Chapter 1

Introduction

Optimization with partial differential equations (PDEs) is a modern field of research in applied mathematics, starting in the early 1970s with the work of Lions [235], although it has a very important predecessor and companion in the research on optimal control of ordinary differential systems that started with the works of the Bernoulli brothers in 1700; see [274, 278].

As in the optimal control case, it is the idea of being able to influence PDE application systems that is attracting enormous research efforts toward PDE optimization. In fact, it is the ultimate aim of any application problem to manipulate systems in a desired way.

The purpose of PDE optimization appears manifold and ranges from the need to control application systems to that of how to optimally change or estimate features of real-world systems modeled by PDEs. An important class of problems in optimization results from optimal control applications. These consist of an evolutionary or equilibrium system including a control mechanism and a functional modeling the purpose of the control. Other important classes of optimization problems are shape design, topology, and parameter optimization. Optimization is also an essential tool for solving many inverse problems. In all these cases we are concerned with systems that are modeled by a set of PDEs. Therefore we are in the framework of infinite-dimensional optimization problems where one distinguishes between state and optimization variables.

Because of the nature of PDE problems, solving the related optimization problems requires realization of optimization strategies having increasing complexity and the ability to solve large-scale problems in an accurate and computationally efficient way. These needs are revolutionizing the scenario of the optimization discipline since many classical methodologies appear overwhelmed by the size of the problems to be solved and by the type of additional requirements that the solution must satisfy. On the other hand, classical PDE solvers cannot be straightforwardly applied to solve optimality systems since new differential structures and a new type of coupling appear.

In this book, we present some recent results and outline present developments in the field of the numerical solution of PDE optimization problems. On the one hand, we give an introduction to well-known optimization methodologies that have been extended to the present case. We discuss these methodologies with less emphasis because they are also the subject of well-written books on optimization. On the other hand, we discuss with greater detail some methodologies that originate from the field of numerical PDE and are less known in the optimization community. Furthermore, we illustrate problems and methodologies like PDE optimization with uncertainty, shape optimization, quantum optimal control, and space-time electromagnetic inverse scattering problems that are emerging topics in PDE optimization.

In Chapter 2, we provide an introduction to optimization problems with PDE constraints using the terminology and notation that is usual in the PDE optimization community. The notions of reduced objective functional, gradient, Hessian and Lagrangian functions, optimality systems, etc., are introduced. A detailed derivation of optimality systems characterizing representative PDE optimization problems is illustrated.

In Chapter 3, we illustrate basic concepts concerning the discretization of optimality systems focusing on finite differences. Accuracy of optimal solutions is discussed considering an elliptic and a parabolic control problem. Further, we discuss the case of higher-order discretization and the case of optimal control problems governed by integral equations.

In Chapter 4, we recall some well-known unconstrained optimization methods. Our purpose is to emphasize some aspects of the implementation and application of these methods in the case of PDE optimization. We discuss nonlinear conjugate gradient schemes, Newton-type methods, and other black-box schemes. Further, we illustrate the main features of semismooth Newton methods and SQP schemes. The issue of preconditioning of KKT systems is also addressed.

In Chapter 5, multigrid methodologies are discussed. We roughly distinguish between the direct multigrid approach where the optimization problem is implemented within the hierarchy of grid levels, the use of multigrid schemes as inner solvers within an optimization scheme, and solution strategies where the multigrid method defines the outer loop.

In Chapter 6, we illustrate recent approaches to computing solutions to PDE optimization problems which are robust with respect to the stochasticity of the application framework. We discuss the treatment of uncertainty in PDE constrained optimization in the case where the coefficients of the PDE models are subject to random perturbations. Further, we discuss the problem of aerodynamic design under geometric uncertainty. A Bayesian approach to quantify uncertainty in PDE optimization problems is also illustrated.

In Chapter 7, we discuss novel applications of PDE optimization with representative models of mathematical physics, that is, shape optimization with Navier–Stokes equations, optimal control of quantum systems governed by the Schrödinger equation, and inverse scattering with Maxwell equations.

A long but certainly incomplete list of references completes this book.