturing process does not allow for perfect surface finishes. These uncertainties about the actual shape must be taken into account

when designing optimisation tools for microstructures. I have presented this approach in the spirit of the linearisation-based framework given by Allaire and Dapogny. In other words, we try to compute a microstructure that generates the desired homogenised tensor and that should also be insensitive to small geometrical perturbations by penalising the shape gradient. Let me give more precise statements.

Assume that, in a given macroscopic domain, there is a periodic distribution of holes inside an isotropic elastic solid phase, with constant elasticity tensor A. The periodicity size is denoted $\alpha > 0$. Let $Y = [0,1]^N$ be the rescaled unit periodic cell, where N is the space dimension. Inside this unit periodicity cell, the solid domain is the subset $\Omega \subset Y$, its complement being holes with boundary $\Gamma = \partial\Omega$. When $\alpha \to 0$, the medium can be considered homogeneous, with an effective constant elasticity tensor A^*. To compute this homogenized tensor A^*, one needs so-called correctors $w_{ij} \in \mathbb{H}^1_{\#}(Y)$ (defined below in sub-section (2.1)), corresponding to the local displacement in the cell Y, defined for each pair $(i,j) \in \{1,2,\ldots,N\}^2$ as the solutions of the following cell problems

$$\left\{ \begin{array}{lll} \operatorname{div}\left(A\left(e_{ij} + \epsilon\left(w_{ij}\right)\right)\right) & = 0 & \text{in } \Omega \\ A\left(e_{ij} + \epsilon\left(w_{ij}\right)\right) \cdot n & = 0 & \text{on } \Gamma \\ y \mapsto w_{ij}(y) & & [0,1]^N - \text{ periodic} \end{array} \right.$$

where $e_{ij} = \frac{1}{2}\left(e_i \otimes e_j + e_j \otimes e_i\right)$ is a basis for symmetric tensors of order 2, n is the normal to the boundary Γ in Ω, and $\epsilon\left(w_{ij}\right) = \frac{1}{2}\left(\nabla w_{ij} + {}^t\nabla w_{ij}\right)$ is the symmetric strain tensor. The family of functions w_{ij} can be used to define the effective tensor $\mathbf{A}^* = \left[A_{ijkl}\right]_{i,j,k,l=1}^N$ in accordance with

$$A^*_{ijkl}(\Omega) = \int_Y A\left(e_{ij} + \epsilon\left(w_{ij}\right)\right) : \left(e_{kl} + \epsilon\left(w_{kl}\right)\right) dy \quad \forall i,j,k,l \in \{1,2,\ldots,N\}$$

Let us consider a given tensor $\mathbf{G} \in \mathbb{R}^{N\times N}_{sym}$ describing the desired material properties. The robust inverse homogenization problem is then: can we find a periodic hole structure (that is a domain Ω) such that the effective tensor is as close as possible to $\mathbf{G}$, while being the least sensitive to geometric perturbations? Let us make this vague statement precise.

We follow the strategy of of the previous work [2] and choose the Frobenius norm on matrices to make precise the notion of closeness between matrices and we define the main objective $J(\Omega)$

$$J(\Omega) = \frac{1}{2}\left\|\mathbf{A}^*(\Omega) - \mathbf{G}\right\|_F^2 = \frac{1}{2}\sum_{1\le i,j\le d}\left(A^*_{ijkl}(\Omega) - G_{ijkl}\right)^2$$

as a least square matching of the desired properties. For $\theta \in \mathbb{W}^{1,\infty}\left(\mathbb{R}^N, \mathbb{R}^N\right)$ a perturbation vector of magnitude $\|\theta\|_{\mathbb{W}^{1,\infty}(\mathbb{R}^N,\mathbb{R}^N)} \le \delta$, the shape gradient of $J(\Omega)$ in the direction θ writes

$$J'(\Omega)(\theta) = \int_\Gamma (\theta \cdot n) k(\Omega)$$

Here, $k(\Omega)$ is the scalar field given by

$$k(\Omega) = \sum_{1\leq i,j,k,l\leq N} \left(A^*_{ijkl}(\Omega) - G_{ijkl}\right) A\epsilon\left(\phi_{ij}\right) : \epsilon\left(\phi_{kl}\right).$$

The robust matching criterion $\mathcal{J}_{2,\delta}(\Omega) = J(\Omega) + \delta\|k(\Omega)\|^2_{L^2(\Gamma)}$ is well defined for $\delta > 0$ in the spirit of Allaire and Dapogny's work. It is shape differentiable for all $\Omega \in \mathcal{A}(Y)$, and its shape derivative is given by

$$\mathcal{J}'_{2,\delta}(\Omega)(\theta) = \int_\Gamma (\theta\cdot n)\left[k(\Omega) + \delta\left(\sum_{1\leq i,j\leq N} A\epsilon\left(\phi_{ij}\right) : \epsilon\left(p_{ij}\right) + \partial_n\left(k(\Omega)^2\right) + \mathcal{H}k(\Omega)\right)\right]$$

where $\mathcal{H}$ is the main curvature to the boundary Γ, and the adjoint states p_{ij} are solutions to the following problems :

$$\int_\Omega A\epsilon\left(p_{ij}\right) : \epsilon(\psi) + 2\sum_{1\leq k,l\leq N}\int_\Omega A\epsilon\left(\phi_{kl}\right) : \epsilon(\psi)\int_\Gamma k(\Omega) A\epsilon\left(\phi_{ij}\right) : \epsilon\left(\phi_{kl}\right) = 0$$

for all $\psi \in \mathbb{H}^1_{\#}(Y)$.

In a second step, I presented an approach to optimize an elastic structure subjected to random mechanical loading, we are interested in the solution of shape optimization problems where the expectation of a polynomial function of the state appears as an objective or among constraints: Find a domain Ω_{opt} minimizing the objective $\mathbb{E}[\mathcal{J}(\Omega, \mathbf{g})]$ over a class of admissible domains where, for all event $\omega \in \mathcal{O}$, the state $\mathbf{u}_\Omega \in \left[\mathrm{H}^1(\Omega)\right]^d$ solves:

$$\begin{cases} -\operatorname{div}\boldsymbol{\sigma}\left(\mathbf{u}_\Omega\right) = \mathbf{0} & \text{in } \Omega, \\ \boldsymbol{\sigma}\left(\mathbf{u}_\Omega(\omega)\right)\mathbf{n} = \mathbf{g}(\omega) & \text{on } \Gamma_{\mathrm{N}}, \\ \boldsymbol{\sigma}\left(\mathbf{u}_\Omega(\omega)\right)\mathbf{n} = \mathbf{0} & \text{on } \Gamma_0, \\ \mathbf{u}_\Omega(\omega) = \mathbf{0} & \text{on } \Gamma_{\mathrm{D}}. \end{cases}$$

The sensitivity analysis of the objective and the constraints is studied following the method of differentiation with respect to the shape in the sense of Hadamard. In order to deal with the random aspects of the problem, we extend the approach of [1] to the case of polynomial functions of degree m of the state. In particular, we provide a deterministic expression for the expectation of the functional of interest and its derivative, which depends only on the first m random moments of the loading. This approach is presented for two application cases. The first one studies the sensitivity of the variance of a quadratic functional to the shape, with the only knowledge of the first four moments of the random variable that models the loading of the structure. The second example is related to the approximation of the L^∞ norm of a real-valued function defined on a domain, by its L^m norm, when m is sufficiently large. In particular, we study a problem where we look for the elastic structure of minimum mass, for which the norm L^m of the von Mises stress is bounded by a constant. A typical result of such a simulation is shown in Figure 1. This approach is particularly interesting for industrial applications

FIGURE 1. Example of minimization of the volume under a bound on the expectation of the L^6 norm of von Mises stress.

because one of the main concerns in the design of structures is to avoid the high concentration of mechanical stresses, in order to avoid damage or cracking of the object.

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Time-Dependent Problems: Nonsmoothness, Optimization and Optimal Control

STEFAN VOLKWEIN

(joint work with Behzad Azmi, Marco Bernreuther, Luca Mechelli, Andrea Petrocchi, Jan Rohleff)

In the first part of the talk, a nonsmooth semilinear parabolic partial differential equation (PDE) is considered. For a reduced basis (RB) approach, a space-time formulation is used to develop a certified a-posteriori error estimator. This error estimator is adopted to the presence of the discrete empirical interpolation method (DEIM) as approximation technique for the nonsmoothness. The separability of the estimated error into an RB and a DEIM part then guides the development of an adaptive RB-DEIM algorithm, combining both offline phases into one. Numerical experiments show the capabilities of this novel approach in comparison with classical RB and RB-DEIM approaches. The results are published in [4] which is an extension of the elliptic case considered in [3].

In the second part of the talk we study a nonlinear elliptic-parabolic system, which is motivated by mathematical models for lithium ion batteries; cf. [1, 12]. One state satisfies a parabolic reaction diffusion equation and the other state a elliptic equation. The states are coupled through a strongly non-linear function, and this makes the evaluation of online-efficient error estimates difficult. First

we prove the well-posedness of the system, then show a possible discretization by the RB-DEIM method and finally describe an algorithm for the evaluation of approximated hierarchical a-posteriori error estimators based on [6]. Then, the numerical results show good approximations and efficiencies with a relatively small number of bases. For that reason we turn to parameter optimization problems for the coupled elliptic-parabolic system. We utilize the RB method with the hierarchical error estimation in an adaptive trust-region framework (cf. [2, 5, 9, 13]) and enrich the RB approximation spaces on-the-fly. Numerical examples illustrate the efficiency of the proposed approach.

Finally, the last part of the talk optimal control problems for linear parabolic PDEs with time-dependent coefficient functions are considered. After applying a finite element (FE) discretization the PDEs can be described by linear time variant (LTV) dynamical systems. The associated first-order optimality system can be interpreted as a coupled LTV dynamical system. Due to the large-dimensional FE discretization reduced order modeling is applied. Here, an empirical gramian approach (cf. [10] and [7, 8]) is directly applied to the optimality system. This strategy is efficiently tested for a multiobjective optimal control problem and a closed-loop problem solved by a model predictive control method. The results are compared with the ones obtained by applying a proper orthogonal decomposition reduced order modeling. The results are published in [11].

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Model Reduction and Learning for PDE Constrained Optimization

Mario Ohlberger
(joint work with S. Banholzer, B. Haasdonk, T. Keil, H. Kleikamp, L. Mechelli, M. Oguntola, F. Schindler, S. Volkwein, T. Wenzel)

Model order reduction for parameterized systems has gained much attention in the last two decades. Classically, it is based on a so-called offline phase, where reduced approximation spaces are constructed and the reduced parameterized system is built, followed by an online phase, where the reduced system can be cheaply evaluated in a multi-query context [1]. In this contribution we propose to overcome this offline-online paradigm in the context of PDE-constrained optimization problems by an adaptive learning or enrichment approach where appropriate surrogate models are constructed on-the-fly within an outer optimization loop.

Specifically, we are interested in efficient approximation strategies to solve general PDE-constrained optimization problems of the form

$$\min_{\mu\in\mathcal{P}_{\mathrm{ad}}} J(\mu,u), \text{ such that } e(u;\mu)=0 \text{ in } W', \tag{1}$$

where $J:\mathcal{P}\times V\to\mathbb{R}$ denotes the objective functional and $e(\cdot;\mu):V\to W'$ a residual encoding the parameter dependent state equation (PDE). $\mathcal{P}, V, W$ denote suitable Banach spaces and $\mathcal{P}_{\mathrm{ad}}\subset\mathcal{P}$ a set of admissible parameters.

As a general class of optimization methods to solve (1) we consider descent methods, i.e., for suitable chosen initial value μ^0 we iteratively compute

$$\mu^{k+1} := \mu^k + t^k d^k(\mu^k, u_{\mu^k}, p_{\mu^k}, \dots),$$

where t^k and d^k are suitably chosen step sizes and descent directions for the objective functional, respectively. Depending on the complexity of the problem at hand, the descent directions may be computed from evaluations of the objective functional, from its gradient or even from its hessian with respect to μ. Typically this does not only involve the solution of the state equation $e(u_{\mu^k};\mu^k)=0$ in W', but also the solution $p_{\mu^k}\in W$ of the adjoint equation and possibly solutions of additional equations to obtain sensitivities of the state and the dual solution, etc. Hence, the efficiency of the method scales inversely with the computational complexity to solve the state and adjoint equations.

The principal idea to speed up such methods is to construct a hierarchy of M approximation models at each iteration step k, i.e., at hierarchy level $m=1,2,\dots,M$,

solving for $u_m^k \in V_m^k$ of

$$e_m^k(u_m^k;\mu) = 0 \text{ in } (W_m^k)', \tag{2}$$

with decreasing model complexity $\mathcal{C}_1^k \geq \mathcal{C}_2^k \geq \dots$ and increasing approximation error $||u - u_1^k|| \leq ||u - u_2^k|| \leq \dots$ with the goal to replace as many costly model evaluations as possible by cheaper ones while keeping a guaranteed accuracy for the overall solution of the optimization problem. Examples of such hierarchies of models are e.g., given by classical finite element type discretization schemes with different grid resolutions as well as corresponding reduced order or machine learning surrogate models.

In [2, 3, 4] we investigated such an approach for optimization problems constrained by second-order elliptic PDEs within a trust region optimization framework. Rigorous a posteriori error estimates were derived and the convergence of the resulting multi-fidelity approximation scheme was proven. The construction of the model hierarchy is thereby based on reduced basis methods that are constructed on the fly during the outer optimization loop without any pre-computation in an offline phase. In [5] this concept has been generalized to localized model order reduction for multi-scale problems within the framework of localized orthogonal decomposition methods [6]. Numerical experiments have been conducted with `PyMOR`[1] [7] for the model reduction as well as `dune-gdt`[2] and the DUNE framework [8] for the finite element type discretizations.

Finally, in [9, 10] the concept has been extended to machine learning based surrogate models for time-dependent PDE-constrained parameter optimization and optimal control. A hierarchical framework of full order, reduced order, and machine learning models is introduced in [9] for parameterized parabolic equations that can be queried in any context with a prescribed accuracy. The resulting hierarchical model adaptively updates its hierarchy if it is queried for parameters where either the machine learning model or the reduced order model is not accurate enough. The accuracy is thereby measured by a rigorous a posteriori error estimator that can be used by both the reduced order and machine learning model since the machine learning model approximates in the same space as the reduced order model. As machine learning approaches, deep neural networks were studied as well as kernel and deep kernel methods [11]. In [10], the hierarchy only consists of a full order model and a deep neural network based machine learning model built from snapshots of the full order model. Therefore, a rigorous a posteriori error analysis of the model reduction is unavailable. However, the hierarchy of available models has still been used for rigorous certification of the overall optimization algorithm.

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