Abstract: This survey article summarizes some ideas of the two principal procedures for solving optimal control problems governed by partial differential (algebraic) equations: the indirect method or first-optimize-then-discretize approach based on first-order necessary conditions, and the direct method or first-discretize-then-optimize approach based on non-linear programming software. The focus of this paper is to discuss some pros and cons when applications come from real-life problems. It also glances at the main method which currently may have the best chance for online applications in PDE constrained optimization. The demonstrator example deals with the optimal control of a certain type of high temperature fuel cell system.

Keywords: Optimal control, partial differential equations, numerical methods, real-time, fuel cell systems

1. INTRODUCTION

When analyzing mathematical models for complex dynamical systems, their analysis and numerical simulation are generally only first steps. Thereafter, one often wishes to complete these investigations by an optimization step to exploit inherent degrees of freedom for optimizing a desired performance index with the dynamical system as side condition. This generally leads to optimization problems of extremely high complexity, particularly if the underlying system is described by (time dependent) partial differential equations (PDEs) or, more generally, by a system of partial differential algebraic equations (PDAEs).

In this survey paper we will summarize the main ideas of optimization subject to PDE constraints and in particular exhibit some of the challenges we are facing and have to cope when solving real-life problems.

For the purpose of motivation three problems from engineering applications shall be examplarily described first:

(1) Hot cracking is a common risk in welding of aluminium alloys. According to a Russian patent [Shumilin et al. (1980)] this risk can be avoided by applying so-called multi-beam laser welding techniques. By two additional laser beams the thermal stress introduced by the main welding laser can be compensated, if the additional laser beams are optimally placed and sized, while they must not melt on the material. Mathematically we obtain a semi-infinite optimization problem with PDE and non-standard state variable inequality constraints, a special case of an optimal control problem for PDEs; see Petzet (2008) and Figs. 1 and 2. The model is briefly sketched in Appendix A.

(2) Future concepts for intercontinental flights of passenger aircraft envisage aircraft which are able to fly at hypersonic speeds. Due to such high velocities the thermal heating of the aircraft is an issue which has to be taken into account. This multi-physics problem leads to an optimal control problem for a system of ordinary differential equations (ODEs) where the aerothermic heating of the aircraft’s body is modelled by a quasilinear heat equation with nonlinear boundary conditions. The temperature of the thermal protection system constitutes a complicated state variable inequality constraint in an ODE-PDE optimal control problem; see Chudej et al. (2008) and Witzgall and Chudej (2012). Figure 3 shows the coupling structure between ODE- and PDE-subsystem. In Fig. 4 the

Challenge in ODE-PDE optimal control: minimum fuel intercontinental hypersonic flights under a limitation of aero-thermal heating.

Numerical results of minimum fuel trajectory optimization without (dashed) and with temperature constraint (solid); cf. Chudej et al. (2008). The boundary arc of the state constraint can be seen (lower line). Note that the state constraint is not observed in the uncritical region in order to save computer time. They are indicated by the horizontal lines of the graphs. The effect of the state constraint on the trajectory is depicted and the appearance of a boundary arc of the heating constraint can be seen. The model is briefly sketched in Appendix B.

The main example, which will be discussed in more detail in this paper, is concerned with the optimal control of certain fuel cell systems for an environmentally friendly production of electricity. Reaction-advection equations describing the electro-chemical reactions in the gas streams of anode and cathode for each compound, a heat equation describing the heating-up of the solid caused by the reactions, as well as additional ordinary, resp. algebraic, resp. integro differential equations sum up to a huge coupled system of up to 28 instationary spatially two-dimensional PDAEs of extremely high complexity. The inflow data into the anode inlet and into the catalytic burner, and the amount of exhaust gas that is fed back from the cathode outlet to the burner are the control variables, cp. Fig. 5. A complete compendium of the research within this project is given in Sundmacher et al. (2007), whereas Chudej et al. (2008) focus on the mathematics behind the project. Figure 6 shows a photo of the type of stationary high temperature fuel cell module under construction. The stack of cells is just positioned into the Hotmodule, which has been investigated in this project and which is particularly suitable for the highly efficient power-heat coupling.
After this motivation a glimpse on the mathematical theory of optimal control problems for one elliptic equation is given to describe the amount of preparatory work that has to be invested when solving optimal control problems by so-called adjoint based methods, i.e. methods which are based on first order necessary conditions. Thereafter two numerical concepts, namely first optimize then discretize and first discretize then optimize are sketched and discussed with respect to their pros and cons when applying to real-life problems. In addition an overview over the present mathematical toolbox from literature is given to show some current trends of research in PDE optimal control. A glimpse on a certain model reduction technique, which may help in case of real-time demands, finalizes this paper.

2. A GLIMPSE ON THE THEORY

2.1 A linear-quadratic elliptic optimal control problem

Let us consider the following elliptic model optimal control problem of so-called tracking type for a distributed control:

\[ \min_{u \in U_{\text{ad}}} J(y, u) := \frac{1}{2} \int_{\Omega} (y - y_d)^2 \, dx + \frac{\lambda}{2} \int_{\Omega} u^2 \, dx \]

subject to the side conditions

\[ -\Delta y + y = u \quad \text{in} \quad \Omega \subset \mathbb{R}^N, \]

\[ \partial_n y = 0 \quad \text{on} \quad \Gamma = \partial \Omega. \]

Here, let \( \Omega \) be a bounded Lipschitz domain, on which the state variable \( y \) and the control variable \( u \in U_{\text{ad}} := \{ u \in L^2(\Omega) : u_{\text{min}} \leq u \leq u_{\text{max}} \text{ a.e.} \} \) live where the set of admissible controls is defined by functions \( u_{\text{min}}, u_{\text{max}} \in L^\infty(\Omega) \). Finally the function \( y_d \) to be tracked is assumed to be of class \( L^2(\Omega) \) and the regularisation parameter \( \lambda \) shall be positive, \( \lambda > 0 \).

According the Theorem of Lax-Milgram the elliptic boundary value problem has a unique solution \( y \in H^1(\Omega) \) so that there exist a linear and continuous solution operator \( S : U_{\text{ad}} \rightarrow H^1(\Omega) \) mapping each control \( u \) to its associated state \( y \). Herewith, we formally arrive the so-called reduced functional

\[ \min_{u \in U_{\text{ad}}} f(u) \]

with \( f : U_{\text{ad}} \rightarrow \mathbb{R} \) via \( f(u) := J(Su, u) \). Hence we obtain an optimization problem in the Hilbert space \( L^2(\Omega) \). Due to the convexity of this problem it has a unique optimal solution which must fulfill the variational inequality

\[ (S(Su^* - y_d) + \lambda u^*, u - u^*)_{L^2(\Omega)} \geq 0 \quad \forall \ u \in U_{\text{ad}}, \]

where \((\cdot, \cdot)_{L^2(\Omega)}\) denotes the scalar product in \( L^2(\Omega) \) and \( S \) the adjoint solution operator. The asterix \((\cdot)^*\) indicates optimal variables. Because of the convexity of the problem, this necessary condition is here sufficient, too.

By obeying \( S u^* - y_d = y^* - y_d \) and replacing \( p := S(y^* - y_d) \), the above variational inequality can be rewritten as

\[ (p + \lambda u^*, u - u^*)_{U_{\text{ad}}} \geq 0 \quad \forall \ u \in U_{\text{ad}} \]

with the adjoint state variable \( p \) satisfying the adjoint equation

\[ -\Delta p + p = y^* - y_d \quad \text{in} \quad \Omega \subset \mathbb{R}^N, \]

\[ \partial_n p = 0 \quad \text{on} \quad \Gamma = \partial \Omega. \]

Moreover, the variational inequality can be replaced by the pointwise control law

\[ u^*(x) = P_{U_{\text{ad}}} \left\{ - \frac{1}{\lambda} p(x) \right\} \]

with the projection operator \( P_{U_{\text{ad}}} \) onto the set of admissible controls.

The original boundary value problem for the state variable \( y \in H^1(\Omega) \) and the boundary value problem for the adjoint state \( p \) being also of class \( H^1(\Omega) \) constitute together with the optimal control law the so-called first-order optimality or Karush-Kuhn-Tucker system. This is a well-defined coupled system for two elliptic equations admitting a unique solution under reasonable assumptions. For more details it is referred to the most recent textbook of this field concerning theory, the book of Tröltzsch (2010).

Such optimality systems can be easily set up by the formal Lagrange technique [cf. Tröltzsch (2010)]. Define the Lagrangian \( L \) and integrate twice by parts

\[ L(y, u, p) := J(y, u) - \int_\Omega (-\Delta y + y - u) \, p \, dx - \int_{\partial \Omega} \partial_n y p \, ds \]

Then a differentiation in the direction of \( h \in H^1(\Omega) \) yields

\[ D_y L(y^*, u^*, p) h = 0 \quad \forall h \in H^1(\Omega) \]

\[ \Rightarrow -\Delta p + p = y^* - y_d, \quad \partial_n p = 0, \]

\[ D_u L(y^*, u^*, p) (u - u^*) \geq 0 \quad \forall u \in U_{\text{ad}} \]

\[ \Rightarrow (p + \lambda u^*, u - u^*)_{U_{\text{ad}}} \geq 0 \quad \forall u \in U_{\text{ad}}. \]

In addition there holds \( f'(u) = D_u L(y^*, u^*, p) \).

2.2 A semilinear-quadratic elliptic optimal control problem

The generalisation to semilinear equations for distributed as well as boundary controls \( v \in V_{\text{ad}}, \text{resp.} \ u \in U_{\text{ad}} \) for an objective function of type

\[ \min_{u \in U_{\text{ad}}, v \in V_{\text{ad}}} J(y, v, u) := \frac{1}{2} \int_{\Omega} (y - y_d)^2 \, dx + \frac{1}{2} \int_\Gamma (y - y_d)^2 \, ds + \frac{\lambda}{2} \int_{\Omega} u^2 \, dx + \frac{\mu}{2} \int_\Gamma v^2 \, ds \]

leads, under suitable assumptions on the non-linearities \( b \) and \( d \), to the following optimality system

\[ -\Delta y + y + b(y) = u \quad \text{in} \quad \Omega \subset \mathbb{R}^N, \]

\[ \partial_n y + d(y) = v \quad \text{on} \quad \Gamma = \partial \Omega, \]

\[ -\Delta p + p + b'(y) p = y - y_d \quad \text{in} \quad \Omega \subset \mathbb{R}^N, \]

\[ \partial_n p + d'(y) p = y - y_d \quad \text{on} \quad \Gamma = \partial \Omega, \]

\[ u(x) = P_{U_{\text{ad}}} \left\{ - \frac{1}{\lambda} p(x) \right\}, \quad v(x) = P_{V_{\text{ad}}} \left\{ - \frac{1}{\mu} p(x) \right\}. \]

For details, see again Tröltzsch (2010).
In this book also general nonlinear functionals as well as instationary partial equations such as parabolic equations are investigated. Note that for this model problem the adjoint equation has the same main part of the differential operator as the original state equation while their nonlinearities are linearized. In case of linear or semilinear parabolic equations with time $t \in (0, t_f)$ the adjoint equation is regressive in time, i.e., the term $y_t$ passes over to a term $-p_t$ with initial conditions given in $t = t_f$ instead of $t = 0$ as for the state variable $y$.

Necessary conditions even for quite general nonlinear problems can be easily set up by the formal Lagrange technique, even in cases, where existence proofs fail, however, without a theoretical justification. Nevertheless, this technique often provides the only possibility to proceed towards adjoint-based numerical methods.

Since PDE models are mostly not nonlinear in the main part of their differential operator, except for quasilinear equations, the possibly severest nonlinearities are often given by the source terms $b$ and $d$. They may then be treated separately by symbolic or automatic differentiation. We will demonstrate this for the MCFC model mentioned in the introduction.

### 3. A GLIMPSE ON THE NUMERICS

Let us write a general problem of optimal control for PDEs in abstract form as follows:

$$(P) \quad \min_{u \in U_{ad}, y \in Y_{ad}} J(y, u) \quad \text{s.t.} \quad PDE(y) = B(u).$$

Here $PDE$ stands for an arbitrary differential equation in the state $y$ and $B$ is an operator acting on the control $u$. The aim in solving those problems efficiently is to keep the ratio of the amount of computation for the optimization versus the amount of computation for the simulation of the problem below a small constant, which obviously cannot undershoot 2 in view of the above theoretical results.

The two essential numerical procedures are known as direct, resp. first discretize then optimize-method, and indirect, resp. first optimize then discretize-method. A direct method can be described as follows:

$$(P_h) \quad \min_{u_h \in U_{ad}, y_h \in Y_{ad}} J_h(y_h, u_h) \quad \text{s.t.} \quad PDE_h(y_h) = B_h(u_h)$$

where the index $h$ indicates discrete variables, resp. discretized operators. Crucial are the choices of the finite dimensional spaces $U_{ad}^h$ and $Y_{ad}^h$ for the state, resp. control variable as well as the discretization of the PDE. This approach leads to a generally huge nonlinear programming problem for which even standard software for large scale constrained nonlinear optimization may today be applicable only for problems of moderate size unless coarse discretizations are accepted, e.g., using the combination of AMPL [The AMPL Company (2012)] and IPOPT [Laird and Wächter (2012)].

In contrast, indirect methods exploit the first order necessary conditions: The minimization of the reduced functional $f(u) := J(S(u), u)$ requires the solution of an optimality system of the form $f'(u) = 0$ which then has to be discretized, i.e., as $F_h(u_h) = 0$. Here appropriate finite dimensional ansatz spaces for the adjoint state and generally also for certain multipliers are to be chosen additionally.

In summary, first discretize then optimize means: replace all quantities of the infinite dimensional optimization problem by finite dimensional substitutes and solve an NLP:

$$\min f(u) = J(S(u), u) \Rightarrow \min f_h(u_h) = J_h(S_h(u_h), u_h),$$

while first optimize then discretize means: derive optimality conditions of the infinite dimensional system, discretize the optimality system and find a solution of the discretized optimality system:

$$f'(u) = 0 \Rightarrow F_h(u_h) = 0.$$

In ideal manner, one should strive for a discrete concept for which both approaches commute; see Vexler et al (2011). A rich mathematical toolbox — not necessarily complete — has been developed so far consisting, e.g., of one-shot-iterations based on the structure of the optimality system (cf. Griewank, Schulz), of non-smooth solution techniques for state constrained problems (cf. Ito, Hintermüller, Kunisch, M. Ulbrich), of multigrid methods (cf. Borzi, Schulz), of tailored discrete concepts (cf. Hinze, Meyer, Rösch), of penalty or barrier methods for the relaxation of constraints (cf. Hintermüller, Kunisch, Schiela), of methods for state-constrained optimal control problems via set optimal control problems using shape calculus (cf. Frey, Bechmann, Pesch, Rund), of various concepts of adaptive algorithms (cf. Becker, Rannacher: Vexler; Hintermüller, Hoppe; Hinze, Günther, and many others), of surrogate models for the PDE system in the optimality system (cf. Hinze et al., Sachs et al., Kunisch, Tröltzsch, S. Ulbrich, Volkwein), of shape optimization methods (cf. Sokolowski, Zolesio; Ganger, Schulz; Hintermüller, Ring; M. Ulbrich, S. Ulbrich), of automatic differentiation tools providing adjoints automatically (cf. Griewank, Walther). Most of the associated references can be found in the textbooks focussing on numerical methods for PDE constrained optimization of Hinze, Pinnau, M. Ulbrich, and S. Ulbrich (2008) and Borzi and Schulz (2011), resp. in the survey article of Herzog and Kunisch (2010), resp. in articles of the aforementioned authors the references of which can be found on their homepages, resp. which can be downloaded from there.

### 4. A REAL-LIFE APPLICATION: OPTIMIZATION OF MOLTEN CARBONATE FUEL CELLS

Fuel cells are apparatuses for an environmentally friendly energy production in which a controlled oxyhydrogen reaction goes on. Fuel cell systems can be classified according to their range of application: mobil or stationary, and to their operating temperature: low, moderate, or high.

Here, we exploit two models of a hierarchy of mathematical models for so-called Molten Carbonate Fuel Cells (MCFCs), a prototype of which is the Hotmodule of MTU Onsite Energy GmbH, Ottobrunn; see Fig. 6. These models have been developed by Heidebrecht (2004) and later simplified by Rund and Chudej (2011). The results, which are summarized for this review, were, in great part, funded by the Federal Ministry of Education and Research of the Federal Republic of Germany from May 2002 until December 2005.
First, the functionality of MCFCs shall be described briefly. MCFCs are high temperature fuel cells that can produce the necessary hydrogen from its fuel gas, e.g., from methane CH\textsubscript{4} because of its high operating temperature. This technique is known as internal reforming and is one of the advantages of MCFCs, since naturally occurring elemental hydrogen is relatively rare on Earth, despite it is the most abundant chemical element.

The two reduction reactions in the anode gas channel (see Fig. 7) are endothermic, hence they consume energy. The anode exhaust gas is completely oxidized in the burning chamber by inserting air. After passing a mixer two oxidation reactions take place in the cathode gas channel which sum up to the second reduction reaction shown in Fig. 7. This reaction is exothermic. Part of the exhaust gas of the cathode can be refed into the catalytic burner; see again Fig. 7. This figure emblematis the simplest model for a MCFC by a spatially 1D counter flow configuration. In contrast, Fig. 8 depicts a spatially 2D cross flow configuration, which is realized in the Hotmodule mentioned above.

In summary, seven chemical compounds indexed by \( k \) (cp. Fig. 8) appear: CH\textsubscript{4}, H\textsubscript{2}O, H\textsubscript{2}, CO, CO\textsubscript{2}, O\textsubscript{2}, and N\textsubscript{2}. Electricity is produced if the anode is provided by hydrogen and the cathode by oxygen. The two electrodes are separated by a special electrolyte, which only let pass carbonate ions CO\textsubscript{3}\textsuperscript{2-}, cp. Fig. 7.

By the way, the exhaust gas at the cathode outlet can be declared as air according to the German Federal Pollution Control Act.

The variables appearing in the PDAE model due to Heidebrecht (2004) can be obtained from Fig. 8. They can be grouped according to their time scales into slow, fast, and very fast variables. The complete system consists of a semilinear heat equation for the solide temperature \( \theta_s \), a set of quasilinear hyperbolic reaction advection equations for the molar fractions \( \chi \) of all chemical compounds indexed by \( k \), the anode and cathode gas temperatures \( \theta_a \) and \( \theta_c \), as well as for the molar flow densities \( \gamma \) the equation of which degenerate, i.e. do not depend of partial derivatives with respect to time \( \tau \). Here the time is scaled due to a transformation of all variables to dimensionless quantities. The spatial variables are denoted by \( z \in [0,1] \) for the 1D counter flow design (Fig. 7) and by \( \zeta_1 \) and \( \zeta_2 \) for the 2D cross flow design (Fig. 8). The potentials \( \Phi \) and the cell current \( U_{cell} \) are given by ordinary differential algebraic equations (DAEs) in each spatial point the nonlinear terms of which depend on integral terms which in turn depend on all other variables. Depending on the complexity of the model the chemical reactions \( \varphi \) in the pores of the electrodes are modelled by additional algebraic equations. The transition from the anode outlet through burner and mixer to the cathode inlet is described by additional algebraic and ordinary differential algebraic equations. Complete models can be found for the 2D cross flow model being of dimension up to 28 in Heidebrecht (2004) and Chudej et al. (2008) and for the 1D counter flow model being of dimension 21 in Rund and Chudej (2011) and Rund (2012).

This dynamical system can be controlled by up to seven controls for the configuration of the inflowing gas streams at the anode inlet and into the burning chamber either from outside or from the cathode outlet via the recirculation device. Finally, \( I_{cell} \) is an input variable to be chosen for load changes. Optimal load changes will be the major task for the optimization of those complicated PDAE models. In doing so large variations of the solid temperature \( \theta_s \) must be avoided to get around material corrosion induced by hot spots.

4.2 Numerical results for the 2D cross flow configuration via the first-discretize-then-optimize approach

In her thesis Sternberg (2007) has investigated models for the 2D cross flow configuration. In particular she has computed optimal trajectories for fast and safe load changes including sensitivity studies. Her first-discretize-then-optimize approach is based on standard discretization schemes, including conservative upwind schemes for the hyperbolic transport equations. Thereby the PDAE model is transferred via semi-discretization in space into a large scale system of DAEs, known as method of lines. Then the code NUDOCCCS of Bäckens (2002) was applied to solve the DAE optimal control problem. Inside NUDOCCCS the sparse NLP solver SNOPT has been employed, the
Fig. 9. Fast load change by tracking the cell current using either the full set of controls (top) or the molar flow density at anode inlet only [Sternberg (2007)].

Fig. 10. Solid temperature $\theta_s$ at final time [Sternberg (2007)]. Note the gas flow directions: in the anode from $\zeta_1 = 0$ to $\zeta_1 = 1$, in the cathode from $\zeta_2 = 1$ to $\zeta_2 = 0$. A hotspot occurs at the anode outlet, resp. at the cathode inlet.

Fig. 11. Anode gas temperature $\theta_a$ at final time [Sternberg (2007)]. The anode reaction is firstly endothermic, then exothermic.

Fig. 12. Cathode gas temperature $\theta_c$ at final time [Sternberg (2007)]. The cathode reaction is uniformly endothermic.

More results can be found in Sternberg (2007) and Chudej et al. (2008). In the latter fast and safe load changes have been obtained by modifying the objective functional

$$\min_{\tau_0} \int_{\tau_0}^{\tau_f} \left( (1 - \varepsilon(\tau)) (U_{\text{cell}}(\tau) - U_{\text{to-be}})^2 \right) \, d\tau$$

$$+ \varepsilon(\tau) \left( \int_{\Omega} \left( \theta_s(\zeta, \tau) - \theta_{\text{ref}}(\zeta, \tau) \right)^2 \, dx \right) \, d\tau$$

with

$$\varepsilon = 0 \text{ on } \left[ 0, 0.1, 1 \right], \quad \varepsilon = 1 \text{ on } \left[ 1, 11.1, 111.1 \right],$$

and \( \varepsilon = 1 \) on \([111.1, 1111.1]\).

Herewith the fast reacting cell current $U_{\text{cell}}$ is initially to be tracked towards $U_{\text{to-be}}$ and, at the end, the functional switches to the slowly varying solid temperature $\theta_s$. This choice avoids too large and therefore risky variations in the solid temperature without employing a pointwise state constraint on it or even a constraint on the gradient of the solid temperature which would be quite a challenge for such a complicated model; see Fig. 13 for the numerical results.

Due to the complexity of the system and the long process time (about 3 hrs.), but mainly due to the non-efficient application of numerical differentiation for the computation of the gradient of the objective function with respect to the discretized control variables only coarse discretizations could be handled. Nevertheless, the numerical results were satisfactory at that time thanks to the smoothing influence of the heat equation. However, the amount of computation went up to days.

Figure 9 shows the optimization of a fast load change from $I_{\text{cell}} = 0.7$ to $I_{\text{cell}} = 0.6$. Hereby, the stationary value of the cell current $U_{\text{cell}}$ associated with the new load is tracked in the $L^2$-norm. Because of this type of functional the entire time interval could be partitioned in a pseudo-logarithmic scale to compensate for the dynamical behaviour of fast variables at the beginning of the process. The optimization was then performed on the resulting subintervals in a suboptimal manner. Since the cell current reacts relatively fast, the new stationary point of the MCFC could be achieved in less than 1 sec. Moreover it turned out that the molar flow density alone is sufficient for controlling fast load changes. Figures 10, 11, and 12 depict the solid temperature $\theta_s$ and the gas temperatures in the anode and cathode channel, $\theta_a$, resp. $\theta_c$. 

Latest version of which can be found in Gill, Murray, and Saunders (2012).
4.3 Numerical results for the 1D counter flow configuration
via the first-optimize-then-discretize approach

Rund (2012) recently succeeded in applying the first-optimize-then-discretize approach to the 1D counter flow design for a modified model where all superfluous variables were omitted. To give an impression of the complexity of this simplified model its differential operator part is presented here in detail while the nonlinear source terms are abbreviated.

Equations prevailing in the gas channels and the solid:

\[
\begin{align*}
\frac{\partial \chi_{k,a}}{\partial t} + \gamma_a \frac{\partial \chi_{k,a}}{\partial z} &= f^{\chi_{k,a}}, \quad k \in \mathcal{I} \\
\frac{\partial \chi_{k,c}}{\partial t} - \gamma_c \frac{\partial \chi_{k,c}}{\partial z} &= f^{\chi_{k,c}}, \quad k \in \mathcal{I} \\
\frac{\partial \theta_a}{\partial t} + \gamma_a \frac{\partial \theta_a}{\partial z} &= f^{\theta_a} \\
\frac{\partial \theta_c}{\partial t} - \gamma_c \frac{\partial \theta_c}{\partial z} &= f^{\theta_c} \\
\frac{\partial (\gamma_a \theta_a)}{\partial z} (z,t) &= f^{\gamma_a \theta_a} \\
-\frac{\partial (\gamma_c \theta_c)}{\partial z} (z,t) &= f^{\gamma_c \theta_c} \\
c_{p,s} \frac{\partial \theta_a}{\partial t} - \frac{1}{v_c} \frac{\partial^2 \theta_a}{\partial z^2} &= f^{\theta_a}
\end{align*}
\]

Equations prevailing in burner and mixer:

\[
\begin{align*}
\chi_{k,b}(t) &= f^{\chi_{k,b}}, \quad k \in \mathcal{I} \\
\theta_b(t) &= f^{\theta_b} \\
\gamma_b(t) &= f^{\gamma_b} \\
\gamma_{air}(t) &= f^{\gamma_{air}} \\
\frac{d\chi_{k,m}}{dt}(t) &= f^{\chi_{k,m}}, \quad k \in \mathcal{I} \\
\frac{d\theta_m}{dt}(t) &= f^{\theta_m} \\
\gamma_m(t) &= f^{\gamma_m}
\end{align*}
\]

Equations describing the cell current and the potential fields:

\[
I_a(t) = \int_0^1 i_a(z,t) \, dz, \quad i_a(z,t) = f^{i_a}
\]

\[
I_c(t) = \int_0^1 i_c(z,t) \, dz, \quad i_c(z,t) = f^{i_c}
\]

\[
\frac{dU_{\text{cell}}}{dt}(t) = f^{U_{\text{cell}}} \\
\frac{\partial \Phi_a}{\partial t}(z,t) = f^{\Phi_a} \\
\frac{\partial \Phi_c}{\partial t}(z,t) = f^{\Phi_c}
\]

Except the nonlinearity in the two degenerated transport equations for the molar flow densities \( \gamma \), which, by the way, can be transformed by introducing auxiliary variables \( v := \gamma \theta_a \), the entire nonlinearity of the system is contained in the \( f^\gamma \)-terms. The full model can be found in Rund (2012). This property seems to be typical for complex multi-physics models and alleviates the derivation of the adjoint equations by applying the formal Lagrange technique with the Lagrangian

\[
\mathcal{L}(\ldots) = J
\]

\[
- \int_0^{t_f} \left( \int_{Q} \left( \frac{\partial \chi_{k,a}}{\partial t} + v_a \frac{\partial \chi_{k,a}}{\partial z} - f^{\chi_{k,a}} \right) \hat{\chi}_{k,a} \, dz \right) dt
\]

\[
- \int_0^{t_f} \left( \int_{Q} \left( \frac{\partial \chi_{k,c}}{\partial t} + v_c \frac{\partial \chi_{k,c}}{\partial z} - f^{\chi_{k,c}} \right) \hat{\chi}_{k,c} \, dz \right) dt
\]

\[
- \int_0^{t_f} \left( \int_{Q} \left( \frac{\partial \theta_a}{\partial t} + v_a \frac{\partial \theta_a}{\partial z} - f^{\theta_a} \right) \hat{\theta}_a \, dz \right) dt
\]

\[
- \int_0^{t_f} \left( \int_{Q} \left( \frac{\partial \theta_c}{\partial t} + v_c \frac{\partial \theta_c}{\partial z} - f^{\theta_c} \right) \hat{\theta}_c \, dz \right) dt
\]

\[
\int_0^{t_f} \left( \int_{Q} \left( \frac{\partial v_a}{\partial t} - \gamma_a \frac{\partial v_a}{\partial z} - f^{v_a} \right) \tilde{v}_a \, dz \right) dt - \int_0^{t_f} \left( \int_{Q} \left( v_a(0,t) - v_{a,in} \right) \tilde{v}_a \, dz \right) dt
\]

\[
- \int_0^{t_f} \left( \int_{Q} \left( \frac{\partial v_c}{\partial t} - \gamma_m \frac{\partial v_c}{\partial z} - f^{v_c} \right) \tilde{v}_c \, dz \right) dt - \int_0^{t_f} \left( \int_{Q} \left( v_c(1,t) - \gamma_m \theta_m \right) \tilde{v}_c \, dz \right) dt
\]
Linearization of the nonlinear terms yield the differential operators for the adjoint equations. Here the tilde and the hat indicate Lagrange multipliers associated with state variables governed by PDEs or other types of equations, resp. multipliers for initial conditions. Then partial integrations with respect to time and space yield the differential operators for the adjoint equations. This can be relatively easily done analytically. For the linearization of the nonlinear terms \( f \) however — cp. the adjoint equation of the semilinear model problem in Subsection 2.2 — one should employ symbolic or automatic differentiation. Further partial integrations may alleviate to read the adjoint system out of the so modified Lagrangian by means of standard variational arguments; cp. the example in Subsection 2.1.

Rund (2012) has developed an efficient discretization scheme for the integration of the optimality system based on an implicit time adaptive integrator, which can handle the different time scales, and, e.g. on upwind schemes for the advection-reaction equations. The two subsystems, state and adjoint system, are integrated successively due to the coupling structure shown in Fig. 14 similar to the well-known backward sweep method of the early days of ODE optimal control. This method is efficient even for many time steps which are to be performed because of the different time scales.

The two subsystems are connected by a set of nonlinear variational inequalities caused by the twofold entry of the controls into the fuel cell; cp. Fig. 14. The iteration is performed by a Quasi-Newton method with BFGS updates not relying on second order information. SQP methods seem to be hardly applicable due to their necessity of providing second order information. For more details see Rund (2012). The amount of computation for the 1D counter flow configuration can thus be reduced to minutes, if not less, e.g., using \( N = 81 \) lines, 160 time steps chosen by the code ode15s (Matlab R2010b) on Intel64 3.3 GHz DC, 8 GB: 5 sec CPU. — In principle this approach is also adaptable for 2D models.

Figure 15 shows the optimal solutions for the anode, cathode, and solid temperature for a load change started at 0.1 sec; cf. Rund (2012)
4.4 Some aspects of online control using model reduction techniques

In order to apply those computed optimal solutions for online control purposes, the complexity of the model must be reduced. Common approaches are known as model reduction techniques such as the Karhunen-Loève decomposition (1946, 1955), known under various names, today preferably called POD (proper orthogonal decomposition); see, e.g., the survey paper of Hinze and Volkwein (2005).

The basic idea can be described as follows. Let \( T \) stand for a state variable of a dynamical system governed by a PDE of type

\[
\frac{\partial T}{\partial t}(t, y, z) = \mathcal{D}T(t, y, z) + f(T(t, y, z))
\]

with the differential operator

\[
\mathcal{D} = a_y \frac{\partial}{\partial y} + a_z \frac{\partial}{\partial z} + b_y \frac{\partial^2}{\partial y^2} + b_z \frac{\partial^2}{\partial z^2}.
\]

Using the ansatz

\[
T(t, y, z) \approx \sum_{i=1}^{N} \bar{T}_i(t) \varphi_i(y, z)
\]

with precomputed basis functions \( \varphi_i(y, z) \) reflecting the main properties of the solution of \( T \). Such basis functions can, for example, be obtained from a simulation with a prescribed control programme to be expected “close enough” to the optimal one. Then take “snapshots” at different time instants \( t_i \), i.e. define \( \varphi_i(y, z) := T(t_i, y, z) \). Orthogonalize these basis functions, e.g. by a singular value decomposition. The PDE model can then be reduced, via the method of weighted residuals

\[
\int_{\Omega} \left( \frac{\partial T}{\partial t} - \mathcal{D}T - f(T) \right) \varphi_j \, dy \, dz = 0, \quad j = 1, \ldots, N,
\]

to an ordinary differential (algebraic) system

\[
\frac{d\bar{T}_i}{dt} = g_i(\bar{T}_1, \bar{T}_2, \ldots, \bar{T}_N), \quad i = 1, \ldots, N.
\]

Generally, \( N \) can be chosen much smaller than the number of discretization points for the semi-discretization in space according to the method of lines.

This approach has been applied in the aforementioned project by Mangold (2006) for the construction of a state estimator from the measurements that are available in the MCFC system (see Fig. 16). Figure 17 shows the high accuracy that can be obtained despite a drastically reduced number of ODEs from the POD ansatz compared to the number of ODEs from the method-of-lines approximation. Figure 17 finally depicts the results of the state estimator for the solid temperature and its gradient developed by Mangold (2006). This state estimator was actually implemented into the Hotmodule fuel cell system at the powerplant of the University Hospital, Magdeburg.

For more details for this approach applied to fuel cell online-control, see Mangold (2006).

Recent results on error estimates for POD approximations can be found, e.g., in Sachs and Volkwein (2010). Error estimates, if available at all at that time, were not taken into account in Mangold (2006).

5. CONCLUSION

The first-discretize-then-optimize approach lacks under a kind of curse of dimension and is applicable only for problems of modest size since the number of variables in NLP problems which can be treated by today’s best solvers are too limited for PDE constrained optimization problems. Important is to use NLP solvers which can extract exact first and second-order gradient information out of the discretization schemes by automatic differentiation, e.g., if they can be linked with the mathematical-modelling-language tool AMPL of The AMPL Company (2012), e.g.
the interior point solver IPOPT of Laird and Wächter (2012), or one uses directly discretization schemes where the two approaches commute.

The first-optimize-then-discretize approach requires the most skilled user and lacks under its difficult handling if non-standard problems like the ones presented here are to be optimized.

In cases where dynamical systems are controlled around their stationary state POD methods seem to be a promising method for online applications. Highly non-linear dynamical behaviour however cannot be treated so far.

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REFERENCES


Appendix A. MODEL OF THE LASER WELDING PROBLEM

To give an impression of the model for the multi-beam laser welding technique we firstly have to understand how the micro structure, particularly of an aluminium alloy, develops during the solidification. In the solid-liquid region, called mushy zone, between the liquidus and solidus isotherms, crystals grow dendritically until they form grains. During this process the liquid and the solid phase of the micro structure, particularly of an aluminium alloy, develop. During the solidification. In the solid-liquid region, called mushy zone, between the liquidus and solidus isotherms, crystals grow dendritically until they form grains. Moreover tensile strains and stresses occur which may initiate an opening displacement, the possible source for a hot crack; see Fig. A.1.

The following thermo-mechanical model is based on the so-called strip expansion technique of Okerblom et al. (1963); cp. Fig. A.2. Let us assume that the strips discretizing vertically the mushy zone can move frictionless and independently from each other and that they are deformable only in y-direction. Then, according to Ploshikhin, Prihodovsky, and Zoch (2003), the opening displacement $u_{od}$ is given by

$$
u_{od}(x_S) = 2\alpha \int_0^B \left[ T(x_L, y) - T(x_S, y) \right] \, dy ,$$

where $T$ denotes the temperature, $x_S < 0$ and $x_L < 0$ are those abscissae of the solidus, resp. liquidus isotherms, i.e. $T = T_S$, resp. $T = T_L$, lying behind the position of the main laser at $(x = 0, y = 0)$, and $\alpha > 0$ (thermal expansion coefficient) as well as $B > 0$ (width of workpieces) are constants; cp. Fig. A.2. This opening displacement must be either minimized or, at least, limited.

The optimization parameters describing position and size of the auxiliary laser beams are described by Fig. A.3. These parameters can be grouped by $p \equiv (p_1, p_{II})^\top$, $p_I \equiv (p_1, p_2, p_3, p_4)^\top$, and $p_{II} \equiv (p_5, p_6)^\top$, where the parameters $p_5 := x_S$ and $p_6 := x_L$ are implicitly defined by the equations $T_S = T(p_5, 0)$, resp. $T_L = T(p_6, 0)$. These two parameters act more like state variable, since only the parameters $p_I$ actually are design parameters to be chosen optimally. Obviously, the temperature depends on these parameters, $T(x, y) = T(x, y; p_I)$. Hence, the abscissae $p_5 := x_S(p_I)$ and $p_6 := x_L(p_I)$ also depend on these design parameters. It turns out that these abscissae have to be determined as precise as possible; see Petzet (2008). Thus, they have to be optimized while the opening displacement is bounded by a critical value $u_{od}^{crit}$.
subject to
\[
-\Delta T(x, y; p_1) - \frac{v}{a} \frac{\partial T}{\partial x}(x, y; p_1) = \frac{h(x, y; p_1)}{\lambda_s} \text{ in } \Omega,
\]
\[
T(x, y; p_1) = T_{amb} \text{ on } \partial \Omega,
\]
\[
\max_{(x, y) \in D_1(p_1)} T(x, y; p_1) \leq T_S,
\]
\[
u_{\text{od}}(p_5) \leq u_{\text{crit}}^{\text{od}}
\]
with the admissible set of parameters
\[
P_{\text{ad}} := \{p \in \mathbb{R}^6 : p_1 \leq 0, p_5 \leq 0, p_6 \leq 0, 0 \leq p_4 \leq q, 0.1 \leq p_3 \leq p_2, p_2 + p_3 \leq B, p_5 \leq p_1 + p_3, p_1 - p_3 \leq p_6, 0 \leq g(p_3) \leq p_3\}.
\]
Here, the constants \(v, a, \lambda, s, T_{\text{amb}}, \) and \(q\) denote velocity of the main laser, thermal diffusivity, thermal conductivity, thickness of plate, ambient temperature, and output power of main laser. The model functions \(h\) and \(g\) describe the area related density of power output of all lasers, resp. a smoothing function for modelling the influence region of the two auxiliary laser beams. See Fig. A.3 and for more details again Petzet (2008).

The temperature distribution is modelled by a quasi-stationary heat equation in a moving reference frame. The objective function is a point-functional. The inequality constraint constitutes a state constraint for avoiding additional weld pools under the auxiliary laser beams which obviously can be transformed to a standard pointwise state constraint acting only on a subregion of \(\Omega\).

Note that the PDE allows a semi-analytical solution which turns out to be numerically inferior to a finite element approximation; see Petzet (2008).

Appendix B. MODEL OF THE HYPERSONIC AIRCRAFT PROBLEM

The equations of motion for a flight along a great circle over a rotational Earth are given by the following ODE system [cf., e.g., Miele (1962)]:

\[
\dot{v} = \frac{1}{m} \left[ T(v, h; \alpha, \delta_T) \cos(\alpha + \sigma_T) - D(v, h; \alpha) \right] - \frac{g(h) \sin \gamma + \omega_E^2 r(h) \sin \gamma}{v}.
\]

\[
\dot{\gamma} = \frac{1}{mv} \left[ T(v, h; \alpha, \delta_T) \sin(\alpha + \sigma_T) + L(v, h; \alpha) \right] + \cos \gamma \left[ \frac{v}{r(h)} - \frac{g(h)}{v} + \omega_E^2 r(h) \right] + 2 \omega_E,
\]

\[
\dot{h} = v \sin \gamma,
\]

\[
\dot{\zeta} = v \cos \gamma,
\]

\[
\dot{m} = -\beta_T(v, h; \alpha, \delta_T).
\]

Here \(v, \gamma, h, \) and \(m\) are the state variables denoting velocity, flight path angle, altitude over Earth, path length, and mass. The control variables are the angle of attack \(\alpha\) and the throttle setting \(\delta_T\). Thrust \(T\), drag \(D\), lift \(L\) as well as instantaneous fuel consumption \(\beta\) are complicated model functions describing special characteristics of the hypersonic aircraft. The functions \(g\) and \(r\) denote the acceleration of gravity, resp. the distance of the aircraft from the geocenter. The time interval \([0, t_T]\) is unsuppressed. All other variables not mentioned are constants.

Minimum fuel trajectories are the goal of optimization, which is equivalent to maximize the mass at the unspeciﬁed terminal time:

\[
\max_{(\alpha, \delta_T) \in U_{\text{ad}}} m(t_T).
\]

Besides appropriate boundary conditions the typical inequality constraints of flight path optimization are further side conditions: box constraints for the two controls deﬁning the set \(U_{\text{ad}}\) of admissible controls, mixed control-state constraints for the load factor, \(0 \leq n(v, h; m; \alpha) \leq 2\), and a pure state constraints for the dynamic pressure, \(10 \leq q(v, h) \leq 50 [kPa]\). For details see Wächter (2004).

Due to the hypersonic flight regime the aero-thermal heating \(\Theta\) of the thermal protection system (TPS) is an important issue, yielding an additional constraint of type

\[
\Theta \leq \Theta_{\text{max}} = 1000 [K]
\]

where the aero-thermal heating \(\Theta\) is governed by a quasi-linear heat equation with nonlinear boundary conditions (because of the Stefan-Bolzmann law)

\[
\begin{align*}
q_{\text{TPS}} c_p(\Theta) \frac{\partial \Theta}{\partial t} & - \text{div} \left[ \lambda(\Theta) \text{grad} \Theta \right] = 0 \text{ in } \Omega \times (0, t_T), \\
\Theta(x, 0) & = \Theta_0(x) = 300 [K] \text{ in } \Omega, \\
\frac{\partial \Theta}{\partial n}(x, t) & = q_{\text{conv}}(v, h, \alpha) - q_{\text{rad}}(\Theta, \Theta_{\text{air}}(h)) \text{ on } \partial \Omega \times (0, t_T).
\end{align*}
\]

The ODE system and the PDE are unilaterally coupled here, but the heat constraint feeds the information from the PDE back to the ODEs.

For more details it is refered to Wächter (2004), Chudej et al. (2008), and Witzgall and Chudej (2012).