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SIMULATION OF MULTIBODY SYSTEMS WITH SERVO CONSTRAINTS THROUGH OPTIMAL CONTROL*

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ABSTRACT. We consider mechanical systems where the dynamics are partially constrained to prescribed trajectories. An example for such a system is a building crane with a load and the requirement that the load moves on a certain path.

Modelling the system using Newton's second law – "The force acting on an object is equal to the mass of that object times its acceleration." – and enforcing the servo constraints directly leads to differential-algebraic equations (DAEs) of arbitrarily high index. Typically, the model equations are of index 5 which already poses high regularity conditions. Also, common approaches for the numerical time-integration will likely fail. If one relaxes the servo constraints and considers the system from an optimal control point of view, the strong regularity conditions vanish and the solution can be obtained by standard techniques.

By means of a spring-mass system, we illustrate the theoretical and expected numerical difficulties. We show how the formulation of the problem in an optimal control context works and address the solvability of the optimal control system. We discuss that the problematic DAE behavior is still inherent in the optimal control system and show how its evidences depend on the regularization parameters of the optimization.

Key words. servo constraints, inverse dynamics, high-index DAEs, optimal control, underactuated mechanical systems

AMS subject classifications. 70Q05, **65L80**

1. Introduction

We consider mechanical systems with servo constraints, see e.g. [16, 5, 24], for which a part of the motion is specified. This includes crane models where we search for an input such that the end effector follows a prescribed trajectory. Thus, we consider an *inverse dynamics* problem.

The direct modeling approach, comprising the equations for the dynamics and the target trajectory as a constraint, comes as a differential-algebraic equation (DAE) of very high index. Note that we consider the DAEs in the so-called *behaviour context*, in which the inputs are regarded as variables [18, Ch. 3.6]. An immediate consequence is that a solution to the problem can only exist if the target trajectory is sufficiently smooth. We will refer to this approach as the DAE setting.

We also investigate the optimal control approach that relaxes the constraints and balances the approximation to the target with the control effort. We will see that this relaxation of the constraint $Cx = y$ softens the strong regularity assumptions from the DAE setting. In theory, the desired trajectory y may be even discontinuous. However, with the reformulation the DAE problematic is not simply gone. The weak coupling of

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the masses and the non-collocated sensors and activators are still in the model and cause oscillations in the output and strong peaks in the (unknown) input.

A remedy is the penalization of the derivatives of the control force at the expense of a worse performance and of less standard systems of equation for the numerical realization. In this paper we analyse the optimal control approach and investigate methods for the solution of the resulting equation systems. With the introduction of suitable penalization parameters we are able to balance the deviation from the trajectory and the control forces which - in applications - correspond to the costs.

Within the paper, we address the following difficulties:

(1) The very weak coupling of input and output that, in the (DAE) limit, will lead to singular actuations. We will investigate the dependency of the penalty or regularization parameters and the behavior in the limit case.
(2) Necessary and sufficient optimality conditions with an emphasis on their use for the solution of the optimization problem. Particularly in the case of holonomic constraints, the formally derived first-order optimality conditions are preferable over alternative formulations but they may not be solvable due to inconsistent data.

To illustrate the ideas and difficulties, we consider the idealized example of two cars connected via a spring, cf. Figure 1.1, as it was used, e.g., in [5, Sect. II].

Example 1.1. We consider a mechanical system with two degrees of freedom, namely the positions x_1, x_2, and one servo constraint. Aim is to find the input force F such that x_1 follows the desired trajectory given by the (sufficiently smooth) function y. The constrained system has the form

$$m_1\ddot{x}_1 = -k(x_1 - x_2 - d), \tag{1.1a}$$

$$m_2\ddot{x}_2 = \quad k(x_1 - x_2 - d) + F, \tag{1.1b}$$

$$x_1 = \quad y. \tag{1.1c}$$

Here, the spring constant k and the spring length d are positive. The given equations of motion form a DAE of (differentiation) index 5. For a definition of the index we refer to [8, Def. 2.2.2]. The generalization to a spring-mass chain of n masses connected by $n-1$ springs is straightforward and can be found in [5, Ex. 2], see also Example 2.3.

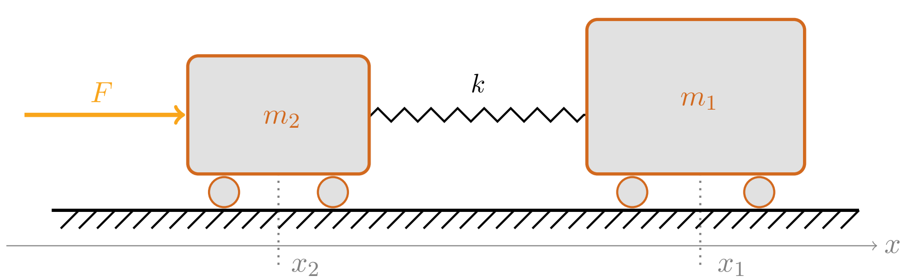

FIGURE 1.1. Illustration of the mechanical system from Example 1.1 including two cars connected by a spring with parameters k and d.

The paper is organized as follows. In Section 2 we give the formulation of the servo constraint problem as a DAE for which we additionally allow holonomic constraints. The counterpart is then presented in Section 3 in which the problem is modeled as an optimal control problem. Here we formulate the optimality conditions, discuss the consistency conditions of the boundary data, and prove the existence of an optimal solution. The relation of the two approaches is then topic of Section 4. In particular, we analyse the optimal control problem in which the input is not penalized. Section 5 gives an overview of the different solution strategies. This includes the DAE case as well as the optimal control approach for which boundary-value problems have to be solved. In Section 6 we compare the two approaches in means of two numerical examples. Finally, we conclude in Section 7.

2. Problem Setting

This section is devoted to the original formulation of the servo constraint problem as high-index DAE. For this, we consider the dynamics of a mechanical system with holonomic and servo constraints. This setting then includes the generalization of Example 1.1 with n cars as well as other simple crane models such as the overhead crane [6, Ex. 4].

Problem 2.1. For a time interval $[0,T]$, initial values x^0, $v^0 \in \mathbb{R}^n$ and a forcing term $f \in \mathcal{C}([0,T];\mathbb{R}^n)$, for $g\colon \mathbb{R}^n \to \mathbb{R}^r$, $M \in \mathbb{R}^{n,n}$ symmetric and strictly positive definite and $A \in \mathbb{R}^{n,n}$, for an output operator $C \in \mathbb{R}^{m,n}$ and a desired output y with $y(t) \in \mathbb{R}^m$, and for an input operator $B \in \mathbb{R}^{n,m}$, find an input $u \in \mathcal{C}([0,T];\mathbb{R}^m)$, a state trajectory $x \in \mathcal{C}^2([0,T];\mathbb{R}^n)$, and a Lagrange multiplier $p \in \mathcal{C}([0,T];\mathbb{R}^r)$ such that

$$M\ddot{x} = Ax + G^{\mathsf{T}}(x)p + Bu + f, \tag{2.1a}$$

$$0 = g(x), \tag{2.1b}$$

$$y = Cx, \tag{2.1c}$$

$$x(0) = x^0, \quad \text{and} \quad \dot{x}(0) = v^0. \tag{2.1d}$$

Note that the Lagrange multiplier p couples the holonomic constraint (2.1b) to the dynamical equations (2.1a) and that G is the Jacobian of the holonomic constraint, i.e., $G(x) = \frac{\partial g}{\partial x}(x) \in \mathbb{R}^{m,r}$.

If there are no holonomic constraints, as in the introductory Example 1.1, equation (2.1b) falls away. In this case, also the $G^{\mathsf{T}}(x)p$ term in equation (2.1a) vanishes and we are left with the following linear ODE servo problem.

Problem 2.2. Consider the setup of Problem 2.1 with $g \equiv 0$. Find an input $u \in \mathcal{C}([0,T];\mathbb{R}^m)$ and a state trajectory $x \in \mathcal{C}^2([0,T];\mathbb{R}^n)$ such that

$$M\ddot{x} = Ax + Bu + f, \tag{2.2a}$$

$$y = Cx, \tag{2.2b}$$

$$x(0) = x^0, \quad \text{and} \quad \dot{x}(0) = v^0, \tag{2.2c}$$

As a generic example, we consider the model equations for a mass-spring chain like in Figure 1.1 but with n cars. This then leads to a DAE of index $2n+1$, cf. [5, Ex. 2].

Example 2.3. A mass-spring chain, where one wants to steer the first mass x_1 along a trajectory y by applying a force u to the last mass x_n, can be modeled as in Problem 2.2, where $x = [x_1\ x_2\ \cdots\ x_n]^{\mathsf{T}}$ is the vector of coordinates, $M \in \mathbb{R}^{n,n}$ is the diagonal matrix of the masses, and $A \in \mathbb{R}^{n,n}$, $B \in \mathbb{R}^{n,1}$, $C \in \mathbb{R}^{1,n}$, and $f \in \mathbb{R}^{n,1}$ are given as

$$A = \begin{bmatrix} -k_1 & k_1 & & & & \\ k_1 & -k_1-k_2 & k_2 & & & \\ & k_2 & -k_2-k_3 & k_3 & & \\ & & \ddots & \ddots & \ddots & \\ & & & k_{n-2} & -k_{n-2}-k_{n-1} & k_{n-1} \\ & & & & k_{n-1} & -k_{n-1} \end{bmatrix}, \quad B = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix},$$

$$C = \begin{bmatrix} 1 & 0 & \dots & 0 \end{bmatrix}, \quad \text{and} \quad f = \begin{bmatrix} k_1 d_1 \\ -k_1 d_1 + k_2 d_2 \\ \vdots \\ -k_{n-2}d_{n-2} + k_{n-1}d_{n-1} \\ -k_{n-1}d_{n-1} \end{bmatrix} \tag{2.3}$$

for given spring constants $k_1, \dots, k_{n-1} > 0$ and spring lengths $d_1, \dots, d_{n-1} > 0$.

In the numerical examples of Section 6 we will consider system (2.2) for the 2-car example which has index 5 like typical examples from engineering such as trajectory tracking of cranes, cf. [6] for a list of examples. However, we will also consider the case of an higher index in Section 6.2.

From the theory of DAEs it is well-known that derivatives of the right-hand side of system (2.1) appear in the solution [8, Ch. 2]. Because of the assumed semi-explicit structure of the system, only derivatives of g and y are part of the solution and, in particular, of the desired input u. One can show that in the index-5 case, the input will depend on the 4-th derivative of y, while for the n-spring-mass chain of Example 2.3 it will depend on $y^{(2n)}$. Thus, the following assumptions are indeed necessary for a continuous solution u of Problem 2.1 or 2.2.

Assumption 2.4 (DAE Setting)**.** In the formulation of Problem 2.1 and Problem 2.2 we assume:

(1) Smoothness of the data: $f \in \mathcal{C}([0,T];\mathbb{R}^n)$ and $y \in \mathcal{C}^{\nu_d-1}([0,T];\mathbb{R}^m)$, where ν_d is the (differentiation) index of the system equations.
(2) Consistency of the initial values with respect to the holonomic constraints: $g(x^0) = 0$ and $G(x^0)v^0 = 0$, if applicable.
(3) Consistency of the initial values with respect to the target output: $Cx^0 = y(0)$ and $Cv^0 = \dot{y}(0)$ but also the conditions which result from the insertion of the differential equation into the servo constraint,

$$\ddot{y} = C\ddot{x} = CM^{-1}(Ax + G^\mathsf{T}(x)p + Bu + f).$$

Remark 2.5. In the n-car example from Example 2.3 the consistency conditions which directly follow from equation (2.2b) are $y(0) = x_1^0$ and $\dot{y}(0) = v_1^0$. Furthermore, we obtain by the combination of equations (2.2a) and (2.2b) the two conditions

$$m_1\ddot{y}(0) = k_1(-x_1^0 + x_2^0 + d_1), \qquad m_1 y^{(3)}(0) = k_1(-v_1^0 + v_2^0).$$

We emphasize that the numerical integration of high-index DAEs involves many difficulties, see e.g. [18, Ch. II]. Furthermore, the high index property and the resulting assumptions hypothesize that the DAE formulation (2.1) does not provide an appropriate model. Thus, we propose a remodeling process which leads to an optimal control problem.

This involves a modeling error which is adjustable by a parameter as we discuss in the following sections.

3. Formulation as Optimal Control Problem

Instead of prescribing the servo constraint (2.1c) in a rigid way, we formulate it as the target of an optimization problem. Accordingly, the solution will not follow the trajectory exactly which allows for a less regular target and which typically leads to smaller input forces.

Problem 3.1. For a $\nu \in \mathbb{N}$, find $u \in \mathcal{C}^{\nu}([0,T];\mathbb{R}^m)$ that minimizes the cost functional

$$\mathcal{J}(x,u) := \mathcal{S}(x(T)) + \int_0^T \mathcal{Q}(x) + \mathcal{R}(u)\,\mathrm{d}t \tag{3.1}$$

with the quadratic performance criteria

$$\mathcal{Q}(x) := \frac{1}{2}(Cx-y)^{\mathsf{T}}Q(Cx-y), \qquad \mathcal{R}(u) := \frac{1}{2}\sum_{i=0}^{\nu} u^{(i)\mathsf{T}}R_i u^{(i)}, \tag{3.2a}$$

$$\text{and}\quad \mathcal{S}(x(T)) := \frac{1}{2}\big(Cx(T)-y(T)\big)^{\mathsf{T}}S\big(Cx(T)-y(T)\big), \tag{3.2b}$$

for given $Q \in \mathbb{R}^{m,m}$, $S \in \mathbb{R}^{m,m}$, and $R_0, \ldots, R_\nu \in \mathbb{R}^{m,m}$ symmetric and positive semi-definite, and with $x = x(u) \in \mathcal{C}^2([0,T];\mathbb{R}^n)$ is related to u through the dynamics (2.1a), the holonomic constraint (2.1b) and the initial conditions (2.1d).

The parameters Q, S, and $R_0, \ldots, R_\nu$ can be chosen to meet certain requirements for the minimization. With this, we may install different kinds of penalizations of the derivatives of this input variable u. Note that $R_0, \ldots, R_\nu$ describe the modeling error compared to the DAE formulation in Problem 2.1, see also the discussion in Section 4.

Note that in Problem 3.1 the fulfillment of the constraint (2.1c) is balanced with the cost of the input u including its derivatives up to order ν. This relaxation also relaxes the necessary smoothness conditions on y for a continuous solution u and also the consistency condition of the initial values with respect to the target output, cf. Assumption 2.4.

Assumption 3.2 (Optimal Control Setting)**.** In the formulation of Problem 3.1 we assume:

1. Smoothness of the data: f and y are continuous on $[0,T]$.
2. Consistency of the initial values with respect to the holonomic constraints: $g(x^0) = 0$ and $G(x^0)v^0 = 0$, if applicable.

3.1. Optimality Conditions.

We derive the *formal* optimality conditions for the optimization problem Problem 3.1, cf. [22, Ch. 6] and [19] for the DAE case, i.e., in the case of holonomic constraints.

Assumption 3.3. For any input u, the state equations (2.1a)-(2.1b) with (2.1d) have a unique solution $x = x(u)$ that depends continuously differentiable on u.

For the considered setups, and in particular the linear problem from Example 2.3, this assumption is readily confirmed. To derive the formal optimality conditions, we consider the Lagrange functional

$$\mathcal{L}(u;\lambda,\mu) = \mathcal{J}(x(u),u) + \int_0^T \lambda^{\mathsf{T}}\big(\ddot{x} - Ax - G^{\mathsf{T}}(x)p - Bu - f\big) + \mu^{\mathsf{T}}g(x)\,\mathrm{d}t \tag{3.3}$$

for formally introduced multipliers $\lambda \in \mathcal{C}^2([0,T];\mathbb{R}^n)$ and $\mu \in \mathcal{C}([0,T];\mathbb{R}^r)$. The formal optimality conditions are derived from the requirement that for suitable (λ, μ) an optimal u^* marks a stationary point of $\mathcal{L}(u;\lambda,\mu)$, i.e.,

$$\frac{\partial}{\partial u}\mathcal{L}(u^*;\lambda,\mu)\delta_u = 0 \tag{3.4}$$

for every variation δ_u, cf. [26, Ch. 14]. This is the case, if (x, p, u, λ, μ) solves the following formal optimality system.

Problem 3.4. Consider the functions and coefficients defined in Problem 2.1 and 3.1. Find (x,p), $(\lambda,\mu) \in \mathcal{C}^2([0,T];\mathbb{R}^n) \times \mathcal{C}([0,T];\mathbb{R}^r)$ and $u \in \mathcal{C}([0,T];\mathbb{R}^m)$ such that

$$M\ddot{x} = Ax + G^\mathsf{T}(x)p + Bu + f, \tag{3.5a}$$

$$0 = g(x), \tag{3.5b}$$

$$M^\mathsf{T}\ddot{\lambda} = A^\mathsf{T}\lambda + \frac{\partial}{\partial x}\big(G(x)^\mathsf{T}p\big)\lambda - G^\mathsf{T}(x)\mu - C^\mathsf{T}QCx + C^\mathsf{T}Qy, \tag{3.5c}$$

$$0 = G(x)\lambda, \tag{3.5d}$$

$$0 = \sum_{i=0}^{\nu}(-1)^i R_i u^{(2i)} - B^\mathsf{T}\lambda \tag{3.5e}$$

with the initial conditions for x as in equation (2.1d) and the terminal conditions for the dual variable λ given by

$$M^\mathsf{T}\lambda(T) = 0, \quad M^\mathsf{T}\dot{\lambda}(T) = C^\mathsf{T}S(Cx(T) - y(T)). \tag{3.6}$$

For u, depending on the parameter ν, we obtain the boundary conditions

$$\sum_{i=1}^{\nu}\sum_{k=1}^{i}(-1)^k \; \delta_u^{(i-k)\mathsf{T}} \; R_i u^{(i+k-1)}\Big|_0^T = 0 \tag{3.7}$$

for all variations δ_u from a suitable subset of $\mathcal{C}([0,T];\mathbb{R}^m)$.

Remark 3.5. For the case $\nu = 0$, by virtue of (3.5e), we obtain the often used algebraic relation

$$0 = -B^\mathsf{T}\lambda + R_0 u$$

and no boundary conditions for the input u.

In general, for $\nu > 0$, the space of suitable variations δ_u depends on the incorporation of the inputs in the optimality problem. Either, one may add the derivatives of the input to the cost functional as in (3.1) without any specifications of initial conditions or the inputs $\dot{u}, \ldots, u^{(\nu-1)}$ are incorporated as part of the state vector as in [22, Rem. 3.8]. In the latter case, initial conditions have to be stated for $u(0), \ldots, u^{(\nu-1)}(0)$ which may be unphysical. Furthermore, the corresponding variations $\delta_u, \dot{\delta}_u, \ddot{\delta}_u, \ldots, \delta_u^{(\nu-1)}$ have to vanish at $t = 0$.

Remark 3.6. If we do not impose restrictions on the admissible u and, thus, on δ_u, for fixed ν and positive definite R_ν the following conditions need to hold:

$$\begin{aligned}
\nu = 1: \quad & \dot{u}(0) = \dot{u}(T) = 0, \\
\nu = 2: \quad & \ddot{u}(0) = \ddot{u}(T) = 0, \\
& R_1\dot{u}(0) - R_2 u^{(3)}(0) = R_1\dot{u}(T) - R_2 u^{(3)}(T) = 0.
\end{aligned}$$

3.2. **First-order Formulation.** In order to apply standard theory and standard numerical routines, we reformulate the optimality system as first-order system. For this, we restrict ourselves to the unconstrained case $r = 0$ with $\nu = 1$. We introduce the variables

$$z = \begin{bmatrix} x \\ \dot{x} \end{bmatrix}, \qquad \zeta := \begin{bmatrix} -\dot{\lambda} \\ \lambda \end{bmatrix}, \qquad v := \begin{bmatrix} u \\ -\dot{u} \end{bmatrix}.$$

The DAE (2.2) in first-order form is given by

$$\tilde{M}\dot{z} = \tilde{A}z + \tilde{B}u + \tilde{f}, \tag{3.8a}$$

$$\tilde{C}z = g, \tag{3.8b}$$

$$z(0) = \begin{bmatrix} x^0 \\ v^0 \end{bmatrix}, \tag{3.8c}$$

with

$$\tilde{M} := \begin{bmatrix} I_n & 0 \\ 0 & M \end{bmatrix}, \quad \tilde{A} := \begin{bmatrix} 0 & I_n \\ A & 0 \end{bmatrix}, \quad \tilde{B} := \begin{bmatrix} 0 \\ B \end{bmatrix}, \quad \tilde{C} := \begin{bmatrix} C & 0 \end{bmatrix}, \quad \tilde{f} := \begin{bmatrix} 0 \\ f \end{bmatrix}.$$

Therein, I_n denotes the identity matrix in $\mathbb{R}^n$. In order to write the resulting optimality system (3.5) as a first-order system, we further introduce the matrices

$$\hat{M}^\mathsf{T} := \begin{bmatrix} M^\mathsf{T} & 0 \\ 0 & I_n \end{bmatrix}, \quad \tilde{J} := \begin{bmatrix} 0 & I_m \\ -I_m & 0 \end{bmatrix}, \quad \tilde{I}_\beta := \begin{bmatrix} -\beta_0 I_m & 0 \\ 0 & \beta_1 I_m \end{bmatrix}, \quad \hat{B} := \begin{bmatrix} \tilde{B} & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ B & 0 \end{bmatrix}.$$

The optimality system with the Lagrange multiplier μ and control v is given via

$$\begin{bmatrix} 0 & \tilde{M} & \\ -\hat{M}^\mathsf{T} & 0 & \\ & & \beta_1 \tilde{J} \end{bmatrix} \begin{bmatrix} \dot{\zeta} \\ \dot{z} \\ \dot{v} \end{bmatrix} = \begin{bmatrix} 0 & \tilde{A} & \hat{B} \\ \tilde{A}^\mathsf{T} & -\tilde{C}^\mathsf{T}\tilde{C} & \\ \hat{B}^\mathsf{T} & & \tilde{I}_\beta \end{bmatrix} \begin{bmatrix} \zeta \\ z \\ v \end{bmatrix} + \begin{bmatrix} \tilde{f} \\ \tilde{C}^\mathsf{T} g \\ 0 \end{bmatrix} \tag{3.9}$$

with the initial and terminal conditions

$$z(0) = \begin{bmatrix} x^0 \\ v^0 \end{bmatrix}, \quad -\hat{M}^\mathsf{T}\zeta(T) = \gamma\tilde{C}^\mathsf{T}(\tilde{C}x(T) - g(T)), \quad \dot{u}(0) = 0, \quad \dot{u}(T) = 0. \tag{3.10}$$

In the case were an initial condition for the input was prescribed, i.e., $u(0) = u^0$ is given, the conditions for u in (3.10) reduce to $\dot{u}(T) = 0$. With appropriate matrices $\mathcal{B}_0$ and $\mathcal{B}_T$ and a vector $\rho \in \mathbb{R}^{4n+2m}$, these boundary conditions can also be written in the form

$$\mathcal{B}_0 \begin{bmatrix} \zeta(0) \\ z(0) \\ v(0) \end{bmatrix} + \mathcal{B}_T \begin{bmatrix} \zeta(T) \\ z(T) \\ v(T) \end{bmatrix} = \rho.$$

This formulation is used in Section 5.2.2 below.

3.3. **Necessary Conditions for the Existence of an Optimal Solution.** If the optimality system (3.5)-(3.7) has a solution, then it provides necessary optimality conditions for $(x(u), u)$. However, in the considered DAE context, i.e., when holonomic constraints are applied, it may happen that the optimization problem has a solution while the *formal* optimality system is not solvable [20]. Apart from the general case that the boundary values do not permit a solution [2], for a DAE, a solution may not exist because of insufficient smoothness of the data or because of inconsistent initial or terminal values.

Thus, it is an important task to establish the necessary conditions for solvability of the formal optimality system. By Assumption 3.2 the initial conditions for x are consistent.

The adjoint equations (3.5b) and (3.5d) have the same differential-algebraic structure, so that from (3.5d), we can read off the consistency conditions for the terminal values for λ, namely

$$G(x(T))\lambda(T) = 0 \quad \text{and} \quad \frac{\mathrm{d}}{\mathrm{d}t}\big(G(x(T))\big)\lambda(T) + G(x(T))\dot\lambda(T) = 0, \tag{3.11}$$

cf. Assumption 3.2(2). Comparing the prescribed terminal conditions (3.6) for λ to (3.11), we obtain the necessary and sufficient condition for consistency as

$$0 = G(x(T))M^{-\mathsf{T}}C^{\mathsf{T}}S(Cx(T) - y(T)). \tag{3.12}$$

Similar conditions in a slightly different formulation have been reported in [23]. There, the authors proposed the variants to remove the end point penalization from the cost functional or to consider a regularization of the dynamical equation. Within this regularization the constraint (2.1b) is replaced by its derivative.

The following theorem shows that instead of the state equations, one can modify the cost functional. This modification ensures consistency while not affecting neither the performance criterion nor the necessity of the formal optimal conditions.

Theorem 3.7 (Ensuring consistency)**.** *Let $P_{x^*(T)}$ be a projector onto the kernel of $G(x^*(T))$, that satisfies $M^{-\mathsf{T}}P^{\mathsf{T}}_{x^*(T)} = P_{x^*(T)}M^{-\mathsf{T}}$. Then, replacing the terminal conditions* (3.6) *for λ by the conditions*

$$M^{\mathsf{T}}\lambda(T) = 0, \quad M^{\mathsf{T}}\dot\lambda(T) = P_{x^*(T)}C^{\mathsf{T}}S(Cx^*(T) - y(T)), \tag{3.13}$$

ensures consistency of the terminal conditions for λ. Moreover, if $(x^*, p^*, u^*, \lambda, \mu)$ solve the optimality system with (3.13)*, then u^* is a stationary point of* (3.3)*.*

Proof. Let u^* be a solution to the optimality system and consider the first variation $\frac{\partial}{\partial u}\mathcal{L}(u^*; \lambda, \mu)$. The relation that defines the terminal condition for $\dot\lambda^{\mathsf{T}}$ is given by

$$0 = \frac{\partial}{\partial u}\big(\mathcal{S}(x^*(T))\big)\delta_u(T) - \dot\lambda^{\mathsf{T}}(T)\delta_{x(\delta_u)}(T) = \frac{\partial}{\partial x}\big(S(x^*(T))\big)\delta_{x(\delta_u)}(T) - \dot\lambda^{\mathsf{T}}(T)\delta_{x(\delta_u)}(T), \tag{3.14}$$

where $\delta_{x(\delta_u)} = \frac{\partial}{\partial u}\big(x^*(u)\big)\delta_u$ is the variation in x^* that is induced by the variation of u. Since $\delta_{x(\delta_u)}$ solves the state equations (2.1a)-(2.1b) linearized about x^* with input δ_u, cf. [25, Ch. 2], it holds that $\delta_{x(\delta_u)}(T)$ fulfills the linearized constraint (2.1b), i.e. $G(x^*(T))\delta_{x(\delta_u)}(T) = 0$ or, equivalently, $\delta_{x(\delta_u)}(T) = P_{x^*(T)}\delta_{x(\delta_u)}(T)$. Thus, relation (3.14) does not change if one replaces $\frac{\partial}{\partial x}\big(S(x^*(T))\big)$ by $\frac{\partial}{\partial x}\big(S(x^*(T))\big)P_{x^*(T)}$. For the considered quadratic cost functional (3.1), this means that the formal conditions (3.12) are equivalent (in the sense that the the first variation of $\mathcal{L}$ is not affected) to

$$\dot\lambda(T) = P_{x^*(T)}\frac{\partial}{\partial x}\big(\mathcal{S}(x^*(T))\big)^{\mathsf{T}} = P_{x^*(T)}C^{\mathsf{T}}S(Cx^*(T) - y(T))$$

which concludes the proof. □

Remark 3.8. In the general case, $P_{x^*(T)}$ is defined implicitly since it depends on the unknown solution x^*. In the case of linear holonomic constraints, $P_{x^*(T)}$ is readily computed, cf. [14, Rem. 8.20]. As in the example presented below, in order to ensure consistency of the terminal conditions one may also use a projection onto a subspace of $G(x(T))$ that is possibly independent of x. This, however, will effectively alter the performance criterion $\mathcal{S}$.

Remark 3.9. If M is symmetric, the condition $M^{-\mathsf{T}}P_{x^*(T)}^{\mathsf{T}} = P_{x^*(T)}M^{-\mathsf{T}}$ is nothing but the orthogonality condition in the inner product induced by M^{-1} which is the natural inner product in PDE applications.

3.4. **Existence of Optimal Solutions.** For Problem 3.1 constrained by linear equations without holonomic constraints as in (2.2a), existence of solutions is provided by well-known results.

Lemma 3.10 (Existence of an optimal solution)**.** *For $\nu \geq 0$ consider the optimal control problem with cost functional* (3.1)*, constrained by* (2.2a) *and let Assumption 3.2 hold. If $R_\nu > 0$ and if $u(0)$, $\dot{u}(0)$, …, $u^{(\nu-1)}(0)$ are given, then system* (3.5) *and the optimal control problem have a unique solution for any $T < \infty$ and initial data x^0 and v^0.*

Proof. Recall that, by the standard order reduction approach, the second-order system (3.5) can be reformulated as an equivalent first-order system, cf. Section 3.2.

Then, for $\nu = 0$ the result is given in [22, Rem. 3.6]. For $\nu = 1$ with $R_1 > 0$, we may introduce a new variable for the derivative of the control u. Interpreting u as a part of the state variable whereas its derivative $v := \dot{u}$ is the new control variable, the same arguments apply, cf. [22, Rem. 3.8]. Note that this ansatz requires an initial value for u. This procedure may be successively repeated for $\nu > 1$. □

Remark 3.11. Note that the existence result in Lemma 3.10 is true for all initial values x^0 and v^0 in contrast to the DAE (2.1), which requires consistent initial data. In the case $\nu = 0$ with $R_0 = 0$, we again need consistent boundary conditions, since this yields again the DAE formulation of the problem. We discuss this case below in Section 4.

For the nonlinear optimality system (3.5) with holonomic constraints, we use the strong but reasonable assumption that the state equations (2.1) have a solution for any input u under consideration and that the solutions of the state equations depend smoothly on the input (Assumption 3.3) to state that existence of a solution to the formal optimality system is indeed a necessary condition.

We first show that the adjoint equations have a solution for every state trajectory and, thus, also at the optimal solution. Then we confer that the smoothness of the input to state map implies that, at an optimal solution, the gradient condition (3.5e) must also be fulfilled.

Lemma 3.12. *Consider a solution (x, p) of* (2.1)*. If g is sufficiently smooth and $G(x(t))$ has full row rank for all $t \in [0, T]$ and if the end condition*

$$M^{\mathsf{T}}\lambda(T) = 0, \quad M^{\mathsf{T}}\dot{\lambda}(T) = C^{\mathsf{T}}S(Cx(T) - y(T)), \tag{3.15}$$

is consistent, then the adjoint equation (3.5c)-(3.5d) *with end condition* (3.15) *has a unique solution.*

Proof. We rewrite the adjoint equations as a first-order system, cf. the second equation of (3.9),

$$\begin{bmatrix} M^{\mathsf{T}} & 0 \\ 0 & M^{\mathsf{T}} \end{bmatrix} \frac{\mathrm{d}}{\mathrm{d}t} \begin{bmatrix} \lambda \\ \dot{\lambda} \end{bmatrix} = \begin{bmatrix} 0 & M^{\mathsf{T}} \\ \tilde{A}^{\mathsf{T}} & 0 \end{bmatrix} \begin{bmatrix} \lambda \\ \dot{\lambda} \end{bmatrix} + \begin{bmatrix} 0 \\ G^{\mathsf{T}} \end{bmatrix} \mu + \begin{bmatrix} 0 \\ \tilde{f} \end{bmatrix}, \tag{3.16a}$$

$$G\lambda = 0, \tag{3.16b}$$

where μ is the multiplier that accounted for the holonomic constraint in (3.3), where we have omitted the dependencies on x and t, and where we have clustered all linear coefficients and inhomogeneities in $\tilde{A}$ and $\tilde{f}$. Then, via another multiplier η, we add the differentiated constraint $\dot{G}\lambda + G\dot{\lambda} = 0$ to the system and consider

$$\begin{bmatrix} M^\mathsf{T} & 0 \\ 0 & M^\mathsf{T} \end{bmatrix} \frac{\mathrm{d}}{\mathrm{d}t} \begin{bmatrix} \lambda \\ \dot{\lambda} \end{bmatrix} = \begin{bmatrix} 0 & M^\mathsf{T} \\ \tilde{A}^\mathsf{T} & 0 \end{bmatrix} \begin{bmatrix} \lambda \\ \dot{\lambda} \end{bmatrix} + \begin{bmatrix} G^\mathsf{T} & \dot{G}^\mathsf{T} \\ 0 & G^\mathsf{T} \end{bmatrix} \begin{bmatrix} \eta \\ \mu \end{bmatrix} + \begin{bmatrix} 0 \\ \tilde{f} \end{bmatrix}, \tag{3.17a}$$

$$\begin{bmatrix} G & 0 \\ \dot{G} & G \end{bmatrix} \begin{bmatrix} \lambda \\ \dot{\lambda} \end{bmatrix} = 0. \tag{3.17b}$$

Since G has pointwise full row rank and since the terminal conditions are assumed to be consistent, we can call on [14, Thm. 8.6] to state that System (3.17) has a unique solution. One can show that the parts (λ, μ) of a solution (λ, η, μ) to (3.17) also solve (3.16). The other way round, by construction and by the smoothness assumption on G, a solution (λ, μ) to (3.16) partially defines a solution to (3.17) and, thus, is unique. □

Theorem 3.13. *Assume that $u \mapsto x$ is Lipschitz continuous. If for a given $(x(u_0), u_0)$, the constraints and the cost functional are Gâteaux differentiable with respect to x at $x(u_0)$ and if the terminal conditions* (3.6) *are consistent, then the optimality system* (3.5) *is a necessary condition for optimality of $(x(u_0), u_0)$.*

Proof. By Lemma 3.12, at every candidate solution $x(u_0)$, the adjoint equation (3.5c) and (3.5d) with (3.6) is solvable. Then, the claim follows from the result given in [14, Thm. 5.5]. □

Concerning sufficiency for the existence of unique global or local solutions, general results for constrained optimization extended to optimal control problems can be consulted, see, e.g., [14, Ch. 5.3].

3.5. **Various Optimality Systems.** In the remaining part of this section, we consider special cases of the optimality system (3.5) for constrained and non-constrained systems and different values of ν. For this, we consider again the cost functional (3.1) and set

$$Q = I_m, \qquad R_i = \beta_i I_m, \qquad S = \gamma I_m.$$

Thus, the remaining parameters for the optimization problem are $\gamma, \beta_0, \dots, \beta_\nu \geq 0$. For different values of ν this then leads to different structures of the optimality system which we further analyse. In this subsection, we always assume $\beta_\nu > 0$. The special case $\nu = 0$ with $\beta_0 = 0$, i.e., with no constraints on the input at all, is then discussed in Section 4.

3.5.1. *Case $r = 0$, $\nu = 0$.* We consider the unconstrained case with $r = 0$, i.e., the optimization is constrained by an ODE instead of an DAE. As mentioned above, we assume here $\beta_0 > 0$. This then leads to the optimality system

$$\begin{bmatrix} 0 & M & \\ M^\mathsf{T} & 0 & \\ & & 0 \end{bmatrix} \begin{bmatrix} \ddot{\lambda} \\ \ddot{x} \\ \ddot{u} \end{bmatrix} = \begin{bmatrix} 0 & A & B \\ A^\mathsf{T} & -C^\mathsf{T}C & \\ -B^\mathsf{T} & & \beta_0 I_m \end{bmatrix} \begin{bmatrix} \lambda \\ x \\ u \end{bmatrix} + \begin{bmatrix} f \\ C^\mathsf{T} y \\ 0 \end{bmatrix}.$$

Thus, we obtain an DAE of index 1 but with initial and terminal conditions of the form

$$x(0) = x^0, \quad \dot{x}(0) = v^0, \quad \lambda(T) = 0, \quad M^\mathsf{T}\dot{\lambda}(T) = \gamma C^\mathsf{T}(Cx(T) - y(T)).$$

3.5.2. *Case $r = 0$, $\nu = 1$.* Again we consider the unconstrained case, i.e., $r = 0$. However, we include the penalization of the first derivative of the input u with parameter $\beta_1 \neq 0$. This then leads to the system

$$\begin{bmatrix} 0 & M & \\ M^\top & 0 & \\ & & \beta_1 I_m \end{bmatrix} \begin{bmatrix} \ddot{\lambda} \\ \ddot{x} \\ \ddot{u} \end{bmatrix} = \begin{bmatrix} 0 & A & B \\ A^\top & -C^\top C & \\ -B^\top & & \beta_0 I_m \end{bmatrix} \begin{bmatrix} \lambda \\ x \\ u \end{bmatrix} + \begin{bmatrix} f \\ C^\top y \\ 0 \end{bmatrix}. \tag{3.18}$$

In contrast to the case with $\nu = 0$, the leading matrix on the left-hand side is invertible. Thus, the optimality system (3.18) is an ODE. The corresponding boundary conditions are given by

$$\begin{gathered} x(0) = x^0, \quad \dot{x}(0) = v^0, \quad \dot{u}(0) = 0, \quad \dot{u}(T) = 0, \\ \lambda(T) = 0, \quad M^\top \dot{\lambda}(T) = \gamma C^\top (Cx(T) - y(T)). \end{gathered}$$

3.5.3. *Case $r = 0$, $\nu = 2$.* In the case $\nu = 2$ also the second derivative of the inputs are penalized, i.e., $\beta_2 \neq 0$. As seen in equation (3.5e), the fourth derivative of u appears in the optimality system. In order to write the system in a second-order form, we introduce a new variable $v := \ddot{u}$. The optimality system then has the form

$$\begin{bmatrix} 0 & M & & \\ M^\top & 0 & & \\ & & 0 & \beta_2 I_m \\ & & I_m & 0 \end{bmatrix} \begin{bmatrix} \ddot{\lambda} \\ \ddot{x} \\ \ddot{u} \\ \ddot{v} \end{bmatrix} = \begin{bmatrix} 0 & A & B & \\ A^\top & -C^\top C & & \\ B^\top & & -\beta_0 I_m & \beta_1 I_m \\ & & 0 & I_m \end{bmatrix} \begin{bmatrix} \lambda \\ x \\ u \\ v \end{bmatrix} + \begin{bmatrix} f \\ C^\top y \\ 0 \\ 0 \end{bmatrix}. \tag{3.19}$$

Thus, we have again an ODE and the corresponding boundary values read:

$$\begin{gathered} x(0) = x^0, \quad \dot{x}(0) = v^0, \quad \ddot{u}(0) = 0, \quad \ddot{u}(T) = 0, \\ \beta_1 \dot{u}(0) = \beta_2 \dot{v}(0), \quad \beta_1 \dot{u}(T) = \beta_2 \dot{v}(T), \\ \lambda(T) = 0, \quad M^\top \dot{\lambda}(T) = \gamma C^\top (Cx(T) - y(T)). \end{gathered}$$

3.5.4. *Case $r > 0$, $\nu = 0$.* Finally, we give an example of the optimality system if the cost functional ist constrained by an DAE. Here, we do not penalize derivatives of the inputs, i.e., $\nu = 0$ and $\beta_0 \neq 0$. Assuming that the Jacobian G is constant, i.e., equation (3.5b) is of the form $0 = g(x) = Gx$, we obtain the optimality system

$$\begin{bmatrix} 0 & M & & & \\ M^\top & 0 & & & \\ & & 0 & & \\ & & & 0 & \\ & & & & 0 \end{bmatrix} \begin{bmatrix} \ddot{\lambda} \\ \ddot{x} \\ \ddot{p} \\ -\ddot{\mu} \\ -\ddot{u} \end{bmatrix} = \begin{bmatrix} 0 & A & G^\top & 0 & -B \\ A^\top & -C^\top C & 0 & G^\top & 0 \\ G & 0 & 0 & & \\ 0 & G & & 0 & \\ -B^\top & 0 & & & -\beta_0 I_m \end{bmatrix} \begin{bmatrix} \lambda \\ x \\ p \\ -\mu \\ -u \end{bmatrix} + \begin{bmatrix} f \\ C^\top y \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

In contrast to the previous cases, we obtain here a DAE of index 3, but again with a mixture of initial and terminal conditions. This can be shown by a look at the special structure which is the same as for constrained multibody systems, cf. [13, Ch. VII.1]. Note that this is no surprise, since we removed only the 'index-5 constraint' by the cost functional.

4. Comparison of DAE and Optimal Control Solutions

To discuss the qualitative behavior of the solutions of the optimal control problem, we consider the linear case without holonomic constraints and, in particular, discuss the n-element mass-spring chains as in Example 2.3 with the matrices $A \in \mathbb{R}^{n,n}$, $B \in \mathbb{R}^n$, $C \in \mathbb{R}^{1,n}$, and the right-hand side $f \in \mathbb{R}^n$ as in (2.3).

In the optimal control setting of Section 3 it is reasonable to assume that R_ν is positive definite. In the sequel, we analyse the limit case with $\nu = 0$ and $R_0 = 0$, i.e., the case in which the control is not constrained at all.

4.1. **Equivalence for $R_0 = 0$.** We show that for Example 2.3 with $\nu = 0$ and $R_0 = 0$ the DAE approach of Problem 2.2 is equivalent to the optimal control formulation in Problem 3.1, provided $Q > 0$. Note that this implies that the corresponding optimality system is only solvable for $y \in \mathcal{C}^{2n}([0,T];\mathbb{R})$. Recall that n denote the number of coupled cars.

It is easy to see that a solution (x, u) of the original DAE (2.2) minimizes the cost functional for $R_0 = 0$. As solution of the DAE, we have $Cx = y$ such that the cost functional $\mathcal{J}$ from (3.1) is minimized since

$$\mathcal{J}(x,u) = \mathcal{S}(x(T)) + \frac{1}{2}\int_0^T (Cx-y)^\mathsf{T} Q (Cx-y)\,\mathrm{d}t = 0.$$

Let us consider the optimality system for the case $R_0 = 0$. Equation (3.5e) reduces to $0 = B^\mathsf{T}\lambda$ which directly implies that the last component of λ vanishes, i.e., $\lambda_n = 0$. As a result, equation (3.5c) has the form

$$\begin{bmatrix} \ddot\lambda_1 \\ \ddot\lambda_2 \\ \vdots \\ \ddot\lambda_{n-1} \\ 0 \end{bmatrix} = \begin{bmatrix} -k_1 & k_1 & & & \\ k_1 & -k_1-k_2 & k_2 & & \\ & \ddots & \ddots & \ddots & \\ & & k_{n-2} & -k_{n-2}-k_{n-1} & k_{n-1} \\ & & & k_{n-1} & -k_{n-1} \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \vdots \\ \lambda_{n-1} \\ 0 \end{bmatrix} - \begin{bmatrix} Q(x_1-y) \\ 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix}.$$

In agreement with the boundary conditions of λ, we obtain successively $\lambda_{n-1} = \cdots = \lambda_1 = 0$. If Q is invertible, this implies that $x_1 = Cx = y$ which then resembles Problem 2.2. In this case, also condition (3.6) is satisfied and thus, the Problems 2.2 and 3.1 are equivalent. If Q is not invertible then the system is not uniquely solvable.

Remark 4.1. The preceding observation is an instance of the general fact that if the linear system without holonomic constraints is controllable and observable and if Q is invertible, then, provided the data is sufficiently smooth, a solution to the optimal control problem Problem 3.1 resembles the solution of the DAE of Problem 2.1. To see this, recall that in the considered situation, the system is observable, if, and only if, $Cx - g = 0$ implies $x_1 = g$, and, by duality, that the system is controllable, if and only if, $B^\mathsf{T}\lambda = 0$ implies that $\lambda = 0$ for all time.

Remark 4.2. The equivalence of the DAE and optimal control approach for $R_0 = 0$ can also be shown for the trolley crane from the example in Section 6.3 below which includes a holonomic constraint. In this case, one can show in a similar manner that the dual variables λ and μ vanish such that the servo constraint $Cx = y$ has to be satisfied.

4.2. **Convergence Barriers.** By Lemma 3.10, if $y \in \mathcal{C}([0,T],\mathbb{R})$ and $R_0 > 0$, then the quadratic Problem 3.1 with $\nu = 0$, subject to linear constraints, has a unique solution. By the results of the previous Section 4.1, for $R_0 = 0$, a solution only exists, if y sufficiently smooth.

In this subsection, we examine how the optimal control u behaves when $R_0 \to 0$ in dependence of the smoothness of y. Consider the n-car example Example 2.3 and the associated adjoint equations

$$M^{\mathsf{T}}\ddot{\lambda} = A^{\mathsf{T}}\lambda - C^{\mathsf{T}}(Cx - y) \tag{4.1}$$

with A and C from (2.3). With

$$\Delta_j := k_j\Big(\frac{\lambda_j}{m_j} - \frac{\lambda_{j-1}}{m_{j-1}}\Big), \quad j = 2, 3, \ldots, n, \tag{4.2}$$

we can rewrite Equation (4.1) as

$$\ddot{\lambda}_1 = -\Delta_2 - (x_1 - y), \tag{4.3a}$$

$$\ddot{\lambda}_2 = \Delta_2 - \Delta_3, \tag{4.3b}$$

$$\vdots$$

$$\ddot{\lambda}_{n-1} = \Delta_n - \Delta_{n-1}, \tag{4.3c}$$

$$\ddot{\lambda}_n = \Delta_n. \tag{4.3d}$$

The gradient condition (3.5e) gives $\lambda_n = R_0 u$ and $\Delta_n = \ddot{\lambda}_n = R_0\ddot{u}$. By a combination of (4.2) and (4.3), we recursively compute λ_{n-1}, λ_{n-2}, $\cdots$, λ_1 via the formulas

$$\lambda_{j-1} = -\frac{1}{k_{j-1}}\Delta_j + \frac{m_{j-1}}{m_j}\lambda_j \quad \text{and} \quad \Delta_{j-1} = \Delta_j - \ddot{\lambda}_{j-1}.$$

Finally, via (4.3a), we can directly relate the difference in the target $x_1 - y$ to the computed input u. Assuming uniform masses m and uniform spring constants k for $n = 2$ we find

$$x_1 - y = R_0\Big(2\ddot{u} - \frac{1}{k}u^{(4)}\Big) \tag{4.4}$$

while for $n = 3$ it must hold that

$$x_1 - y = R_0\Big((\frac{1}{k} + 1)u^{(4)} - \frac{1}{k}(\frac{1}{k} + 1)u^{(6)}\Big). \tag{4.5}$$

We observe that

- For nonsmooth y, where we cannot expect convergence of x_1 to y, the control u will have strong peaks in its derivatives in order to fulfill (4.4) or (4.5) for $R_0 \to 0$.
- For moderate values of R_0, the tracking error $x_1 - y$ is affected by the oscillations in the derivatives of u multiplied by multiples of $\frac{1}{k}$ depending on the length of the considered chain.
- For $k \to \infty$, i.e., when the connections between the cars become more rigid, the higher derivatives of u are damped out from the tracking error. In fact, if one connection is rigid, the two connected cars can be considered as one and the index of the system reduces.

5. Solution Strategies

Within this section, we review several concepts how to solve numerically mechanical problems with servo constraints. First, we comment on the classical approach where the model is given by the DAE (2.1). In this case, index reduction methods are applied which then allow to integrate the resulting equations. Second, using the optimal control ansatz (3.1), we consider the two cases of either solving directly the optimality system, which is a boundary value problem (BVP), or the resulting Riccati equations. The latter approach may then be used to define a feedback control.

5.1. **Solving High-index DAEs.** As mentioned already in the introduction, the computation of the inverse dynamics of a discrete mechanical system given by a specification of a trajectory is a highly challenging problem [4, 5]. The reason is the high-index structure of the resulting DAEs. In the here considered case of underactuated mechanical systems, the systems are often of (differentiation) index 5 but may be arbitrarily high as shown in Example 2.3.

In order to realize the so-called *feedforward control* of the system, one has to solve this high-index DAE. Here, it is advisable to apply index reduction methods instead of solving the equations directly [8, Ch. 5.4]. A well-known approach based on a projection of the dynamics was introduced in [5], see also [7]. For this, one has to compute time-dependent projection matrices in order to split the dynamics of the underactuated system into constrained and unconstrained parts.

Instead of the projection approach one may also use the index reduction technique called *minimal extension* [17]. This technique profits from the given semi-explicit structure of the dynamical system and can be easily applied. The application to a wide range of crane models can be found in the recent paper [1]. Therein, it is shown that the method of minimal extension may even be applied a second time which then leads to a DAE of index 1 for which the numerical integration works essentially as for stiff ODEs [13, Ch. VI.1].

We remark that index reduction techniques are inevitable for numerical simulations of high-index problems. However, for applications like the n-car example given in the introduction, which is of index $2n+1$, the DAE approach does not seem to be applicable. The here presented modeling as an optimal control problem still works properly for the general case. For a numerical example including a 3-car model, we refer to Section 6.

5.2. **Direct Solution of the Optimality BVP.** In this subsection, we discuss the application of the finite difference method as well as a shooting approach in order to solve the optimality system (3.5).

5.2.1. *Finite Differences.* The optimality system includes both initial and terminal conditions, so that the application of standard time-stepping methods is not possible. A straight-forward approach is to introduce a grid of the time domain and to apply the method of finite differences to the differential coupled equations leads to a (large but block-sparse) algebraic system. Alternatively, one can apply finite elements or more general collocation methods.

5.2.2. *Shooting Method.* For the application of the shooting method, we consider the first-order system (3.9), i.e., we consider again the case with $r = 0$ (no additional holonomic constraint) and $\nu = 1$.

For notational reasons, we write system (3.9) short as $\mathcal{M}\dot{y} = \mathcal{K}y + h$, i.e., the vector y includes all state, input, and dual variables. Recall that the boundary conditions can be written in the form $\mathcal{B}_0 y(0) + \mathcal{B}_T y(T) = \rho$. Because of the special structure of the given boundary conditions (initial and terminal conditions are not mixed), we may assume a reordering of the variables in order to get a system of the form

$$\mathcal{M}\dot{y} = \mathcal{K}y + h, \qquad \begin{bmatrix} \mathcal{B}_{01} \\ 0 \end{bmatrix} y(0) + \begin{bmatrix} 0 \\ \mathcal{B}_{T2} \end{bmatrix} y(T) = \begin{bmatrix} \rho_1 \\ \rho_2 \end{bmatrix}.$$

The aim of the shooting method is to restore the initial conditions for the entire vector y such that methods for initial value problems are applicable again. Since the initial values of the state variables and $\dot{u}$ (respectively u, if initial data for the input was prescribed) are already given, we can apply the so-called *reduced superposition* [2, Ch. 4.2.4]. This reduces the computational effort of the method. Within the following algorithm, we denote by s the size of the original system and thus, $2s$ the size of the first-order system we want to solve.

Step 1: Search for the fundamental solution of the corresponding homogenous system. However, using the reduced superposition, it is sufficient to compute $Y \in \mathbb{R}^{2s,s}$ solving

$$\mathcal{M}\dot{Y} = \mathcal{K}Y, \qquad Y(0) = \begin{bmatrix} I & & 0 & & & \\ & I & & 0 & & \\ & & & & I & 0 \end{bmatrix}^\top.$$

Step 2: Find a solution $w \in \mathbb{R}^{2s}$ of the initial value problem

$$\mathcal{M}\dot{w} = \mathcal{K}w + h, \qquad w(0) = \begin{bmatrix} 0 & 0 & x^0 & v^0 & 0 & 0 \end{bmatrix}^\top.$$

Step 3: Find coefficients $c \in \mathbb{R}^s$, given by the linear system

$$\mathcal{B}_{T2} Y(T) c = \rho_2 - \mathcal{B}_{T2} w(T),$$

which then gives the solution of the BVP as $y = Yc + w$. Thus, an approximation of y can be either given directly, if the matrices Y and w were stored on the entire time grid, or by solving the IVP

$$\mathcal{M}\dot{y} = \mathcal{K}y + h \qquad \text{with} \quad y(0) = Y(0)c + w(0).$$

Remark 5.1 (comparison of computational effort)**.** Assume that we always use the same time step size with N grid points. Then, the finite difference method leads to a system of size $2sN$ such that the computational effort is quadratic in N. For the shooting method we have to solve several initial value problems (each using N time steps). Note that the size of the systems is bounded by the size of the original BVP such that the overall costs are only linear in N (but with a large constant depending on s^2).

Remark 5.2. An extension of the (single) shooting method which is more stable is called the *multiple shooting method* [2, Ch. 4.4.3]. For this, the time interval $[0, T]$ is partitioned by shooting points $0 = t_1 < t_2 < \cdots < t_{N+1} = T$. On each subinterval $[t_i, t_{i+1}]$ we may compute a solution $y_i(t) = Y_i(t)c_i + w_i(t)$ similarly as above. The coefficient vectors $c_i \in \mathbb{R}^s$ are given by a linear system which contains the boundary as well as the continuity conditions in-between the time steps.

Remark 5.3. For the other cases, i.e., for $r > 0$ (with holonomic constraints) or different values of ν, we may need to use different techniques, depending in the structure of the BVP. In the case $r = 0$, $\nu = 0$, cf. Section 3.5.1, where we obtain as optimality system an index-1 DAE, we have to consider shooting methods for such systems. For this, we refer to [21]. In the case $r > 0$, for which we obtain index-3 systems, we refer to [9] or, after an index reduction to index 2, also to [12].

5.3. **Riccati Approach.** In the linear case and if $\nu = 0$, i.e., if no derivatives of u appear in the optimality system (3.5), the BVP can be solved via a Riccati decoupling. This requires the formulation as a first-order system as in (3.9) which already is in the standard form considered, e.g., in [22, Ch. 5]. In the case of holonomic constraints, one can call on the results on constrained Riccati equations given in [14] that readily apply to constrained multibody equations in the *Gear-Gupta-Leimkuhler* formulation [11].

6. Numerical Examples

In this section, we provide several numerical experiments. First, we consider the two-car system from Example 1.1, i.e., an example without holonomic constraints. Second, we add a third car which then gives a index-7 DAE in the original formulation. Finally, we consider an overhead crane as an example with $r > 0$, i.e., with a holonomic constraint. The code is written in *Python* and can be obtained from the author's public *Github* repository [15].

6.1. **Two-car Example.** We consider the two-car example from the introduction, see Figure 1.1. Recall that the equations of motion (1.1) form a DAE of index 5. As in [6, Ex. 3] the following parameters were used within the computations:

$$m_1 = 2kg, \qquad m_2 = 1kg, \qquad k = 1\tfrac{N}{m}, \qquad d = 0.5m.$$

6.1.1. *Comparison of DAE and Optimal Control Solution.* The initial values within the computations are given by

$$x_1^0 = 0.5m,\ v_1^0 = 0\tfrac{m}{s}, \qquad x_2^0 = 0m,\ v_2^0 = 0\tfrac{m}{s}.$$

For the definition of a rest-to-rest maneuver we introduce the polynomial

$$p(s) = 1716s^7 - 9009s^8 + 20020s^9 - 24024s^{10} + 16380s^{11} - 6006s^{12} + 924s^{13}.$$

With this and $y_0 = 0.5m$, $y_{\mathrm{f}} = 2.5m$, we define on the time interval $[0, 4s]$ the target trajectory

$$y(t) = \begin{cases} y_0, & \text{if } 0 \le t < 1, \\ y_0 + p\big(\tfrac{t-1}{2}\big)(y_{\mathrm{f}} - y_0), & \text{if } 1 \le t \le 3, \\ y_{\mathrm{f}}, & \text{if } 3 < t \le 4. \end{cases} \tag{6.1}$$

Note that y is smooth enough, such that the DAE solution (to which we refer to as exact solution) exists. Recall that this requires consistent initial positions and initial velocities of the cars as mentioned in Remark 2.5, namely

$$y(0) = x_1^0, \quad \dot{y}(0) = v_1^0, \quad m_1\ddot{y}(0) = -(x_1^0 - x_2^0 - d), \quad m_1 y^{(3)}(0) = -(v_1^0 - v_2^0).$$

We compare the exact solutions, that are readily computable from the systems equation, to the trajectories and input forces obtained from solving the associated optimal control problem Problem 3.1 with the parameters $Q = S = 1$ and for varying $R_0 = \beta \in \mathbb{R}$. The occurring linear boundary value problem is solved by finite differences on a regular grid of size $\tau = 0.01s$.

As expected, depending on the penalization parameter β, the optimal control approach leads to input forces that are smaller than the exact force F, see Figure 6.1(left). The reduction of the amplitude is best seen for large values of β. The optimal control problem is a compromise of costs and accuracy, as can be seen from the deviations from the target trajectory that decrease for smaller values of the penalization parameter β, cf. Figure 6.1(right).

6.1.2. *Feedback Representations of the Optimization Solutions.* Another advantage of the optimization approach is that the optimal control can be realized as a feedback. In fact, the first-order optimality conditions (3.5) suggest that u depends linearly on λ which depends, possibly nonlinearly, on the state x. For the considered linear case of Example 1.1, the optimality system can be solved via a differential Riccati equation [22, Ch. 5.1], which directly leads to a feedback representation of the optimal control.

We stay with the example of the 2-car setup to illustrate the benefits of the feedback representation. If one simply applies the known exact control solution to the considered

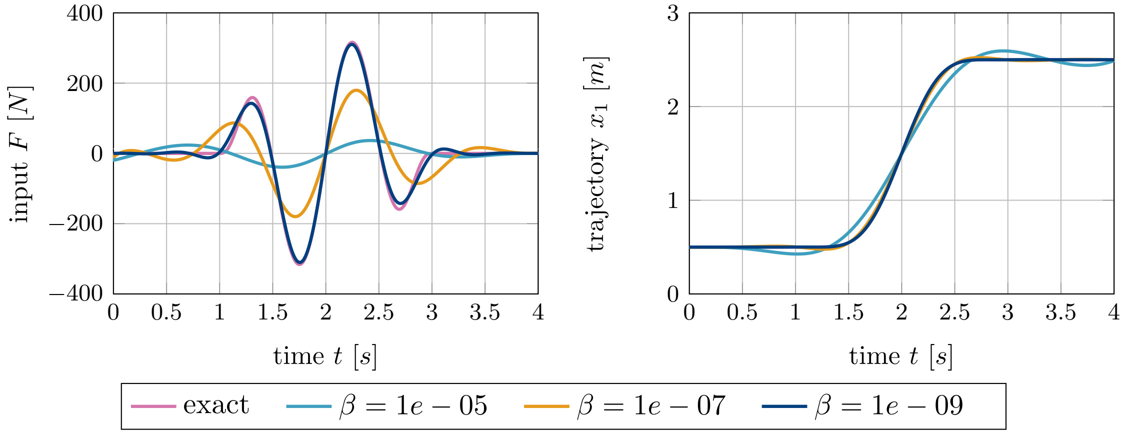

FIGURE 6.1. The exact input force F (DAE solution) and the forces obtained through the optimal control formulation for different values of the penalization parameter β (left) and the corresponding trajectories (right) for the 2-car example.

system, a perturbation, e.g. in the initial position or initial velocity, will necessarily lead to a drift off the desired trajectory, cf. Figure 6.2(left). In contrast, the feedback solution of the optimal control problem with $\beta_0 = 10^{-9}$ will detect and damp possible perturbations, cf. Figure 6.2(right).

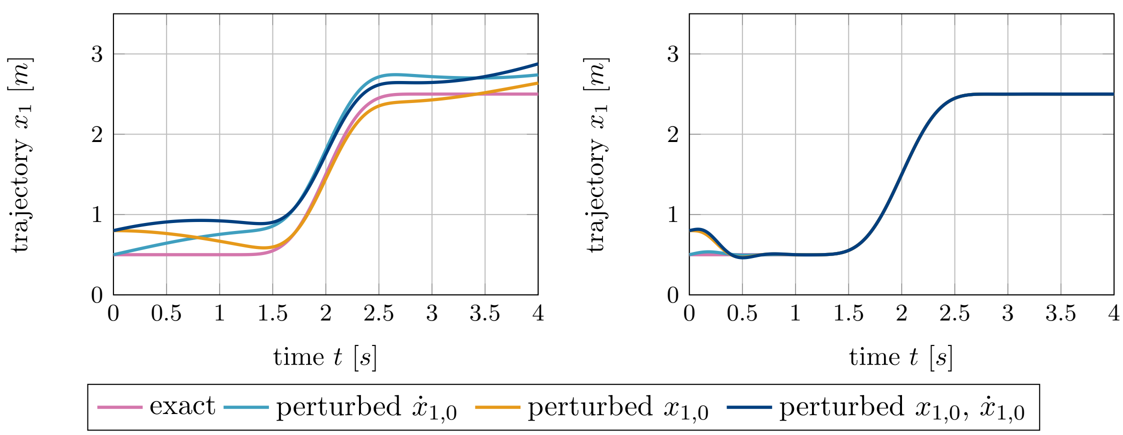

FIGURE 6.2. Benefits of the feedback representation: The output obtained from applying the exact control solution directly (left) and the output obtained via a feedback representation of the control solution of the optimal control problem (right) in the case of perturbed initial values.

6.2. **Three-car Example.** In this subsection, we add an additional car, i.e., we consider Example 2.3 with $n = 3$. This means that the positions of the bodies are given by x_1, x_2, and x_3 where the trajectory of x_1 is prescribed by y. Recall that this gives a DAE of index 7 rather than index 5 as in the previous example. As parameters we set

$$m_1 = m_2 = 1kg, \qquad m_3 = 2kg, \qquad k = 1\frac{N}{m}, \qquad d = 0.5m.$$

As initial conditions we have

$$x_1^0 = 0.5m,\ v_1^0 = 0\frac{m}{s}, \qquad x_2^0 = 0m,\ v_2^0 = 0\frac{m}{s}, \qquad x_3^0 = -0.5m,\ v_3^0 = 0\frac{m}{s}.$$

For the simulation we consider the same rest-to-rest maneuver as in (6.1). As required, the prescribed trajectory is 6-times continuously differentiable and the initial conditions satisfy all consistency conditions, cf. Assumption 2.4 and Remark 2.5.

The exact solution as well as the results from the optimal control problem for different values of the penalization parameter are shown in Figure 6.3. The weak coupling from the input on the third car to the output measured on the first car is apparent in the large peaks in the exact input force. The optimization approach leads to significantly reduced amplitudes in the input at the expense of a certain deviation from the prescribed target trajectory.

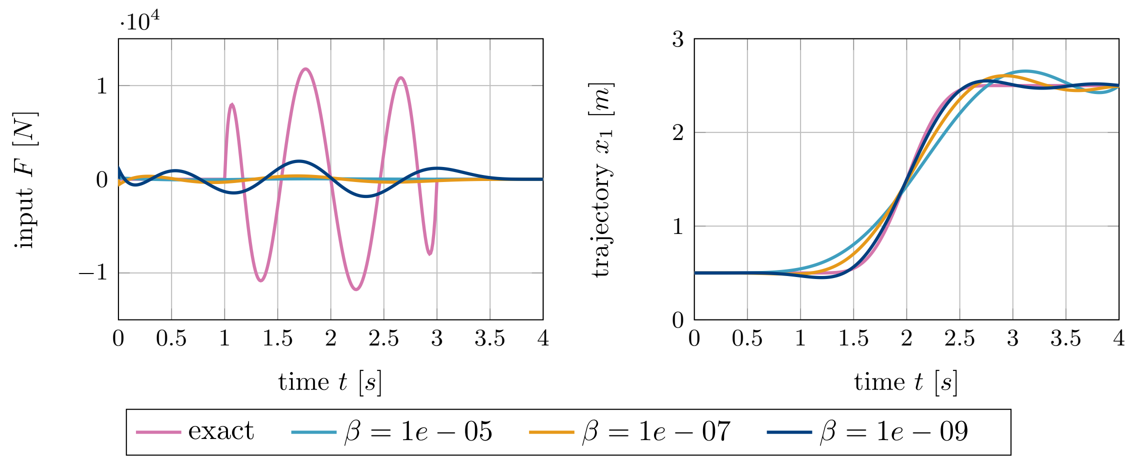

FIGURE 6.3. The exact input force F (DAE solution) and the forces obtained through the optimal control formulation for different values of the penalization parameter β (left) and the corresponding trajectories (right) for the 3-car example.

6.3. **Overhead Crane.** The servo constraint problem of this section was originally formulated in terms of minimal coordinates in [6] and was recast in redundant coordinates in [3], see Figure 6.4. We follow here the latter approach which then fits into the framework of Section 2. For this, we consider the state and input variables

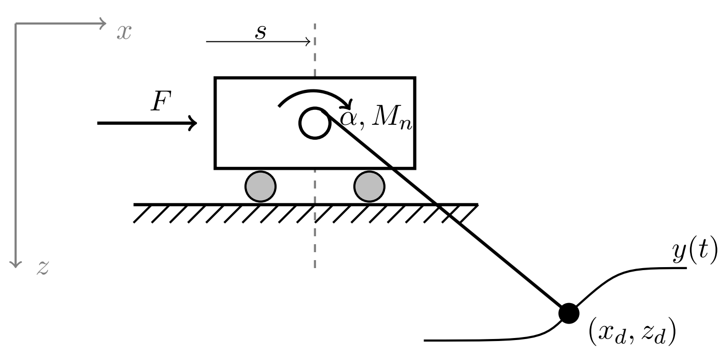

FIGURE 6.4. Overhead trolley crane with the notation of the rotationless formulation introduced in [3].

$$x = [s,\ \alpha,\ x_d,\ z_d]^{\mathsf{T}}, \quad u = [F,\ M_n]^{\mathsf{T}}.$$

With these redundant coordinates (one additional variable as well as one additional equation) we need to add one holonomic constraint and a corresponding Lagrange multiplier $p \in \mathbb{R}$. The overall system reads

$$\begin{bmatrix} m_t & & & \\ & J & & \\ & & m & \\ & & & m \end{bmatrix} \begin{bmatrix} \ddot{s} \\ \ddot{\alpha} \\ \ddot{x}_d \\ \ddot{z}_d \end{bmatrix} - G^\mathsf{T}(x)p - \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} u = \begin{bmatrix} 0 \\ -rmg \\ 0 \\ mg \end{bmatrix}, \tag{6.2a}$$

$$(x_d - s)^2 + z_d^2 - (r\alpha)^2 = 0, \tag{6.2b}$$

$$\begin{bmatrix} x_d \\ z_d \end{bmatrix} - y = 0 \tag{6.2c}$$

with

$$G(x) = 2 \begin{bmatrix} s - x_d & -r^2\alpha & x_d - s & z_d \end{bmatrix}, \quad \left(G(x)^\mathsf{T} p\right)_x = 2p \begin{bmatrix} 1 & 0 & -1 & 0 \\ 0 & -r^2 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

In the optimal control approach, with a cost functional as in Problem 3.1, the solution is obtained through the solution of the additional adjoint equations (3.5c) and (3.5d), the gradient condition (3.5e), and the boundary conditions (3.6) and (3.7).

We consider the system parameters

$$m_t = 10kg, \qquad J = 0.1Nm, \qquad m = 1kg, \qquad r = 0.1m, \qquad g = 9.81\tfrac{m}{s^2},$$

with initial values

$$x_0 = [0m,\ 40m,\ 0m,\ 4m]^\mathsf{T} \qquad \text{and} \qquad \dot{x}_0 = [0,\ 0,\ 0,\ 0]^\mathsf{T}.$$

Furthermore, we consider a target trajectory as defined in (6.1) but on the time interval $[0, 6s]$ and with the vector valued starting and terminal points

$$y_0 = [0,\ 4]^\mathsf{T} \qquad \text{and} \qquad y_f = [1,\ 5]^\mathsf{T}.$$

We linearize the resulting nonlinear boundary value problems with holonomic constraints around the constant solution that is obtained with $u \equiv [0,\ 0]^\mathsf{T}$ and solve it via finite differences. The computed approximation to the optimal control is then evaluated in the actual nonlinear model (6.2a,b) and compared to the analytical solution of (6.2a-c).

As the plots in Figure 6.5 show, this combined linearization and optimal control approach leads to decent approximation of the actual control that can be obtained without the direct solution of the high-index DAE [1] or finding the *flat inputs* [10].

7. Conclusion

Within this paper, we have considered mechanical systems with a partly specified motion which are usually modeled by DAEs of index ≥ 5. Such models require high regularity assumptions and their numerical treatment is extremely challenging because of the sensitivity to perturbations. Because of this, we have introduced an alternative modeling approach which relaxes the prescribed servo constraint and considers a minimization problem instead. By this, we decrease the possible errors which occur in the simulation of an high-index DAE but include an additional error, since we do not satisfy the constraint exactly. However, this modeling error is controllable by the penalization parameters.

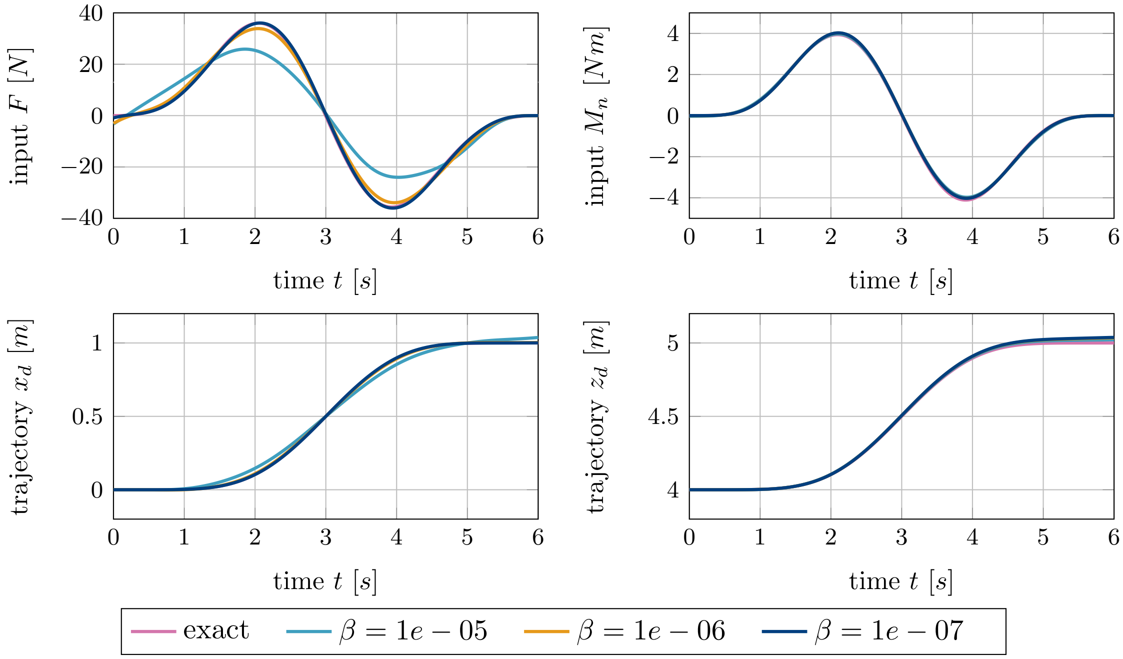

FIGURE 6.5. The forces F and M_n obtained through linearization and optimization for varying penalization parameter β (top) and the resulting trajectories (bottom) for the example of the overhead crane.

By means of the numerical examples, we have shown the advantages of the optimal control approach. First, the resulting control effort is much smaller at the price of only a small error in the constraint and thus, more realistic as this corresponds to a reduction of costs in real-world applications. Second, the approach is less sensitive to perturbations such as inconsistent initial data.

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