Optimization and Engineering (2018) 19:515–520
https://doi.org/10.1007/s11081-018-9398-1

RESEARCH ARTICLE

# An introduction to partial differential equations constrained optimization

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Received: 23 July 2018 / Revised: 23 July 2018 / Accepted: 23 July 2018 /
Published online: 9 August 2018


**Abstract**
Partial differential equation (PDE) constrained optimization is designed to solve control, design, and inverse problems with underlying physics. A distinguishing challenge of this technique is the handling of large numbers of optimization variables in combination with the complexities of discretized PDEs. Over the last several decades, advances in algorithms, numerical simulation, software design, and computer architectures have allowed for the maturation of PDE constrained optimization (PDECO) technologies with subsequent solutions to complicated control, design, and inverse problems. This special journal edition, entitled "PDE-Constrained Optimization", features eight papers that demonstrate new formulations, solution strategies, and innovative algorithms for a range of applications. In particular, these contributions demonstrate the impactfulness on our engineering and science communities. This paper offers brief remarks to provide some perspective and background for PDECO, in addition to summaries of the eight papers.

**Keywords** Partial differential equations · Constraints · Optimization

## 1 Challenges

The state of numerical simulation has reached impressive levels of maturity enabling prediction of complicated dynamics from transport to thermo-mechanical systems and from medical imaging to material science. An important challenge is to

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utilize numerical modeling to support decision making and specifically solve optimal design, control and inversion problems. This motivates the need for algorithms and computational methods that are efficient, accurate, and applicable in the context of complicated dynamics. To this end, PDE-constrained optimization (PDECO) provides techniques designed to solve large-scale nonlinear problems constrained by complex systems. However, the culmination of mathematics, algorithmic design, software implementation, and PDE discretization including all the associated technologies, motivate a range of challenges including problem size, implementation intrusiveness of PDE solvers, globalization, inexactness, treatment of inequalities, and time dependence.

## 2 Algorithmic overview

PDECO problems are originally posed in function spaces and thus their numerical treatments require solutions with very high-dimensional state and optimization variables, which strain even the most powerful computational architectures in terms of memory, efficiency, and parallelism. The problem size however ranges from a handful to the equivalent of the number of state variables. For instance, optimal control of source terms or boundary conditions will explore fewer decision variables than the mesh-dependent decision variables in topological optimization. Inverse problems can span the spectrum with reconstruction of source terms, boundary conditions or material properties. Accordingly, the foundation of algorithmic design is based on achieving optimality and feasibility but often demands customization to accommodate formulation, dynamics, software, and computer architectures.

PDECO embodies analysis, discretization, and the development of dedicated optimization methods for minimization problems constrained by partial differential equations. Several challenges must be addressed to solve these problems, consisting of ill-conditioning, nonlinearities, computational requirements, and software implementation. To address these challenges several key algorithmic and computational techniques are adopted. First, exact gradients are enabled through direct or adjoint-based sensitivities. The motivation for accuracy and efficiency is to address the large scale nature of the PDECO problem and nonlinearities associated with the physics and the optimization formulation. Typically, finite difference methods to calculate gradient and Hessian information are ineffective and computationally intractable. Second, the dynamics are represented by PDEs which need to be discretized (e.g. finite elements, finite differences, discontinuous Galerkin, etc.) and therefore proper handling of function spaces is crucial to ensure consistent and mesh-independent convergence properties. Third, for transient dynamics, implicit time integration methods are required. Fourth, because of the large-scale nature of the problems, embedded interfaces are necessary to exchange optimization, state, and other vectors between the optimization and forward simulation solvers. Consequently, software design plays an important role to make PDECO algorithms available to different numerical simulation codes.

Solution strategies are typically based on variants of Newton's method applied to the optimality conditions, also known as the Karush–Kuhn–Tucker (KKT) system.

A full-space solution strategy requires linear solvers with appropriate preconditioners. Sequential Quadratic Programing (SQP) is a full space strategy that can conveniently incorporate inequality constraints. The elimination of state variables is known as a reduced space formulation and is a popular solver strategy because it offers a more convenient implementation path than full space methods. Severe nonlinearities with poorly conditioned matrices are possible as a result of PDE constraints. Furthermore, large scale PDE solvers are inexact and must be accounted for in optimization software. To address these issues, standard line search and trust-region methods are commonly deployed with more customized algorithms such as continuation methods, mesh sequencing, regularization techniques, initial guess approximations, and adaptive approaches to address inexactness.

## 3 Advancements

Despite the aforementioned challenges and complications, significant advances have been made to where complex engineering and science problems are being solved with impact on decision-making. The contributions in this special journal edition features design, control, and inversion problems applied to material science, transport, electrical engines, biomedical science, magneto-statics, thermo-mechanical systems, and manufacturing. In each case, better designs, optimal control, accurate reconstructions are presented not just for standard PDECO problems but for more advanced formulations, including optimization under uncertainty, design of sensor locations for inverse problems, topological optimization solutions, control of parameters, and real-time performance for data assimilation. These contributions highlight the applicability of PDECO and demonstrate the many extensions of the field. In the following section, summaries of each paper are provided.

## 4 Summary of contributions

Adam et al. (2018) study a topology optimization problem for the cross section (aperture design) of a strained photonic device. The full system couples PDE models for elasticity, semiconductors, and optics. The paper focuses on the linear elasticity part and addresses the optimal placement of several materials within a domain using a phase field approach. The differentiability properties of the control-to-state mapping are investigated and existence of solutions as well as first and second order optimality conditions are proved. The authors propose three numerical methods—gradient flow, projected gradient, and interior point approaches—and compare them for two test cases on a hierarchy of meshes.

The paper by Antil et al. (2018) investigates an optimal control strategy for steering drug concentration to a desired target location. The underlying PDE is a drift-diffusion equation that contains the Kelvin (magnetic) force. The proposed approach solves an optimization problem to approximate a desired Kelvin force field by a superposition of dipoles. The control variables are the dipoles' magnetic field intensity, direction, and their location. Existence of solutions and optimality conditions are derived for two cases where either the dipole positions or their directions are fixed. Convergent discretizations are proposed and investigated. Numerical results for several test cases are presented. The authors also propose a discretization scheme for the convection-dominated drift-diffusion equation that results after inserting the approximated force field.

Herzog et al. (2018) study the optimal sensor placement for joint parameter and state estimation in a large dynamical system, e.g., a semi-discretized unsteady PDE. First, the initial state and further parameters are estimated based on $m$ state measurements and then the dynamical system is solved with these data to obtain a quantity of interest (QOI) that depends on the final time state. The goal is to select $m$ out of $\ell > m$ state measurements to estimate the QOI in an optimized way. The approach uses an approximate covariance matrix of the joint initial state and parameter estimates. From this matrix, which depends on the selected measurements, encoded as a 0–1 vector $w$, an approximate covariance matrix of the QOI is derived that enters the cost function of the optimal sensor placement problem. The authors relax the 0–1-constraints on $w$ and propose a simplicial decomposition method that exploits the problem structure. Numerical results for a thermo-mechanical system demonstrate the capabilities of the approach.

The article by Hintermüller et al. (2018) studies adaptive discretizations based on goal-oriented a posteriori error estimation for optimal control problems governed by a Cahn–Hilliard–Navier–Stokes system. A double well potential is used which results in an unsteady PDE system that couples a fourth order variational inequality with the Navier–Stokes equations. Optimal control of the semi-discrete problem is considered, which constitutes an infinite-dimensional mathematical program with complementarity constraints (MPCC) for which suitable stationarity conditions are derived. The main focus of the paper is the development of a goal-oriented adaptive finite element approach for this challenging problem class. Numerical experiments for the splitting of a bubble by a spatially localized control and the stabilization of a rising bubble in a capillary by tangential Dirichlet boundary control are presented.

Kärcher et al. (2018) investigate certified reduced basis (RB) approximations for parametrized four-dimensional variational (4D-Var) data assimilation problems. Both, the strong-constraint case, which targets at estimating the initial data from measurements, and the weak-constraint case, which estimates a forcing term that represents model errors, are considered. In terms of optimal control, the control is given by the initial condition in the strong- and by the model error in the weak-constraint case. The state equations contain a parameter vector. The paper develops RB approximations for state, adjoint state, and control including efficiently computable a posteriori error bounds. The RB is obtained by a POD-greedy method that samples the parameter set. The efficiency of the approach is documented for a spatially 2D convection diffusion equation with the Péclet number as the parameter.

The paper by Kolvenbach et al. (2018) develops a robust optimization approach for shape optimization problems under uncertainty. The uncertain parameters live in an ellipsoid and the cost and constraint functions are robustified by taking the worst case over this uncertainty set. Quadratic approximations with respect to the uncertain parameters are used to achieve a good compromise between accuracy and tractability. They are obtained either by Taylor expansion or by interpolation. Adjoint-based techniques for computing the required derivatives as well as subgradients of the worst case functions are developed. The worst case functions are value functions of trust region (TR) problems. Different approaches are presented and compared that either use the value functions or formulate an MPCC with the TR optimality systems as constraints. Applications to shape optimization of an elastic structure and of an electrical engine are considered and a numerical comparison of the different approaches is performed for these problems.

Leithäuser et al. (2018) consider optimal shape design problems for polymer spin packs. This problem class arises in the production of synthetic fibers and non-woven materials. The design goal is achieved by adjusting the wall shear stress (WSS) at the boundary. Two setups are discussed, one in 3D and governed by Stokes flow, and one in 2D, where the Stokes system is rewritten as a biharmonic equation and additional geometric and state constraints (lower bound on the WSS) are considered. The 3D problem is solved by a gradient method in a subspace of $H^2$ based on the Riesz representation of the shape derivative of the tracking-type cost function. In the 2D case, the biharmonic equation reformulation is transformed to a reference domain by combining the method of mappings with conformal maps. The resulting problem is solved by an interior point method using the discretize-then-optimize approach. Numerical results for both setups are presented.

The article by Mang et al. (2018) provides a survey of PDE constrained optimization techniques for medical imaging applications. As concrete examples, the authors discuss image registration as well as data assimilation for brain tumor imaging. Also cardiac motion estimation is briefly addressed. The applications are formulated as PDE-constrained optimal control problems with a tracking-type functional and regularization. The image registration problem inverts for the velocity field in a transport equation while the brain tumor imaging problem identifies the initial condition of a nonlinear parabolic PDE. Numerical aspects of the PDE discretization, computational details of the optimization method, and an adjoint-based globalized Gauss–Newton–Krylov algorithm, are discussed. Several large-scale numerical experiments are showcased.

## 5 Conclusions and future opportunities

PDECO is deeply rooted in engineering and science and will continue to advance as a result of the ever-growing demand for analysis to support decision-making processes. Many exciting areas of future research can be identified. The presence of uncertainty in the dynamics, boundary conditions, initial conditions, measurements, or the computational infrastructure motivates an important field of research in the area of optimization under uncertainty, potentially leveraging robust optimization, risk-averse methods, and optimal experimental design. The incorporation of integer optimization variables demands new mathematical innovation to couple mixed integer programming and PDECO. Competing objective functions suggest the consideration of game theory concepts which combined with PDE constraints will require new algorithmic designs. In addition to many more potential algorithmic research areas, the need to solve new engineering and science problems will drive interesting research extensions. For example non-smooth behavior from phase changes, contact friction, visco-plastic flows, and electrical circuits are driving new research in variational inequalities, complementarity systems, and semismooth Newton algorithms. It should be noted that terms in the optimization formulation can also cause non-smoothness (e.g. regularization, risk measures). A final challenge worth mentioning, especially in light of exascale computer architectures, is the development of software to enable efficient and flexible processing.

**Acknowledgements** Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under Contract DE-NA-0003525. This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

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