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MODEL REDUCTION AND LEVEL SET METHODS FOR SHAPE OPTIMIZATION PROBLEMS

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Toni Lassila: *Model reduction and level set methods for shape optimization problems*; Helsinki University of Technology Institute of Mathematics Research Reports A593 (2010).

Abstract:

In this work two topics related to mathematical shape optimization are considered. Topological optimization methods need not know the correct topology (number of connected components and possible holes) of the optimal shape beforehand. Shape optimization can be performed by a topological gradient descent algorithm. Computational applications of topological optimization and level set based shape optimization involve the optimal damping of vibrating structures and an inverse problem of reconstructing a shape based on noisy interferogram measurements.

For parametric shape optimization with partial differential constraints the model reduction approach of reduced basis methods is considered. In the reduced basis method a basis of snapshot solutions is used to construct a problem-dependent approximation space that has much smaller dimension than the underlying finite element approximations. The state constraints for optimization are then replaced with their reduced basis approximation, leading to efficient shape optimization methods. Computational examples involve the optimal engineering design of airfoils in potential and thermal flow.

AMS subject classifications: 35R35, 49Q10, 65K10

Keywords: shape optimization, topological optimization, level set method, model reduction, reduced basis method, partial differential equations

Toni Lassila: *Mallien redusointi ja tasa-arvojoukkojen menetelmät muodon optimoinnin tehtäville*

Tiivistelmä:

Tässä työssä tarkastellaan kahta matemaattiseen muodon optimointiin liittyvää aihetta. Topologiset optimointimenetelmät eivät tarvitse etukäteistietoa optimaalisen muodon oikeasta topologiasta (yhtenäisten komponenttien tai mahdollisten reikien lukumäärä). Muodon optimointia voidaan suorittaa topologisen gradienttimenetelmän avulla. Topologisen optimoinnin ja tasa-arvojoukkojen menetelmään perustavan muodon optimoinnin laskennallisia sovelluksia työssä ovat värähtelevän rakenteen optimaalinen vaimennus sekä inversio-ongelma, jossa muoto päätellään kohinaisista interferometrimittauksista.

Parametrista riippuviin muodon optimointitehtäviin sovelletaan redusoidun kannan menetelmää tehtävän laskennallisen kustannuksen pienentämiseksi, kun tehtävään liittyy osittaisdifferentiaaliyhtälörajoitteita. Redusoidun kannan menetelmässä rakennetaan tehtävästä riippuva approksimaatioavaruus, jonka dimensio on paljon pienempi kuin vastaavan elementtimenetelmän tuottaman approksimaation. Tilanyhtälörajoitteet korvataan redusoidun kannan antamilla approksimaatioilla, mikä johtaa tehokkaaseen muodon optimoinnin menetelmään. Laskennallisia esimerkkejä esitellään optimaalisesta suunnittelusta potentiaalivirtauksessa sekä lämpövirtauksissa.

Avainsanat: muodon optimointi, topologinen optimointi, tasa-arvojoukkojen menetelmä, mallin redusointi, redusoidun kannan menetelmä, osittaisdifferentiaaliyhtälöt

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Otaniemi, September 2010,

Toni Lassila

List of included publications

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[A] Toni Lassila. Optimal damping of a membrane and topological shape optimization. *Structural and Multidisciplinary Optimization*, **38(1)** (2009), 43–52.

[B] Timo Eirola, Toni Lassila. Optimization of convex shapes: an approach to crystal shape identification. In: Xue-Cheng Tai, Knut Mørken, Marius Lysaker, Knut-Andreas Lie (Eds.) *Proceedings of the 2nd International Conference on Scale Space and Variational Methods in Computer Vision*, Voss, Norway. Lecture Notes in Computer Science, Springer (2009), 660–671.

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Author's contribution

The author of the thesis is the primary author of all the articles and is responsible for the computational examples presented in them. In article [D] Gianluigi Rozza and Andrea Manzoni contributed some additional computational examples of the error bounds. Articles [A] and [B] were prepared under the supervision and collaboration of Prof. Timo Eirola at the Institute of Mathematics, Helsinki University of Technology. Articles [C] and [D] were prepared under the supervision of Prof. Alfio Quarteroni and in collaboration with Dr. Gianluigi Rozza at the Institute of Analysis and Scientific Computing, École Polytechnique Fédérale de Lausanne during the author's nine month visit there in 2008–09. Article [E] is a continuation of the work done in [C] and [D].

Contents

I Summary

1 Introduction

This thesis develops and analyzes new numerical methods for shape optimization as well as free boundary problems that can be treated with similar methods. Shape optimization is a part of the field of mathematical optimization theory that is concerned with finding a geometric shape (open subset of Euclidean space with piecewise smooth boundary) that is optimal with respect to some cost functional that depends explicitly or implicitly on the shape. The implicit dependence on the shape is often through the solution of a partial differential equation (PDE), in which case it is called a PDE constrained shape optimization problems. Applications of PDE constrained shape optimization arise for example in industrial design of structures. Shape optimization is usually divided into two schools: parametric shape optimization and shape sensitivity analysis. Another recent trend are the so-called topological optimization methods.

Parametric shape optimization works by introducing first a way to describe the admissible shapes using a finite-dimensional parameter vector. The shape optimization problem is then written as a finite-dimensional nonlinear programming problem [9] with the parameters as the design variables. This approach is common is engineering applications such as aero- and hydrodynamic design [52] and structural design [41], because it can be readily coupled with existing optimization software. The parameterizations can be obtained using techniques such as boundary splines [25], basis shapes [68], or free-form deformations [70], to mention a few options from literature.

Shape sensitivity analysis extends the concept of derivatives as a measure of sensitivity of the cost functional to small changes in the shapes. By computing analytical expression for the shape derivative [74] it is possible to talk about descent directions for shape functionals and thus extend existing finite-dimensional optimization algorithms to the infinite-dimensional manifold of admissible shapes [75]. The shape sensitivity analysis can be performed either in continuous or discrete setting [77]. It should be noted that the resulting optimal design can be different depending on which step is performed first (*discretize first then optimize* vs. *optimize first then discretize*) [24].

Topological optimization methods remove the requirement that the shape be described explicitly by its boundary curve/surface. Instead they use implicit descriptions of the shapes using methods such as level sets [16, 18] or phase-fields [12]. The first concepts of topological sensitivity can be found in the works of Jean Céa in the 1970s [23]. Topological methods do not a priori assume that the shape in question has a fixed topology. That is to say, its number of connected components and their genus do not need to be fixed, but can vary during the course of the optimization iteration. The shape and topological optimization methods have also been successfully combined [73, 78]. For a comprehensive review of topological optimization, see [30].

A common feature in many shape optimization problems is the existence of an underlying physical system that is modelled using partial differential equations [31]. The shape defines the computational domain for the state equations in PDE form, which can be solved to obtain the state of the system. The value of the shape functional can then depend on both the state as well as the shape. When deriving shape sensitivities the sensitivity of the state solution must also be taken into account. This is often accomplished through defining an adjoint state [45], which turns out (in the linear case) to be the solution of a related PDE on the same domain. Together the state and adjoint state can be used to compute the shape gradient in PDE-constrained shape optimization problems. The adjoint approach has the benefit of minimizing the number of PDE solutions needed to evaluate the shape gradient. This is especially important in the nonparametric setting, or in parametric shape optimization when the number of shape parameters is large.

The solution of the state and adjoint state equations is the computationally most involving part of PDE-constrained shape optimization problems. As analytical solutions of PDEs are available only in very simple domains the applied shape optimization methods found in literature almost always rely on numerical approximations to the PDE solutions. The most popular choice for discretization is the finite element method (FEM) [13], where a discrete mesh is constructed on the given domain and the solution to the variational formulation of the PDE is sought in a finite-dimensional subspace of piecewise polynomial functions that have support only on a limited number of elements of the discrete mesh. The FEM results in a large system of linear equations to be solved with methods of computational linear algebra [33]. In realistic applied shape optimization problems these systems can have millions of degrees of freedom. In shape optimization problems there is the additional cost of reassembling the matrix corresponding to the linear system, because the mesh and by extension the matrix depend heavily on the domain (and thus the shape). Because the cost of the PDE solutions dominates the computational workload of applied shape optimization, there is much interest in more efficient methods for approximating the solutions of the state and adjoint state equations. This leads to the model reduction techniques for parametric PDEs discussed in this thesis.

The structure of this thesis is the following: in Sect. 2 the most important aspects of numerical methods for shape optimization are briefly reviewed. In Sect. 3 a prototype shape optimization problem with elliptic PDE constraints is defined. In Sect. 4 the approach of describing the shapes with implicit functions is introduced, and level set methods for shape optimization are discussed. A special case of these are the topological level set methods. In Sect. 5 the attention turns to the question of surrogate optimization via a model reduction of the state equations. The reduced basis method is introduced, as well as the related empirical interpolation method. In Sect. 6 the contributions of the thesis to the state of the art are outlined. The rest of the thesis contains the actual research contributions in the form of five independent research articles.

2 Review of numerical methods for shape optimization

Numerical methods for shape optimization require first choosing how to represent the shapes. A geometric shape can be represented in a multitude of ways, and the choice of its representation dictates the type of numerical scheme. Three different approaches can be identified. These are boundary tracking methods, immersed boundary methods, and fixed domain methods.

In *boundary tracking methods* there exists an explicit description of the boundary of the shape at all times, and it is possible to construct a discrete mesh on geometry that matches the boundary. Then the FEM can be applied on the discrete mesh to compute numerical approximations for the shape gradients, a descent step can be performed in the discrete sense by moving the boundary mesh points in such a way that the value of the cost functional is expected to decrease, and then the mesh is updated to reflect the new geometry and this step is iterated until a sufficiently improved design has been found. The gradients are usually computed by the adjoint approach for computational efficiency, and can either be derived analytically or obtained through a process known as algorithmic differentiation [36]. The latter refers to the application of the chain rule of derivation directly to algorithmic program codes, and enables the applied shape optimization of very complicated systems where the analytical derivatives are not easily forthcoming.

In *immersed boundary methods* an explicit description of the boundary is not used. While an approximation of the boundary can usually be constructed, it is preferred to work without it. When the shape optimization problem includes partial differential equation constraints, the computational domain is extended from just the (a priori unknown) shape to a fixed exterior domain and then the PDE coefficients become the optimization variables that codify the geometric shape to be optimized. This is the fictitious domain approach [38]. The classical idea of discrete 0-1 optimization, where each discretization cell either contains material or doesn't, has been largely abandoned [11] as refining the discretization mesh tends to result in unwanted "swiss cheese" type optimal solutions. The homogenization approach [2], where the design variables vary continuously in the range $(0, 1)$, is preferred. The drawback is that sometimes the resulting optimal shapes have fuzzy boundaries and a post-processing step may be required to recover the final shape.

In this thesis the *fixed domain approach* is also applied. This means that the admissible shapes are taken to be images of a fixed reference shape under a smooth, invertible mapping. The shape mapping can be defined as a function of a finite-number of parameters, which makes it a parametric shape optimization problem. The state equations are then mapped back to the reference domain and become parameter-dependent PDEs on a fixed domain. This approach is suitable for small deformations of shapes, without any topological changes. The difficulties relating to geometric variability are removed, but the parameter-dependence of the PDE coefficients makes the analysis and numerical solution of these equations more challenging.

3 Prototype shape optimization problem

To fix terms and the notation a prototype PDE constrained shape optimization problem is introduced next. Let $\mathcal{S}_{ad}$ be the set of admissible shapes $\Omega \subset \mathbb{R}^d$. Define for each Ω the Hilbert space $X(\Omega)$ of functions on Ω with norm $||\cdot||_X$. Let $J : X(\Omega) \to \mathbb{R}$ be lower-semicontinuous functional in a suitable topology, i.e.:

> For every convergent sequence $\{v_n\}_{n=1}^{\infty}$ s.t. $v_n \to v_0$ it holds that $\liminf_{v \to v_0} J(v) \geq J(v_0)$

The prototype for a PDE constrained shape optimization problem is to find the optimal shape Ω^* that solves

$$\begin{aligned} \min_{\Omega \in \mathcal{S}_{ad}} \quad & J(u(\Omega)) \\ s.t. \quad & \mathcal{A}(u(\Omega), v) = F(v) \quad \text{for all } v \in V(\Omega), \end{aligned} \tag{3.1}$$

where $V(\Omega) \subset X(\Omega)$ is a subspace of all functions v satisfying the Dirichlet boundary condition

$$v \equiv 0 \quad \text{on } \Gamma_d \subset \partial\Omega. \tag{3.2}$$

The PDE is given in the variational form with $\mathcal{A} : X(\Omega) \times X(\Omega) \to \mathbb{R}$ an elliptic bilinear form, i.e. there exist constants $\alpha > 0$ and $\gamma > 0$ s.t.

$$\begin{aligned} \mathcal{A}(v, v) &\geq \alpha ||v||_X^2, && \text{for all } v \in X(\Omega) \quad \text{(coercivity)} \\ |\mathcal{A}(u, v)| &\leq \gamma ||u||_X ||v||_X, && \text{for all } u, v \in X(\Omega) \quad \text{(continuity)} \end{aligned} \tag{3.3}$$

and $F : X(\Omega) \to \mathbb{R}$ a continuous linear form. The function $u(\Omega)$ is called the state solution on a given domain Ω. By suitable regularity assumptions for the admissible shapes $\mathcal{S}_{ad}$, for example the ε-cone property or the uniform Lipschitz property [62], one can prove the existence of an optimal shape Ω^* via an argument of a minimizing sequence and the lower-semicontinuity of J. For further analysis on the requirements for $\mathcal{S}_{ad}$ and the topologies used to guarantee the existence of solutions to shape optimization problems, see [39].

The discrete version of the prototype problem (3.1) involves for each Ω a domain-dependent quasi-uniform ([13], p.108) triangular mesh $\mathcal{T}_{h,\Omega}$ with elements $K \in \mathcal{T}_{h,\Omega}$ having diameter h_K s.t. $h := \max_{K \in \mathcal{T}_{h,\Omega}} h_K$, and the finite element subspace of continuous piecewise-polynomial functions

$$V_h(\Omega) := \{v \in V(\Omega) \cap C(\Omega) \ : \ v|_K \in \mathcal{P}_k(K)\} \tag{3.4}$$

where $\mathcal{P}_k(K)$ denotes the space of polynomials of degree no greater than k on K. Denote the set of all polygonal domains as $\mathcal{S}_{poly}$. The discretized shape optimization problem is to find the optimal polygonal shape Ω_h^* that solves

$$\begin{aligned} \min_{\Omega_h \in \mathcal{S}_{ad} \cap \mathcal{S}_{poly}} \quad & J(u_h(\Omega_h)) \\ s.t. \quad & \mathcal{A}(u_h(\Omega_h), v_h) = F(v_h) \quad \text{for all } v_h \in V_h(\Omega_h). \end{aligned} \tag{3.5}$$

The discrete problem satisfies the mesh-independence principle [46] if its solution for h small enough is independent of the choice of the discretization mesh $\mathcal{T}_{h,\Omega}$. The convergence of $\Omega_h^* \to \Omega^*$ as $h \to 0$ is discussed e.g. in [29].

4 Level set methods in shape optimization

In the level set formulation the shapes Ω are represented as the level sets of Lipschitz-continuous functions $\phi : \mathbb{R}^d \to \mathbb{R}$, called implicit functions. Define

$$\Omega = \{\boldsymbol{x} \mid \phi(\boldsymbol{x}) < 0\}, \quad \Omega^c = \{\boldsymbol{x} \mid \phi(\boldsymbol{x}) \geq 0\}. \tag{4.6}$$

In addition the requirement that $\nabla\phi(\boldsymbol{x}) \neq 0$ almost everywhere on $\partial\Omega$ is imposed. This enforces a sharp interface between Ω and its open complement. The benefit of the implicit function approach is that there is no need for an explicit description for the boundary of the shape, which simplifies the implementation of numerical schemes because the mesh does not necessarily have to conform to the boundary of the shape.

4.1 Shape functionals for implicit functions

In the shape optimization problem (3.1) the shape Ω can now be replaced with its implicit function representant ϕ. For the two elementary types of shape functionals, the area and perimeter functionals, the transformation rules are obtained as in [18]

$$J(\Omega) = \int_\Omega f(\boldsymbol{x})\, d\boldsymbol{x} \quad \Longleftrightarrow \quad J(\phi) = \int_{\mathbb{R}^d} H(-\phi(\boldsymbol{x}))f(\boldsymbol{x})\, d\boldsymbol{x} \tag{4.7}$$

$$J(\Omega) = \int_{\partial\Omega} g(\boldsymbol{x})\, ds \quad \Longleftrightarrow \quad J(\phi) = \int_{\mathbb{R}^d} \delta_0(\phi(\boldsymbol{x}))|\nabla\phi(\boldsymbol{x})|g(\boldsymbol{x})\, d\boldsymbol{x} \tag{4.8}$$

where $H(\phi)$ is the Heaviside step function and $\delta_0(\phi)$ the delta distribution at $\phi = 0$. The classical shape sensitivity analysis can now be performed in terms of the implicit function ϕ. Let $\boldsymbol{w} \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$ be a smooth velocity field. If the level sets of ϕ are transported according to the velocity field $\boldsymbol{w}$ in time t, their evolution is described by the level set partial-differential equation

$$\begin{aligned} \frac{\partial\phi(\boldsymbol{x},t)}{\partial t} + \boldsymbol{w}(\boldsymbol{x}) \cdot \nabla\phi(\boldsymbol{x},t) = 0, \qquad & (\boldsymbol{x},t) \in \mathbb{R}^d \times (0,T) \\ \phi(\boldsymbol{x},0) = \phi_0(\boldsymbol{x}), \qquad & \boldsymbol{x} \in \mathbb{R}^d. \end{aligned} \tag{4.9}$$

The left-hand side is simply the Eulerian (material) derivative of ϕ. Note that the choice and scaling of the function $\phi_0(\boldsymbol{x})$ do not matter away from the boundary $\partial\Omega$. The classical shape derivative of J at Ω in the direction $\boldsymbol{w}$ can then be computed using the speed method [79] and the implicit function as the Gâteaux-derivative

$$d_S J(\Omega; w) = \lim_{\tau \to 0^+} \frac{J(\phi(\cdot,\tau)) - J(\phi(\cdot,0))}{\tau}, \tag{4.10}$$

where $\phi(\boldsymbol{x},\tau)$ satisfies (4.9). There are also alternative implicit function approaches that can be used to treat PDE constrained shape optimization problems, see [54].

4.2 Shape gradients and the descent algorithm

In addition to facilitating the computation of the shape derivatives, the level set formulation also allows one to write a descent algorithm for shape optimization. The Hadamard-Zolésio structure theorem [26] states that with some mild regularity assumptions the shape derivative takes the form

$$d_S J(\Omega; \boldsymbol{w}) = \int_{\partial\Omega} (\boldsymbol{w} \cdot \boldsymbol{n}) \nabla J(\boldsymbol{x}) \, ds, \tag{4.11}$$

where $\boldsymbol{n}$ is the exterior unit normal field at the boundary $\partial\Omega$, and $\nabla J \in L^2(\partial\Omega)$ is called the shape gradient (in the L^2 sense) that has support only on the boundary of the shape. Once the gradient has been computed, evaluations of the derivatives for different directions $\boldsymbol{w}$ is inexpensive. It is also possible to define different gradients by changing the inner product. Given any subspace $V \subset L^2(\partial\Omega)$ endowed with an inner product $\langle v_1, v_2 \rangle_V$ that makes the space complete the gradient with respect to the inner product in V can be defined as the unique element $\nabla_V J$ that satisfies

$$\langle \nabla_V J, v \rangle_V = \int_{\partial\Omega} (\nabla_V J) v \, d\Omega, \quad \text{for all } v \in V. \tag{4.12}$$

Note that for the implicit function ϕ the exterior unit normal $\boldsymbol{n}$ at the boundary $\partial\Omega$ can be computed by $\boldsymbol{n} = \nabla\phi/|\nabla\phi|$.

A gradient descent algorithm for shapes proceeds as follows: Let Ω_0 be an initial guess for the shape and ϕ_0 a corresponding implicit function. For each iteration $k = 0, 1, 2, \ldots$ the shape gradient $\nabla_V J$ at Ω_k is computed and in (4.9) the normal velocity field set equal to the negative gradient, $\boldsymbol{w} = -(\nabla_V J)(\nabla\phi/|\nabla\phi|)$. This results in the evolution equation for the kth descent step

$$\begin{aligned} \frac{\partial\phi(\boldsymbol{x},t)}{\partial t} - \nabla_V J(\boldsymbol{x})|\nabla\phi(\boldsymbol{x},t)| = 0, \qquad & (\boldsymbol{x},t) \in \mathbb{R}^d \times (0, \Delta t) \\ \phi(\boldsymbol{x},0) = \phi_k(\boldsymbol{x}), \qquad & \boldsymbol{x} \in \mathbb{R}^d. \end{aligned} \tag{4.13}$$

to be solved for a short pseudo-time step $\Delta t > 0$. The shape for the next iteration, Ω_{k+1}, is given as the 0-level set of $\phi(\cdot, \Delta t)$. If the pseudo-time step is small enough this iteration will result in a sequence of shapes $\{\Omega_k\}_{k=1}^{\infty}$ that gives monotonically decreasing values in $J(\Omega_k)$. To choose the length of the pseudo-time step Δt without an expensive line search procedure, one can use e.g. the Armijo rule [6].

Equation (4.9) is nonlinear evolution equation of the Hamilton-Jacobi class of PDEs:

$$\frac{\partial\phi(\boldsymbol{x},t)}{\partial t} + H(\nabla\phi(\boldsymbol{x},t)) = G(\boldsymbol{x},t), \quad (\boldsymbol{x},t) \in \mathbb{R}^d \times (0,T). \tag{4.14}$$

Typically, existence and uniqueness of solutions can be shown in the weak sense of viscosity solutions [49]. This means the equation is converted to a hyperbolic-parabolic type

$$\frac{\partial\phi(\boldsymbol{x},t)}{\partial t} - \nabla_V J(\boldsymbol{x})|\nabla\phi(\boldsymbol{x},t)| = \varepsilon\triangle\phi(\boldsymbol{x},t), \quad (\boldsymbol{x},t) \in \mathbb{R}^d \times (0,T), \tag{4.15}$$

by adding an artificial viscosity term, where $\triangle = \sum_{i=1}^{d} \partial_{x_i x_i}$ denotes the Laplace operator, and studying the convergence of solutions as $\varepsilon \to 0$. Numerical solution schemes for level set equations are based on shock-capturing schemes [37, 47] originally designed for the numerical resolution of hyperbolic conservation laws, which retain the sharp boundary of the evolving interface without excessively smoothing out the details as is usually the case with artificial viscosity schemes. For more details on the numerical solution of level set equations, see [60, 71].

4.3 Topological level set methods

While the level set approach does permit certain types of topological changes due to the implicit description of the boundary of the shape, the speed method is still limited to diffeomorphic images of the initial shape and thus in practice can be slow or even unable to discover the correct topology in the case that the optimal shape consists of disjoint components. The topological derivative was defined in [72] as

$$d_T J(\Omega; \boldsymbol{x}^0) = \begin{cases} \lim\limits_{\rho \to 0^+} \dfrac{J(\Omega \cup B(\boldsymbol{x}^0, \rho)) - J(\Omega)}{|B(\boldsymbol{x}^0, \rho)|}, & \boldsymbol{x}^0 \notin \overline{\Omega} \\ \lim\limits_{\rho \to 0^+} \dfrac{J(\Omega \cap B(\boldsymbol{x}^0, \rho)) - J(\Omega)}{|B(\boldsymbol{x}^0, \rho)|}, & \boldsymbol{x}^0 \in \Omega \end{cases} \tag{4.16}$$

where $B(\boldsymbol{x}^0, \rho)$ denotes a ball of radius ρ centered at $\boldsymbol{x}^0$, and $|B|$ its d-dimensional measure. Intuitively, the topological derivative measures the change of J when a small ball is added to Ω at $\boldsymbol{x}^0$ (when $\boldsymbol{x}^0 \notin \Omega$) or when a small hole is created in Ω at $\boldsymbol{x}^0$ (when $\boldsymbol{x}^0 \in \Omega$). The challenge in implementing topological methods is related to deriving the exact asymptotic expression of the derivative from (4.16), which typically requires sophisticated mathematical analysis tools. With certain assumptions on the state equations (mainly a Dirichlet boundary condition) a simpler computation can provide the desired topological sensitivity [40].

It turns out that topological derivatives have a strong connection with the classical shape derivative (4.10) [58]. For many problems, such as the minimum compliance problem of linear elasticity, the topological derivative turns out to be equivalent to the shape gradient up to a constant [22]. When the topological derivative exists and can be computed, similarly to the shape gradient, a gradient descent algorithm for the implicit function can be formulated and implemented by solving the evolution equation

$$\frac{\partial \phi(\boldsymbol{x}, t)}{\partial t} = \nabla_T J(\phi, \boldsymbol{x}, t), \quad (\boldsymbol{x}, t) \in \mathbb{R}^d \times (0, T), \tag{4.17}$$

where the topological gradient is defined as in [17]

$$\nabla_T J(\phi, \boldsymbol{x}, t) = -\text{sgn}\,[\phi(\boldsymbol{x}, t)]\, d_T(\Omega(t); \boldsymbol{x}). \tag{4.18}$$

4.4 Extension to geometric inverse problems

Many geometric inverse problems can be cast as shape optimization problems and solved by the level set approach by following the formulation in [16, 69]. Examples include various inverse scattering problems [27] and the inverse elasticity problem [10]. The general setup of the *forward problem* is: given the system state u an observation y is made

$$y = \mathcal{G}(u) \tag{4.19}$$

where the imaging operator $\mathcal{G} : X(\Omega) \to Y$ maps the state to some topological space Y of observations. In the *inverse problem* context the observation y is given, but the state u is unknown and to be reconstructed. It is assumed that the state depends as before on a variable domain Ω, so that $u = u(\Omega)$, and also an approximation to Ω is to be reconstructed. The difficulty lies in the fact that the inverse operator $\mathcal{G}^{-1}$ is typically not continuous with respect to the observations, i.e. the inverse problem is ill-posed. Furthermore, the measurement y is often polluted with noise, $y = \widehat{y} + \varepsilon$, where $\widehat{y}$ is the true observation and ε is a realization of a noise process. Thus it is usual to minimize the least-squares functional

$$\min_{\Omega \in \mathcal{S}_{reg}} \quad ||\mathcal{G}(u(\Omega)) - y||^2, \tag{4.20}$$

where the subset of admissible shapes $\mathcal{S}_{reg} \subset \mathcal{S}_{ad}$ consists of suitably regularized shapes that recover the continuous dependence of the state u on the observation y. The inverse problem is now written as a shape optimization problem of the type (3.1), and the level set based approach detailed above can be used. Another way to regularize the inverse problem is to use alternative gradients of the type (4.12) and the evolution equation (4.13) in the descent algorithm, see e.g. [16, 64].

5 Model reduction in parametric shape optimization

A large part of the complexity of solving PDE constrained shape optimization problems is the cost of the PDE solution. Numerical optimization algorithms tend to involve a large number of constraint and cost functional evaluations, and since every one of these involves the solution of a potentially highly complex and computationally expensive PDE, there is a need for more efficient solution methods. Model reduction and surrogate optimization ideas have been very popular for shape optimization problems with PDE constraints. The theory of model order reduction for linear systems of ordinary differential equations [5] and PDEs is well-known; unfortunately in shape optimization the problems are inherently nonlinear (the solution of the PDE depends on the domain Ω in a strongly nonlinear way) and therefore new approaches in model reduction that also work with nonlinear problems need to be developed.

In surrogate optimization [65] the full PDE-constrained optimization problem is replaced with an inexpensive approximate optimization problem. This

can involve replacing the cost function with a simpler one, replacing the constraints with near-equivalent ones, or a combination of both techniques. The space mapping approach [7] considers a two-level approach, where a coarse level model is used for the majority of the optimization steps, while a more accurate fine level model is used periodically to guarantee that the resulting designs do not become too unrealistic. The reduced basis surrogate optimization method was first presented in [59], where the state equations, their linear outputs, as well as their first- and second-order sensitivities were all treated with the reduced basis method to obtain a comprehensive surrogate optimization framework. In that work the error bounds for solutions of the reduced state equations were taken into account in the modified cost function to obtain a type of optimization method "in the presence of (modelling) uncertainty". For optimization in time-dependent systems there are also approaches using the proper orthogonal decomposition (POD) [48] that looks for a set of principal eigenmodes of an ensemble of trajectories of a dynamical system. The subspace spanned by these eigenmodes can be used as a type of surrogate model [15] of the state equations in time.

The main interest in this thesis lies in the model reduction of the parametric shape optimization when the shape parameters have been incorporated into the PDE constraints by a geometric transformation back to a fixed reference domain.

5.1 Parameterization of the computational domain

The first step in casting (3.1) as a parametric shape optimization problem is to introduce a reference domain Ω_0, a finite-dimensional parameter vector $\boldsymbol{\mu} \in \mathcal{D}$, a low-dimensional parameter range $\mathcal{D} \subset \mathbb{R}^P$ (e.g. $P < 20$), and a parametric map $F(\,\cdot\,;\boldsymbol{\mu}) : \Omega_0 \to \Omega(\boldsymbol{\mu})$ that is at least C^1 smooth and invertible. The admissible shapes Ω are then assumed to belong in the range of the parametric domain map when applied to the reference shape, that is for all $\Omega \in \mathcal{S}_{ad}$ there exists a $\boldsymbol{\mu} \in \mathcal{D}$ s.t.

$$\Omega(\boldsymbol{\mu}) = F(\Omega_0; \boldsymbol{\mu}). \tag{5.21}$$

Using this map as a transformation it is possible map the PDE constraints in (3.1) on to a fixed domain. For example, the standard elliptic bilinear form

$$\mathcal{A}(u, v) = \int_\Omega \left[A(\boldsymbol{x})\nabla u \cdot \nabla v + b(\boldsymbol{x})uv\right]\, d\boldsymbol{x}, \tag{5.22}$$

where $A(\boldsymbol{x}) \in L^\infty(\mathbb{R}^d, \mathbb{R}^{d\times d})$ is symmetric and uniformly positive definite over all of Ω, i.e.

$$\frac{\langle A(\boldsymbol{x})v, v\rangle}{||v||^2} \geq a_0 > 0 \quad \text{for all } v \neq 0, \boldsymbol{x} \in \Omega, \tag{5.23}$$

and $b(\boldsymbol{x}) \geq 0$, transforms into

$$\widetilde{\mathcal{A}}(\widetilde{u}, \widetilde{v}; \boldsymbol{\mu}) = \int_{\Omega_0} \left[\widetilde{A}(\widetilde{\boldsymbol{x}}, \boldsymbol{\mu})\widetilde{\nabla}\widetilde{u} \cdot \widetilde{\nabla}\widetilde{v} + \widetilde{b}(\widetilde{\boldsymbol{x}}, \boldsymbol{\mu})\widetilde{u}\widetilde{v}\right]\, d\boldsymbol{x} \tag{5.24}$$

according to

$$\widetilde{A}(\widetilde{\boldsymbol{x}}, \boldsymbol{\mu}) := J_F^{-T}(\widetilde{\boldsymbol{x}}; \boldsymbol{\mu}) A(F(\widetilde{\boldsymbol{x}}; \boldsymbol{\mu})) J_F^{-1}(\widetilde{\boldsymbol{x}}; \boldsymbol{\mu}) \, |J_F(\widetilde{\boldsymbol{x}}; \boldsymbol{\mu})| \tag{5.25}$$

$$\widetilde{b}(\widetilde{\boldsymbol{x}}, \boldsymbol{\mu}) := b(F(\widetilde{\boldsymbol{x}}; \boldsymbol{\mu})) \, |J_F(\widetilde{\boldsymbol{x}}; \boldsymbol{\mu})|, \tag{5.26}$$

where J_F denotes the Jacobian matrix of F, i.e. $[J_F]_{ij} := \frac{\partial F_i}{\partial \widetilde{x}_j}$, and $|J_F|$ its determinant. The transformed problem coefficients now depend explicitly on the parameters, and it can be easily verified that also the transformed problem is elliptic. All quantities denoted with tildes live on the fixed reference domain Ω_0 and can be mapped to their counterparts on the original domain Ω. The parametric shape optimization problem in the fixed domain is

$$\begin{aligned} \min_{\boldsymbol{\mu} \in \mathcal{D}} \quad & J(\widetilde{u}(\boldsymbol{\mu})) \\ s.t. \quad & \widetilde{\mathcal{A}}(\widetilde{u}(\boldsymbol{\mu}), \widetilde{v}; \boldsymbol{\mu}) = \widetilde{F}(\widetilde{v}; \boldsymbol{\mu}) \quad \text{for all } \widetilde{v} \in V(\Omega_0). \end{aligned} \tag{5.27}$$

The bilinear form $\widetilde{\mathcal{A}}$ and the linear form $\widetilde{F}$ are now parametric, that is to say the coefficient functions depend explicitly on the parameter vector $\boldsymbol{\mu}$. Once the parametric shape optimization problem has been obtained, model reduction methods for the efficient evaluation of the parametric PDE constraint can be studied. The focus from here on is on the discrete model problem (3.5). To this end the discrete version of the aforementioned problem can be defined in a similar way:

$$\begin{aligned} \min_{\boldsymbol{\mu} \in \mathcal{D}} \quad & J(\widetilde{u}_h(\boldsymbol{\mu})) \\ s.t. \quad & \widetilde{\mathcal{A}}(\widetilde{u}_h(\boldsymbol{\mu}), \widetilde{v}_h; \boldsymbol{\mu}) = \widetilde{F}(\widetilde{v}_h; \boldsymbol{\mu}) \quad \text{for all } \widetilde{v}_h \in V_h(\Omega_0). \end{aligned} \tag{5.28}$$

Assume that existence of solutions can be shown for the infinite-dimensional problems (3.1) and (5.27), that the mesh-independence principle is in effect, and that the discretization parameter h is chosen small enough in the FEM. After these assumptions it suffices to work with a fixed mesh $\widetilde{\mathcal{T}}_h$ on the reference domain Ω_0. The parametric formulation with the fixed domain/fixed mesh -assumptions enable the use of the reduced basis methods for model reduction of the state PDEs, which shall be discussed next.

5.2 Reduced basis methods

A generic model reduction framework for parametric PDEs are the reduced basis methods [61, 67]. The idea was developed in the 1980s in the nonlinear structural mechanics community [3, 32, 57, 63]. The aim is to construct a low-dimensional approximation for the discretized state equations in the PDE constraint of (5.28). To accomplish this, a parametric manifold of PDE solutions is sampled at a few well-chosen parametric points and snapshot solutions of the PDE are computed using the finite element method for solving PDEs numerically. The snapshots are used to construct a low-dimensional space, where Galerkin projection is used for the approximation. To guarantee

approximation stability, a posteriori estimators for the error between the reduced basis approximation and the finite element solution are constructed.

Because the bilinear form depends on the parameter, a parameter independent norm should be first defined. Choose a reference parameter $\bar{\boldsymbol{\mu}} \in \mathcal{D}$ and define the parameter-independent inner product

$$\langle \widetilde{u}, \widetilde{v} \rangle_X := \widetilde{\mathcal{A}}(\widetilde{u}, \widetilde{v}; \bar{\boldsymbol{\mu}}) \tag{5.29}$$

and the norm

$$||\widetilde{v}||_X := \sqrt{\langle \widetilde{v}, \widetilde{v} \rangle_X}. \tag{5.30}$$

In the reduced basis framework a small collection of parameter values $\{\boldsymbol{\mu}_n\}_{n=1}^N$ are used to construct a basis for Galerkin projection for the parametric PDE. Let $\{\widetilde{u}_h(\boldsymbol{\mu}_n)\}_{n=1}^N$ be the finite element solutions for the chosen parameter values, and define

$$V_h^N := \text{span}(\widetilde{u}_h(\boldsymbol{\mu}_1), \widetilde{u}_h(\boldsymbol{\mu}_2), \ldots, \widetilde{u}_h(\boldsymbol{\mu}_N)) \tag{5.31}$$

the reduced basis approximation space. First construct an X-orthogonal basis for V_h^N with the Gram-Schmidt procedure

$$\begin{cases} \zeta^1 = \widetilde{u}_h(\boldsymbol{\mu}_1)/||\widetilde{u}_h(\boldsymbol{\mu}_1)||_X & \\ z^n = \widetilde{u}_h(\boldsymbol{\mu}_n) - \displaystyle\sum_{k=1}^{n-1} \zeta_k \frac{\langle \zeta^k, \widetilde{u}_h(\boldsymbol{\mu}_n) \rangle_X}{||\zeta^k||_X^2} & \text{for } n = 2, 3, \ldots, N\,. \\ \zeta^n = z^n/||z^n||_X & \text{for } n = 2, 3, \ldots, N \end{cases} \tag{5.32}$$

This step in necessary because otherwise the conditioning of the linear system deteriorates for even small N. The reduced basis Galerkin method then looks for a solution $\widetilde{u}_h^N(\boldsymbol{\mu}) \in V_h^N$ s.t.

$$\widetilde{\mathcal{A}}(\widetilde{u}_h^N(\boldsymbol{\mu}), \zeta^n; \boldsymbol{\mu}) = \widetilde{F}(\zeta^n; \boldsymbol{\mu}), \quad \text{for all } n = 1, 2, \ldots, N. \tag{5.33}$$

Now $\widetilde{u}_h^N(\boldsymbol{\mu})$ gives an approximation to the finite element solution $\widetilde{u}_h(\boldsymbol{\mu})$. When the dimension of the reduced basis space N is much smaller than the dimension of the finite element space $\mathcal{N}$ it is to be expected that the problem (5.33) is efficiently solvable for any $\boldsymbol{\mu}$. The surrogate optimization algorithm that is obtained by replacing the full state equations with their reduced basis counterparts reads:

$$\begin{aligned} \min_{\mu \in \mathcal{D}} \quad & J(\widetilde{u}(\boldsymbol{\mu})) \\ s.t. \quad & \widetilde{\mathcal{A}}(\widetilde{u}_h^N(\boldsymbol{\mu}), \widetilde{v}; \boldsymbol{\mu}) = \widetilde{F}(\widetilde{v}; \boldsymbol{\mu}) \quad \text{for all } \widetilde{v} \in V_h^N. \end{aligned} \tag{5.34}$$

A priori the complexity of solving the reduced basis system (5.33) depends only on N, but it turns out that to obtain an efficient method for assembling the system without an explicit workload dependence on $\mathcal{N}$, the following assumption of affine parametric dependence is needed:

$$\widetilde{\mathcal{A}}(\widetilde{u}, \widetilde{v}; \boldsymbol{\mu}) = \sum_{q=1}^{Q_a} \Theta_a^q(\boldsymbol{\mu}) \widetilde{\mathcal{A}}^q(\widetilde{u}, \widetilde{v}) \tag{5.35}$$

and

$$\widetilde{F}(\widetilde{v};\boldsymbol{\mu}) = \sum_{q=1}^{Q_f} \Theta_f^q(\boldsymbol{\mu})\widetilde{F}^q(\widetilde{v}), \tag{5.36}$$

where the parametric coefficient functions Θ_a^q and Θ_f^q should be efficiently evaluable. Then the problem (5.33) splits into parameter-dependent and -independent parts

$$\sum_{q=1}^{Q_a} \Theta_a^q(\boldsymbol{\mu})\widetilde{\mathcal{A}}^q(\widetilde{u}_h^N(\boldsymbol{\mu}),\zeta^n) = \sum_{q=1}^{Q_f} \Theta_f^q(\boldsymbol{\mu})\widetilde{F}^q(\zeta^n), \quad \text{for all } n = 1,2,\ldots,N \tag{5.37}$$

or in matrix form

$$\left(\sum_{q=1}^{Q_a} \Theta_a^q(\boldsymbol{\mu})\underline{A^q}\right) U = \sum_{q=1}^{Q_f} \Theta_f^q(\boldsymbol{\mu})\underline{F^q}, \tag{5.38}$$

where

$$[\underline{A^q}]_{n,n'} := \widetilde{\mathcal{A}}^q(\zeta^{n'},\zeta^n), \quad [\underline{F^q}]_n := \widetilde{F}^q(\zeta^n). \tag{5.39}$$

Thus the system matrices $\underline{A}^q$ and right-hand sides $\underline{F}^q$ can be assembled once in the beginning (offline stage), stored, and then for every $\boldsymbol{\mu}$ the parametric coefficients can be evaluated to assemble and solve the system (5.39) (online stage).

The accuracy and convergence of the reduced basis approximation u_h^N affect the optimization results obtained from the surrogate problem (5.34). It is to be expected that a poor approximation to the state equations results in either suboptimal or infeasible designs because the constraints are not properly enforced. There is little a priori convergence theory for reduced basis approximations. In the best case the convergence is exponential [14, 51], so that the relative error of the reduced basis approximation behaves like

$$\frac{||\widetilde{u}_h - \widetilde{u}_h^N||_X}{||\widetilde{u}_h||_X} \leq Ce^{-kN} \tag{5.40}$$

for some constants $C, k > 0$ after a critical cutoff point $N > N_{\text{crit}}$ has been reached. Therefore much interest lies in the construction of reliable and efficient a posteriori error estimates for $||\widetilde{u}_h - \widetilde{u}_h^N||_X$. One option (see [61], Chapter 4 for the full details) is to use the residual-based estimator

$$\Delta_n(\boldsymbol{\mu}) := \frac{||R_n(\cdot;\boldsymbol{\mu})||_{X'}}{\alpha_{LB}(\boldsymbol{\mu})}, \tag{5.41}$$

where the residual is defined as the dual element

$$R_n(\widetilde{v};\boldsymbol{\mu}) := F(\widetilde{v};\boldsymbol{\mu}) - a(\widetilde{u}_h^n(\boldsymbol{\mu}),\widetilde{v};\boldsymbol{\mu}) \in X'(\Omega_0) \tag{5.42}$$

and $\alpha_{LB}(\boldsymbol{\mu}) > 0$ is a computable lower bound for the coercivity constant $\alpha_0(\boldsymbol{\mu})$, i.e.

$$\alpha_{LB}(\boldsymbol{\mu}) \leq \alpha_0(\boldsymbol{\mu}) \leq \frac{\widetilde{\mathcal{A}}(\widetilde{u},\widetilde{u};\boldsymbol{\mu})}{||\widetilde{u}||_X^2} \quad \text{for all } \widetilde{u} \in X_h. \tag{5.43}$$

A parametric lower bound α_{LB} for the coercivity constant can be constructed by sampling the parameter space to find a proper set of linear constraints that bounds the smallest eigenvalue from below, the so-called successive constraint method [42, 43]. Estimator (5.41) satisfies

$$||\widetilde{u}_h - \widetilde{u}_h^n||_X \leq \Delta_n(\boldsymbol{\mu}) \quad \text{for all } \boldsymbol{\mu} \in \mathcal{D}. \tag{5.44}$$

Until now the strategy for choosing the parameter values used to construct the snapshots has not been addressed. With the a posteriori estimate Δ_n in hand it is possible to use a greedy algorithm for the selection of a good reduced approximation basis. The greedy approach was first proposed in [35], and has since become the standard basis selection algorithm. Let $\Xi_{train} \subset \mathcal{D}$ be a large training sample of parameter points. From Ξ_{train} choose the first parameter value $\boldsymbol{\mu}_1$ according to some rule, and then proceed to find a hierarchical set of parameter points

$$\boldsymbol{\mu}_n = \underset{\boldsymbol{\mu} \in \Xi_{train}}{\arg\max} \quad \Delta_{n-1}(\boldsymbol{\mu}), \qquad \text{for } n = 2, 3, \ldots, N. \tag{5.45}$$

Intuitively: at each iteration add the parameter point that produces the snapshot solution that is worst approximated by the previous reduced basis approximation space. It is known that such a greedy algorithm does not produce the optimal approximation subspace V_*^N of dimension N, but there are some recent indications [14] that the approximation spaces given by the reduced basis greedy algorithm are not too far from the optimal ones.

5.3 Empirical interpolation method

One of the topics of this thesis relates to the fact that for parametric shape optimization problems, assumption (5.35) is almost never valid unless special care is taken to construct a suitable geometric decomposition (see [67], Sect. 5). The recently developed empirical interpolation method [8, 34, 50] has been successfully applied to reduced basis reduction of nonaffinely parameterized problems, such as shape optimization. The empirical interpolation method is a model reduction scheme that replaces the nonaffinely parameterized bilinear form $\widetilde{\mathcal{A}}(\widetilde{u}, \widetilde{v}; \boldsymbol{\mu})$ with an affinely parameterized approximation of the form

$$\widetilde{\mathcal{A}}(u, v; \boldsymbol{\mu}) = \sum_{q=1}^{Q_{\text{EIM}}} \vartheta_a^q(\boldsymbol{\mu}) \widetilde{\mathcal{A}}_{\text{EIM}}^q(\widetilde{u}, \widetilde{v}) + \varepsilon_{\text{EIM}}(\widetilde{\boldsymbol{x}}, \boldsymbol{\mu}), \tag{5.46}$$

where the error term ε_{EIM} needs to be controlled to an acceptable tolerance.

Assume there exists a scalar function $g(\boldsymbol{x}, \boldsymbol{\mu}) \in C^0(\mathcal{D}; L^\infty(\Omega))$ depending on both the spatial coordinates and the parameters in a nonaffine way. The extension to matrix-valued functions via an elementwise procedure is obvious. The objective is to find an approximate expansion of the form

$$g_M(\boldsymbol{x}, \boldsymbol{\mu}) = \sum_{j=1}^{M} \Theta_j(\boldsymbol{\mu}) \zeta_j(\boldsymbol{x}). \tag{5.47}$$

In the empirical interpolation one seeks a set of interpolation points $\boldsymbol{x}^j \in \Omega$ and a set of shape functions $\zeta_j(\boldsymbol{x})$ s.t. the expansion (5.47) is obtained through solving the Lagrange interpolation problem

$$\sum_{j=1}^{M} [B]_{i,j}^{M} \Theta_j(\boldsymbol{\mu}) = g(\boldsymbol{x}^i, \boldsymbol{\mu}), \quad \forall\, i = 1, \ldots, M \tag{5.48}$$

where the $M \times M$ interpolation matrix is defined elementwise as $[B]_{i,j}^{M} := \zeta_j(x^i)$ for $i, j = 1, \ldots, M$. The method is detailed in Algorithm 1.

Algorithm 1 Empirical interpolation procedure as defined in [8]

Require: initial parameter value $\boldsymbol{\mu}_1$ and large training set $\Xi_{train} \subset \mathcal{D}$

1: Let $m = 1$.

2: Set the first shape function $\zeta_1(\boldsymbol{x}) := g(\boldsymbol{x}, \boldsymbol{\mu}_1)$, the approximation space $G_1 := \text{span}(\zeta_1)$, and the interpolation point $\boldsymbol{x}^1 := \underset{\boldsymbol{x} \in \Omega}{\text{argmax}} |\zeta_1(\boldsymbol{x})|$.

3: **repeat**

4: Solve the linear programming problem

$$\boldsymbol{\mu}_{m+1} := \underset{\boldsymbol{\mu} \in \Xi_{train}}{\text{argmax}} \inf_{v \in G_m} ||g(\cdot, \boldsymbol{\mu}) - v||_{L^\infty(\Omega)}. \tag{5.49}$$

5: Set the next shape function $\zeta_{m+1}(\boldsymbol{x}) := g(\boldsymbol{x}, \boldsymbol{\mu}_{m+1})$ and the approximation space $G_{m+1} := \text{span}(\zeta_1, \ldots, \zeta_{m+1})$.

6: Solve the interpolation problem

$$\sum_{j=1}^{m} [B]_{i,j}^{m} \Theta_j^m = \zeta_{m+1}(\boldsymbol{x}^i), \quad \forall\, i = 1, \ldots, m \tag{5.50}$$

with interpolation matrices $[B]_{i,j}^{m} := \zeta_j(\boldsymbol{x}^i)$ for $i, j = 1, \ldots, m$.

7: Compute the residual

$$r_{m+1}(\boldsymbol{x}) := \zeta_{m+1}(\boldsymbol{x}) - \sum_{j=1}^{m} \Theta_j^m \zeta_j(\boldsymbol{x}). \tag{5.51}$$

8: Set the next interpolation point $\boldsymbol{x}^{m+1} := \underset{\boldsymbol{x} \in \Omega}{\text{argmax}} |r_{m+1}(\boldsymbol{x})|$.

9: Let $m \to m + 1$.

10: **until** the error $\max\limits_{\boldsymbol{\mu} \in \Xi_{train}} \inf\limits_{v \in G_{m-1}} ||g(\cdot, \boldsymbol{\mu}) - v||_{L^\infty(\Omega)} < \text{TOL}$

Without additional assumptions on the function g, the error of the empirical interpolation approximation is bounded above by the best approximation in the space G_M [8]

$$||g(\cdot, \boldsymbol{\mu}) - g_M(\cdot, \boldsymbol{\mu})||_{L^\infty(\Omega)} \leq (1 + \Lambda_M) \inf_{v \in G_M} ||g(\cdot, \boldsymbol{\mu}) - v||_{L^\infty(\Omega)}, \tag{5.52}$$

but the Lebesgue constant only satisfies $\Lambda_M \leq 2^M - 1$, which would indicate a possibly poor quality approximation. With added parametric regularity it is possible to give better bounds for the interpolation error [28]. In practice the EIM has been quite useful for solving nonaffinely parameterized PDEs with the reduced basis method [34, 56, 66].

Introducing the EIM approximation to the reduced basis equation (5.33) requires modifications to the a posteriori error estimator (5.44). This was first done in [55, 56]. The augmented estimator is of the form

$$||\widetilde{u}_h - \widetilde{u}_h^N||_X \leq \Delta_N(\boldsymbol{\mu}) + \Delta_{N,M}^{\text{EIM}}(\boldsymbol{\mu}). \tag{5.53}$$

The term $\Delta_{N,M}^{\text{EIM}}(\boldsymbol{\mu})$ is a consistency error term that does not converge to 0 even as $N \to \infty$ if the number of terms M in the affine expansion is kept fixed. This is called the *plateau effect* [34].

5.4 Extension to free boundary problems

A more general class called free boundary problems can be solved using similar techniques as presented previously for shape optimization. Assume that the boundaries of the admissible shapes consist of a suitably parameterized free boundary part $\Sigma(\boldsymbol{\mu})$, and a fixed boundary part Γ, s.t. for all $\Omega(\boldsymbol{\mu}) \in \mathcal{S}_{ad}$ it holds that

$$\partial\Omega(\boldsymbol{\mu}) = \Sigma(\boldsymbol{\mu}) \cup \Gamma. \tag{5.54}$$

The fixed domain approach is again taken to map from Ω_0 to $\Omega(\boldsymbol{\mu})$. An abstract free boundary problem is to solve for $\widetilde{u}(\boldsymbol{\mu}) \in V(\Omega_0)$ that satisfies the state equation

$$\widetilde{\mathcal{A}}(\widetilde{u}(\boldsymbol{\mu}), \widetilde{v}; \boldsymbol{\mu}) = \widetilde{F}(\widetilde{v}; \boldsymbol{\mu}) \quad \text{for all } \widetilde{v} \in V(\Omega_0) \tag{5.55}$$

plus an auxiliary equation for determining the configuration of the free boundary $\Sigma(\boldsymbol{\mu})$

$$\Psi(\widetilde{u}(\boldsymbol{\mu}), \Sigma(\boldsymbol{\mu})) = 0 \tag{5.56}$$

that closes the equation system.

The prototype shape optimization problem (3.1) can be formulated as an abstract free boundary problem by taking the necessary optimality condition that the shape derivative (4.11) must vanish at the optimal shape Ω^*, i.e.

$$\int_{\Sigma^*(\boldsymbol{\mu}) \cup \Gamma} (\boldsymbol{w} \cdot \boldsymbol{n}) \nabla J(\boldsymbol{x}) \, ds = 0 \quad \text{for all } \boldsymbol{w} \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d) \tag{5.57}$$

as the weak form of an auxiliary equation (5.56). Conversely, the free boundary problem can be formulated as a parametric shape optimization problem for example as a least-squares problem

$$\begin{aligned} \min_{\boldsymbol{\mu} \in \mathcal{D}} \quad & |\Psi(u(\boldsymbol{\mu}), \Sigma(\boldsymbol{\mu}))|^2 \\ s.t. \quad & \mathcal{A}(\widetilde{u}(\boldsymbol{\mu}), \widetilde{v}; \boldsymbol{\mu}) = \widetilde{F}(\widetilde{v}) \quad \text{for all } \widetilde{v} \in V(\Omega_0). \end{aligned} \tag{5.58}$$

6 Contribution to the state of the art

This thesis addresses two main topics in applied shape optimization. The first is shape optimization using level set methods, the other reduced basis methods for model reduction in parametric shape optimization. In addition to pure optimal shape design problems, this thesis also applies the techniques developed for the aforementioned problems to a free boundary problem of fluid-structure interaction.

6.1 Level set methods and shape optimization

In [A] a topological shape optimization method for the optimal damping of the two-dimensional wave equation is studied. The objective is to find the optimal design of a damper that has a fixed area and that minimizes the energy at a fixed final time. While the topological derivative defined according to (4.16) was not available for this problem at the time, in [53] it is shown that the topological and shape derivatives for this particular problem differ only by a factor of $o(a)$ for small damping coefficients $a > 0$. Therefore, a topological level set method originally proposed in [4] could be applied to the problem to obtain a topological optimization algorithm that discovers the correct number of disjoint components in about one fifth the number of level set iterations needed. While all level set methods allow certain topological changes of the shapes they can also get stuck in a shape bifurcation point and generally do not permit new components to form away from the current shapes. The topological method of [A] suffers from neither problem and therefore it is a true topological level set method, unlike e.g. the method proposed in [53].

The level set approach to shape optimization is applied in [B] to an inverse problem of reconstructing a shape from its interferogram that is recast into the form (4.20). Convexity of the admissible shapes is proved to be a sufficient condition for the inverse problem to have a unique solution. Here the interest is not to find the correct topology, but rather to modify the level set method in such a way that the feasible shapes are restricted to be convex. The convexity constraint can be difficult to handle in numerical computations, and previous works on this topic [1, 19, 20, 21, 44] have involved a variety of approaches. In contrast these previous works, [B] instead uses a curvature penalization method that allows convexity to be temporarily broken. An important aspect in the inverse problem context is the presence of noise in the data that necessitates regularization before the shape optimization formulation can be used. It turns out that replacing the standard L^2 shape gradient in the descent method with an H^1-version defined by (4.12) is a form of regularization.

6.2 Reduced basis for parametric shape optimization

Article [C] studies a surrogate shape optimization method. The domain parameterization is done with free-form deformations [70], which are a technique for flexible, mesh-independent shape parameterizations. The problem is then mapped to a fixed reference domain according to (5.24), (5.25), and (5.26), and the parameters enter the coefficients of the PDE. Reduced basis methods are used to evaluate the state constraints efficiently. The proposed approach is a generic parametric shape optimization framework. The benefits of the optimization method are demonstrated on a classical problem of inverse design of an airfoil in potential flow.

In [D] the same airfoil geometry is considered, but this time the PDE model is the advection-diffusion equation and the optimization problem resembles a turbine blade configuration problem in an exterior thermal flow. The work concentrates on the a posteriori estimation of the reduced basis approximation error, which had been missing in previous works such as [76]. The nonaffine parameterization arising from the free-form deformations necessitates the use of the empirical interpolation approximation (5.46) for the diffusive coefficients, which in turn creates an additional error term in the reduced basis approximation. The error estimate of [55, 56] is extended to the advection-diffusion case, and a reduced basis surrogate optimization method with certified error bounds for such problems is obtained.

Article [E] utilizes the combination of free-form deformations and reduced basis methods introduced in [C] for the efficient solution of a free boundary problem of fluid-structure interaction. Steady incompressible flow in a channel with a flexible wall is modelled as a coupled problem involving the Stokes equations for the fluid, and a 1-d elliptic equation for the displacement of the flexible wall. The coupling condition (auxiliary equation (5.56) in this case) states that the traction applied to the wall by the fluid should match the displacement of the wall caused by the applied stress. These conditions are treated in terms of the geometric parameters, by least squares minimization (5.58) of the parametric structural displacement and the assumed displacement caused by the traction applied by the fluid.

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