

Preface

Solving optimization problems subject to constraints given in terms of partial differential equations (PDEs) with additional constraints on the controls and/or states is one of the most challenging problems in the context of industrial, medical and economical applications, where the transition from model-based numerical simulations to model-based design and optimal control is crucial. For the treatment of such optimization problems the interaction of optimization techniques and numerical simulation plays a central role. After proper discretization, the number of optimization variables varies between 10^3 and 10^{10} . It is only very recently that the enormous advances in computing power have made it possible to attack problems of this size. However, in order to accomplish this task it is crucial to utilize and further explore the specific mathematical structure of optimization problems with PDE constraints, and to develop new mathematical approaches concerning mathematical analysis, structure exploiting algorithms, and discretization, with a special focus on prototype applications.

The present book provides a modern introduction to the rapidly developing mathematical field of optimization with PDE constraints. The first chapter introduces to the analytical background and optimality theory for optimization problems with PDEs. Optimization problems with PDE-constraints are posed in infinite dimensional spaces. Therefore, functional analytic techniques, function space theory, as well as existence- and uniqueness results for the underlying PDE are essential to study the existence of optimal solutions and to derive optimality conditions. These results form the foundation of efficient optimization methods in function space, their adequate numerical realization, mesh independence results and error estimators. The chapter starts with an introduction to the necessary background in functional analysis, Sobolev spaces and the theory of weak solutions for elliptic and parabolic PDEs. These ingredients are then applied to study PDE-constrained optimization problems. Existence results for optimal controls, derivative computations by the sensitivity and adjoint approaches and optimality conditions for problems with control-, state- and general constraints are considered. All concepts are illustrated by elliptic and parabolic optimal control problems. Finally, the optimal control of instationary incompressible Navier-Stokes flow is considered.

The second chapter presents a selection of important algorithms for optimization problems with partial differential equations. The development and analysis of these methods is carried out in a Banach space setting. This chapter starts with introducing a general framework for achieving global convergence. Then, several variants of generalized Newton methods are derived and analyzed. In particular, necessary and sufficient conditions for fast local convergence are derived. Based on this, the concept of semismooth Newton methods for operator equations is introduced. It is shown how complementarity conditions, variational inequalities, and optimality systems can be reformulated as semismooth operator equations. Applications to constrained optimal control problems are discussed, in particular for elliptic

partial differential equations and for flow control problems governed by the incompressible stationary Navier-Stokes equations. As a further important concept, the formulation of optimality systems as generalized equations is addressed and the Josephy-Newton method for generalized equations is analyzed. This provides an elegant basis for the motivation and analysis of sequential quadratic programming (SQP) algorithms. The second chapter concludes with a short outline of recent algorithmic advances for state constrained problems and a brief discussion of several further aspects.

The third chapter gives an introduction to discrete concepts for optimization problems with PDE constraints. As models for the state elliptic and parabolic PDEs are considered which are well understood from the analytical point of view. This allows to focus on structural aspects in discretization. The approaches *First discretize, then optimize* and *First optimize, then discretize* are compared and discussed, and a variational discrete concept is introduced which avoids explicit discretization of the controls. Special focus is taken on the treatment of constraints. This includes general constraints on the control, and also pointwise bounds on the state, and on the gradient of the state. The chapter presents the error analysis for the variational discrete concept and accomplishes the analytical findings with numerical examples which confirm the analytical results.

Finally, the fourth chapter is devoted to the study of two industrial applications, in which optimization with partial differential equations plays a crucial role. It provides a survey of the different mathematical settings which can be handled with the general optimal control calculus presented in the previous chapters. The chapter focuses on large scale optimal control problems involving two well-known types of partial differential equations, namely elliptic and parabolic ones. Since real world applications lead generally to mathematically quite involved problems, in particular nonlinear systems of equations are studied. The examples are chosen in such a way that they are up-to-date and modern mathematical tools are used for their specific solution. The industrial fields covered are modern semiconductor design and glass production. Each section starts with a modeling part to introduce the underlying physics and mathematical models, which are then followed by the analytical and numerical study of the related optimal control problems.

Acknowledgements

This Book is based on lecture notes of the autumn school *Modellierung und Optimierung mit Partiellen Differentialgleichungen* which was held in September 2005 at the Universität Hamburg. It was supported by the Collaborative Research Center 609, located at the Technische Universität Dresden, and by the Priority Programme 1253, both sponsored by the Deutsche Forschungsgemeinschaft, as well as by the Schwerpunkt Optimierung und Approximation at the Department Mathematik of the Universität Hamburg. All support is gratefully acknowledged.

Finally we would like to thank a number of colleagues whose collaboration and support influenced the material presented in this book. These include Günter Bärowolf, Martin Burger, Klaus Deckelnick, John Dennis, Michael Ferris, Andreas

Günther, Matthias Heinkenschloss, Michael Herty, Michael Hintermüller, Axel Klar, Karl Kunisch, Günter Leugering, Ulrich Matthes, Christian Meyer, Danny Ralph, Ekkehard Sachs, Anton Schiela, Alexander Schulze, Mohammed Seaid, Norbert Siedow, Guido Thömmes, Philippe Toint, Fredi Tröltzsch, Andreas Unterreiter, Luís Vicente, and Morten Vierling.

<http://www.springer.com/978-1-4020-8838-4>

Optimization with PDE Constraints

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2009, XII, 270 p., Hardcover

ISBN: 978-1-4020-8838-4