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EXPLOITING INVARIANTS IN THE NUMERICAL SOLUTION OF MULTIPOINT BOUNDARY VALUE PROBLEMS FOR DAE *

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Abstract. This paper presents a new approach to the numerical solution of boundary value problems for higher index differential algebraic equations. Invariants known for the original DAE as well as invariants of the reduced index 1 formulation are exploited to stabilize initial value problem integration, derivative generation and nonlinear and linear systems solution of an enhanced multiple shooting method. Extensions to collocation are given. Applications are presented for two important problem classes: parameter estimation in multibody systems given in descriptor form, and singular and state constrained optimal control problems. In particular, generalizations of the "internal numerical differentiation" technique to DAE with invariants and a new multistage least squares decomposition technique for DAE boundary value problems are developed, which are implemented in the multiple shooting code PARFIT and in the collocation code COLFIT. Further, a method is described which minimizes the number of necessary directional derivatives in the presence of multipoint conditions and invariants. As numerical applications a parameter identification problem for a slider crank mechanism and a periodic cruise optimal control problem for motor glider aircraft are treated.

Key words. invariants, boundary value problems, higher index differential-algebraic equations, parameter identification, descriptor form for multibody systems, optimal control, singular control, state constraints

AMS subject classifications. 65L10, 65L60

0. Introduction. Initial value problems (IVP) for differential algebraic equations (DAE) have received significantly more attention in the previous years than boundary value problems (BVP). In particular, there has been a very rapid development of new integration techniques and software for multibody systems.

The present paper concentrates on two important classes of boundary value problems for DAE:

- parameter estimation in descriptor form models for multibody systems
- treatment of singular controls and state constraints in optimal control

Both problems have in common that they lead to DAE with invariants that arise from index reduction. Additional physical invariants may appear, such as the total energy in conservative mechanical systems or the Hamiltonian in optimal control problems. The focus of this paper is on the numerical exploitation of these invariants in solution algorithms for multipoint boundary value problems. Two difficult application problems are treated in order to demonstrate the resulting benefits. In a parameter estimation problem for a descriptor form multibody system, the condition number of the linear system is reduced, and the number of Gauß-Newton iterations is decreased significantly. A family of optimal control problems is solved far beyond the previously reached point along a homotopy path.

The numerical solution of nonlinear DAE boundary value problems by multiple shooting exhibits two major additional difficulties as compared to ODE boundary value problems and DAE initial value problems. First, the iteration process solving

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the nonlinear BVP equations generates inconsistent local initial values at the shooting nodes when the algebraic condition is nonlinear, but consistent values are needed for the IVP integration on subintervals. Second, higher index DAE cannot be treated directly in many cases. Index reduction must then be performed, which eliminates higher order information from the DAE, thus causing numerical IVP solutions to drift off from the true solution manifold.

Few approaches to the numerical treatment of DAE boundary value problems have been reported in the literature. Here we do not give a complete list of all contributions, but rather an overview over the general directions of work in this field. In [11] a multiple shooting method is outlined for the treatment of constrained least squares boundary value problems in semi-explicit DAE of index 1. This paper proposes a relaxation technique to deal with inconsistent local initial values at the shooting nodes. A multistage least squares framework based on [10] is outlined for the treatment of under- and over-determined boundary value problems. A general theory of shooting and difference methods for implicit transferable DAE is developed by Griepentrog and März in [18,29]. In [27], Lentini and März investigate the conditioning of DAE boundary value problems. Lamour has proposed and implemented several shooting algorithms [24] and presents in [25] a well-posed multiple shooting method for implicit transferable DAE. Consistency of the converged local initial values is enforced by an additional Newton step on the algebraic conditions after each major Newton iteration on the discretized BVP. Collocation methods for DAE boundary value problems are described by Ascher, Mattheij and Russell [3]. Hanke [21] presents least-squares collocation methods for linear DAE boundary value problems. The code COLDAE of Ascher and Spiteri [6] treats semi-explicit DAE of index at most 2 and fully implicit DAE of index at most 1. It is based on a selective projective collocation method. Both [25] and [6] do not treat invariants. To our knowledge, DAE multipoint boundary value problems—especially over- or underdetermined ones—as they appear in optimal control and in parameter estimation, are up to now only considered in [11].

In the present paper we choose such a general problem class in order to be able to treat optimal control problems and parameter identification problems in a joint framework. The relaxation technique for algebraic constraints introduced in [11] is extended to hierarchies of invariants resulting from index reduction. These invariants are taken into account when solving the local IVP on each shooting interval, which prevents drift-off from the solution manifold by re-introducing the lost higher order information. Necessary extensions to the technique of internal numerical differentiation (IND) due to the invariants are described. Based on [10], a new multistage least squares approach is formulated in detail, which makes it possible to use invariants for numerical stabilization of the boundary value problem solution. A method is described which further exploits the invariants to minimize the number of necessary directional derivatives in the presence of multipoint conditions and invariants. Finally, practical applications demonstrate the stabilizing effect of the exploitation of invariants.

1. Preliminaries. The general type of DAE considered in this paper are semi-explicit DAE of index $r \geq 1$ of the form

$$\begin{aligned} \dot{y}_1 &= f(y_1, y_2), \\ 0 &= g(y_1, y_2), \end{aligned} \tag{1}$$

which allow index reduction to obtain an index 1 system of the same form, or of the quasi-linear form

$$B(y_1)\begin{pmatrix}\dot y_1\\ y_2\end{pmatrix} = f(y_1), \quad B(y_1) \text{ non-singular.}$$

(Typical DAE in this class are systems in Hessenberg form, cf. [13].) We will always use the index 1 form in numerical BVP solution, and therefore require reducibility. The generalized invariants defined in the following definition play the key role in treating index reduced DAE boundary value problems.

DEFINITION 1. A function $h(t, y)$ is called an *invariant of order* k, if

$$\left(\frac{d}{dt}\right)^k h(t, y(t)) \equiv \text{const}$$

along any IVP solution $y(t) = (y_1(t), y_2(t))$ of the DAE (1).

The classical notion of invariants is included in this definition as a special case, namely as invariants of order zero, satisfying $h(t, y) \equiv$ const along any IVP solution. In (mechanical) Hamiltonian systems such invariants correspond to "strong" invariants in the sense of Dirac [15] (see also [26]), while invariants of order 1 correspond to "weak" invariants.

LEMMA 1. *When index reduction is performed on DAE (1), the algebraic conditions of index* $r, r-1, \ldots, 2$ *will become invariants of order* $r-2, \ldots, 0$*, respectively, of the resulting index 1 DAE. We call this a* hierarchy of invariants.

Proof. This follows immediately from the definition. ☐

The boundary value problems considered in this paper are a rather general class of multipoint boundary value problems (MPBVP). Given a (time) interval $[t_0, t_f]$ and interior points $t_0 < t_1 < \cdots < t_{f-1} < t_f$, we seek differential variables y_1, algebraic variables y_2, and parameters p which minimize the least-squares function

$$\|r_1(y(t_0), \ldots, y(t_f), p)\|_2^2 = \min \tag{2}$$

while satisfying the index 1 DAE

$$\begin{aligned} \dot y_1 &= f(y_1, y_2, p), \\ 0 &= g(y_1, y_2, p), \end{aligned} \qquad \frac{\partial g}{\partial y_2} \text{ non-singular} \tag{3}$$

with multipoint boundary conditions

$$r_2(y(t_0), \ldots, y(t_f), p) = 0. \tag{4}$$

In addition there may be a hierarchy of invariants due to index reduction, and possibly also invariants of the original index r DAE.

The parameters p appearing in the above formulation can be regarded as special differential variables (with derivative zero); for ease of presentation they will be dropped in the remainder of the paper, except when parameter identification is discussed.

A condition for the local uniqueness of a solution $y^*(t) \in \mathbb{R}^n = \mathbb{R}^{n_1} \times \mathbb{R}^{n_2}$ of the boundary value problem can be given using the matrices

$$E_i = \sum_{j=0}^{f} \left[\frac{\partial r_i}{\partial y_1(t_j)} - \frac{\partial r_i}{\partial y_2(t_j)}\hat G(t_j)\right] V(t_j, t_0), \quad i = 1, 2, \qquad E = \begin{pmatrix}E_1\\ E_2\end{pmatrix},$$

where $\hat{G}(t) = g_{y_2}(y^*(t))^{-1} g_{y_1}(y^*(t))$, and V satisfies the variational initial value problem

$$\dot{V}(t,t_0) = [f_{y_1}(y^*(t)) - f_{y_2}(y^*(t))\hat{G}(t_j)]V(t,t_0), \qquad V(t_0,t_0) = I.$$

The solution is locally unique if E_2 has full rank ($\le n_1$) and $\operatorname{rank}(E) = n_1$. If E_2 has full rank and $\operatorname{rank}(E) < n_1$, then the boundary value problem is underdetermined and may have multiple solutions in any neighborhood of y^*. These conditions are a generalization of the uniqueness condition for DAE two-point BVP in [18] to the case of least-squares multipoint BVP. However, we restrict ourselves to the special case of semi-explicit DAE rather than treating fully implicit DAE.

For the numerical treatment of multipoint boundary value problems we apply a generalized Gauß-Newton iteration in connection with multiple shooting or collocation (see section 4). In the case of multiple shooting, the initial values on subintervals are in general inconsistent during the iteration, i.e., $g(y^0) \neq 0$. As in [11] we maintain the initial level on each shooting interval by integrating a modified index 1 DAE with relaxed algebraic condition, and include the consistency condition $g(y^0) = 0$ at each node as interior point condition in the boundary value problem. These consistency conditions determine the algebraic variables, whereas continuity conditions are specified only for the differential variables.

Of course, the hierarchical invariants (higher index algebraic conditions) are in general also unequal zero at the nodes. However, since they are related to the index 1 condition, we can use these functions for stabilizing the IVP integration. This will be achieved by defining relaxed versions which depend on the specific local initial values; these relaxed versions remain zero during numerical IVP solution by maintaining the initial level of a hierarchical invariant.

Additional invariants of the original index r DAE are usually *not* invariants of the reduced index 1 formulation. But they provide useful information on the BVP solution, and are therefore included in the BVP formulation together with the consistency conditions for the hierarchical invariants.

In order to distinguish the different usage of invariants for numerical stabilization of IVP solution and BVP iteration, we call them *initial value problem invariants* and *boundary value problem invariants*, respectively.

DEFINITION 2. (a) The initial value problem

$$\begin{aligned} \dot{y}_1 &= f(y_1,y_2), \\ 0 &= \hat{g}(y_1,y_2;t,t^0,y^0), \end{aligned} \qquad y(t^0) = y^0, \tag{1a}$$

is called a *relaxation* of the index 1 initial value problem

$$\begin{aligned} \dot{y}_1 &= f(y_1,y_2), \\ 0 &= g(y_1,y_2), \end{aligned} \qquad y(t^0) = y^0, \qquad \frac{\partial g}{\partial y_2} \text{ non-singular,}$$

if $\hat{g}(y^0;t^0,t^0,y^0) \equiv 0$, i.e., $\hat{g}$ is consistent with arbitrary initial values (t^0,y^0), and $\hat{g}(y;t,t^0,y^0) = g(y) + \gamma(t,t^0,y^0)$ with a differentiable function γ.

(b) A function $\hat{h}(t,y;t^0,y^0)$ is called an *initial value problem invariant* of (1a), if

$$h(t,y(t;t^0,y^0);t^0,y^0) \equiv \text{const}$$

along any solution $y(t;t^0,y^0)$ for arbitrary initial values (t^0,y^0).

(c) A function $\tilde{h}(t,y)$ is called a *boundary value problem invariant* of (2–4) on interval $[t_a,t_b]$, if

$$\tilde{h}(t,y^*(t)) \equiv \text{const} \quad \text{on } [t_a,t_b]$$

along the solution $y^*(t)$ of the BVP.

Remarks. It is not unusual for BVP invariants to apply on subintervals $[t_a, t_b] \subset [t_0, t_f]$ only, such as on constraint arcs or singular arcs. The role of the extended formulation of the algebraic condition in (1a) will be made clear in the examples given below. As a typical example for an extended formulation consider the relaxation

$$\hat{g}(y; t, t^0, y^0) := g(y) - g(y^0)\beta(t - t^0),$$

which is consistent with any initial value y^0 in (1a) if the function β satisfies $\beta(0) = 1$. IVP invariants $\hat{h}$ may then be, e.g., integrals of $\hat{g}$. Hierarchical invariants obtained from index reduction may always serve as both IVP invariants and BVP invariants.

It is well known that Baumgarte's method [7] can be used to stabilize index 1 initial value problems resulting from index reduction of index 3 systems. However, Baumgarte's method has the disadvantage that it depends sensitively on the choice of certain parameters in order to produce a stabilizing effect, and typically leads to a stiff system. The present paper demonstrates that one can obtain essentially the same stabilizing effect using projection methods, without having to deal with stiffness problems and critical parameters.

In the following section the problem classes and associated types of invariants are presented. In section 3 the numerical solution of DAE with IVP invariants and the computation of derivatives with respect to initial values and parameters are discussed. The principle of Internal Numerical Differentiation is generalized to the case of DAE with invariants, which can then be used for integration in the context of multiple shooting. In the fourth section basic features of multiple shooting and collocation are recalled. Section 5 presents generalizations of multiple shooting and collocation which include BVP invariants in the system of continuity and boundary conditions within the framework of a multistage optimization approach. Finally, the efficiency of the new approach is demonstrated by applying it to the parameter identification of a crank slider mechanism in descriptor form and to the optimal control problem of periodic cruise of a motor glider aircraft.

2. The problem classes. In this section the properties of the two boundary value problem classes treated in this paper are presented. IVP and BVP invariants are discussed in detail for multibody systems in descriptor form.

2.1. Hierarchical invariants in multibody systems in descriptor form. The dynamics of a holonomic multibody system in descriptor form is described by a DAE of index 3,

$$M(p)\ddot{p} = f(p, \dot{p}, t) - G^T(p)\lambda \tag{5}$$

$$0 = g_p(p) \tag{6}$$

where $G := \partial g_p/\partial p$ is the derivative of the position constraint g_p, and M is the mass matrix which is known to be positive definite on the kernel of G. Using *index reduction*, i.e., repeated differentiation of g_p with respect to t, one obtains the constraints on velocity and acceleration level, g_v and g_a.

$$0 = g_v(p, \dot{p}) = G(p)\dot{p} \tag{7}$$

$$0 = g_a(p, \dot{p}, \ddot{p}) = G(p)\ddot{p} + \dot{p}^T \frac{\partial}{\partial p} G(p)\dot{p} \tag{8}$$

Equations (5) and (8) form a DAE of index 1. The original constraint (6) and its derivative (7) now play the role of invariants of orders 1 and 0, respectively, of the system. Such systems can be solved efficiently and stably by special techniques which exploit the inherent structure of the reduced system (cf., e.g., [12,16,1]).

Initial values $(p_0, \dot p_0)$ are called *consistent* if they satisfy the constraints on velocity and position level. Initial values $(p_0, \dot p_0, \lambda_0)$ are called *consistent* if there exists an initial acceleration $\ddot p_0$ such that all the equations (5–8) are satisfied. Note that the constraint on acceleration level, g_a, can always be satisfied choosing an appropriate λ. In case of nonlinear algebraic conditions, however, it is often recommendable to allow for free initial values of the algebraic variable, too. Naturally, during the solution process of boundary value problems, the initial values cannot be guaranteed to be always consistent. Therefore, in [11] a relaxation technique was introduced, which alters the DAE system in order to make arbitrary initial values $(p_0, \dot p_0, \lambda_0)$ or $(p_0, \dot p_0, \ddot p_0)$ consistent,

$$\begin{aligned} \hat g_a(p,\dot p,\ddot p; p_0,\dot p_0,\ddot p_0,t) &:= g_a(p,\dot p,\ddot p) - g_a(p_0,\dot p_0,\ddot p_0) \\ \hat g_v(p,\dot p; p_0,\dot p_0,\ddot p_0,t) &:= g_v(p,\dot p) - g_v(p_0,\dot p_0) - (t-t_0) g_a(p_0,\dot p_0,\ddot p_0) \\ \hat g_p(p; p_0,\dot p_0,\ddot p_0,t) &:= g_p(p) - g_p(p_0) - (t-t_0) g_v(p_0,\dot p_0) \\ &\qquad - \tfrac{1}{2}(t-t_0)^2 g_a(p_0,\dot p_0,\ddot p_0) \end{aligned} \tag{9}$$

Consistency of the original higher index constraints must then be assured via interior point conditions which are equivalent to the BVP invariants $g_a = g_v = g_p = 0$. For their treatment see section 5. Obviously, $\hat g_v \equiv \hat g_p \equiv 0$ are invariants of the initial value problem

$$\begin{aligned} \begin{pmatrix} M(p) & G(p)^T \\ G(p) & 0 \end{pmatrix} \begin{pmatrix} \ddot p \\ \lambda \end{pmatrix} &= \begin{pmatrix} f(p,\dot p) \\ -\dot p^T \frac{\partial}{\partial p} G(p)\dot p + g_a(p_0,\dot p_0,\ddot p_0) \end{pmatrix}, \\ p(t_0) &= p_0, \\ \dot p(t_0) &= \dot p_0 \quad \text{(and } \lambda \text{ corresponding to the condition on } \hat g_a). \end{aligned} \tag{10}$$

Here $\ddot p_0$ may be chosen in order to produce a prescribed initial value λ_0. Vice versa, λ_0 may be chosen in order to produce a prescribed initial value $\ddot p_0$. In the latter case $\ddot p_0$ is replaced by λ_0 in the equations (9,10).

In addition to making arbitrary initial values consistent, damping can be introduced if the algebraic constraint (8) is replaced by a different relaxation,

$$0 = \bar g_a = g_a + 2\alpha g_v + \alpha^2 g_p - \beta(p_0, \dot p_0, \ddot p_0, t). \tag{11}$$

This approach, which is due to Baumgarte, has the following advantage. By definition,

$$g_a = \ddot g_p, \quad g_v = \dot g_p.$$

Therefore, (11) can be considered an ODE for $\Phi(t) := g_p$. If the inhomogeneity β is chosen as $[g_a(p_0,\dot p_0,\ddot p_0) + 2\alpha g_v(p_0,\dot p_0) + \alpha^2 g_p(p_0)]\, exp(-\alpha(t-t_0))$, i.e., such that any initial values $(p_0,\dot p_0,\ddot p_0)$ are consistent, then the solution is

$$\Phi(t) := \left(a_0 + a_1(t-t_0) + \frac{1}{2} a_2 (t-t_0)^2 \right) e^{-\alpha(t-t_0)}$$

where

$$\begin{aligned} a_0 &:= g_p(p_0) \\ a_1 &:= g_v(p_0, \dot{p}_0) + \alpha g_p(p_0) \\ a_2 &:= g_a(p_0, \dot{p}_0, \ddot{p}_0) + 2\alpha g_v(p_0, \dot{p}_0) + \alpha^2 g_p(p_0) \end{aligned}$$

(cf. [7,20]). Thus, one may either choose (11), or the condition

$$g_a(p, \dot{p}, \ddot{p}) - \ddot{\Phi}(t) = 0 \tag{12}$$

as the relaxed algebraic constraint of type (1a). In [20] this alternative relaxation technique is introduced in order to cope with inconsistent initial values. In the light of definition 2 we see that the functions

$$\bar{g}_p := g_p - \Phi(t), \quad \bar{g}_v := g_v - \dot{\Phi}(t)$$

become IVP invariants. Boundary value problem invariants are $g_a = g_v = g_p = 0$. Note that the choice of (12) avoids stiffness in the system, which would occur in formulation (11) when large positive values of α are chosen.

2.2. Parameter estimation for multibody systems in descriptor form. The parameter estimation task is to identify unknown system parameters θ, such as masses, moments of inertia, damping and stiffness coefficients, etc., from given measured data of the state history. The measured data are assumed to be perturbed values of functions ϕ_i of an exact solution of the system equations,

$$\eta_{i,j} = \phi_i(y(t_j), \theta) + \varepsilon_{i,j} \quad (y \text{ includes } p, \dot{p}, \lambda),$$

with measurement errors distributed according to a normal distribution with mean value 0 and known variances $\sigma_{i,j}^2$. A Maximum Likelihood estimator for the parameters is the minimizer of the weighted output functional

$$\min_{y,\theta} \ell_2(y, \theta) := \sum_{i,j} \sigma_{i,j}^{-2} (\eta_{i,j} - \phi_i(y(t_j), \theta))^2.$$

This functional is minimized subject to the model DAE and additional boundary conditions. The resulting problem is an overdetermined multipoint boundary value problem. After discretization by multiple shooting or collocation this leads to a nonlinear, constrained least squares optimization problem of the form (2–4). There are efficient methods available for this problem class, for example [10,11,33,34].

2.3. Hierarchical invariants in optimal control problems. When Pontryagin's maximum principle is applied to optimal control problems, singular controls or state constraints may lead to higher index algebraic conditions. (Cf., e.g., [14,23,8]). (A singular control of *order* k has *index* $2k+1$, and a state constraint of *order* k has *index* $k+1$.) Index reduction then produces a hierarchy of invariants. Consider an autonomous optimal control problem for ODE

$$\dot{y} = f(y, u) \quad \text{on } [t_0, t_f]. \tag{13}$$

The aim is to

$$\text{minimize } \phi(y(t_f), t_f)$$

subject to boundary conditions

$$r(y(t_0), y(t_f), t_f) = 0.$$

Let u^* be an optimal control and y^*, λ^* optimal state and costate vectors. According to the maximum principle the Hamiltonian

$$H(\lambda, y, u) = \lambda^T f(y, u)$$

is maximized point-wise by $u^*(t)$ along $(\lambda^*(t), y^*(t))$ almost everywhere,

$$H(\lambda^*(t), y^*(t), u^*(t)) = \max_{v \in \Omega} H(\lambda^*(t), y^*(t), v). \tag{14}$$

Here Ω denotes the set of admissible control values, and the costates λ satisfy the adjoint equations

$$\dot{\lambda}^T = -\lambda^T f_y(y, u) \tag{15}$$

and (for some multiplier α) the transversality conditions

$$\begin{aligned} \lambda(t_0)^T &= \alpha^T r_{y_0}(y(t_0), y(t_f), t_f), \\ -\lambda(t_f)^T &= \alpha^T r_{y_f}(y(t_0), y(t_f), t_f) + \phi_y(y(t_f), t_f), \\ H(t_f) &= \alpha^T r_{t_f}(y(t_0), y(t_f), t_f) + \phi_t(y(t_f), t_f). \end{aligned}$$

(Note that the controls u are the algebraic variables here, while states and costates x, λ are both differential variables.)

It is a well-known fact that from (13–15) follows

$$H(\lambda(t), y(t), u(t)) = \text{const}_1 = H(t_f)$$

along the solution (λ^*, y^*, u^*). In addition, one easily shows that

$$H(\lambda(t), y(t), u(t)) = \text{const}_2(\lambda^0, y^0)$$

for any y, λ solving (13,15) for arbitrary initial values (λ^0, y^0) when u^* is determined according to (14), i.e.,

$$u^*(\lambda, y) = \arg\max_{v \in \Omega} H(\lambda, y, v). \tag{16}$$

In the following we will consider the two most important special cases.

(1) The Hamiltonian is regular, i.e., $H_{uu} > 0$, and $u^*(t) \in \text{int}(\Omega)$ almost everywhere. Then

$$H_u(\lambda, y, u^*) = 0 \tag{16'}$$

follows from (16). The satisfaction of this algebraic condition for u^* implies that the Hamiltonian H is an IVP invariant for the canonical system (13,15).

(2) The Hamiltonian is singular, i.e., the control appears linearly in H (consider a scalar control $u \in [-1,+1]$ only),

$$H(\lambda, y, u) = \lambda^T(p(y) + s(y)u) = P(\lambda, y) + S(\lambda, y)u.$$

The switching function $S(\lambda, y)$ determines the behavior of the optimal control on bang-bang arcs ($S \neq 0$). From the maximum principle (14) follows

$$\begin{aligned} &\text{(a) if } S(\lambda, y) < 0 \text{ then } u^* = -1, \\ &\text{(b) if } S(\lambda, y) > 0 \text{ then } u^* = +1. \end{aligned}$$

Obviously, $H(\lambda, y, u^*(\lambda, y))$ is an IVP invariant if y, λ solve (13,15) and u^* is given by (a), (b). If

$$\text{(c) } S(\lambda, y) \equiv 0$$

on some interval $[t_a, t_b]$, then u^* is not determined by the maximum principle and u is called singular. However, from (c) follows

$$S^i(\lambda, y, u) = \left(\frac{d}{dt}\right)^i S(\lambda, y) \equiv 0, \qquad i = 0, 1, \ldots$$

It is easy to show that $\partial S^1/\partial u \equiv 0$. Assume for simplicity that the singular control has index 3 (equivalent to order 1),

$$\frac{\partial}{\partial u} S^2(\lambda, y, u) \neq 0, \tag{17}$$

and hence u^* can be determined from the algebraic constraint

$$S^2(\lambda, y, u) = 0. \tag{18}$$

In that case the functions S^2, S^1, S^0 yield a system of algebraic equations and IVP invariants which may be formulated in a relaxed form according to system (11),

$$\begin{aligned} S^0(\lambda, y) - S^0(\lambda(t_a), y(t_a)) - (t - t_a)S^1(\lambda(t_a), y(t_a)) &= \hat{S}^0 \equiv 0, \\ S^1(\lambda, y) - S^1(\lambda(t_a), y(t_a)) &= \hat{S}^1 \equiv 0, \end{aligned}$$

are IVP invariants for system (13,15) if u^* is chosen *consistent* according to (18). Note that in this case the Hamiltonian is a BVP invariant along the optimal solution of the BVP, but H is not an IVP invariant on $[t_a, t_b]$ as long as S^0, S^1 and possibly S^2 are inconsistent.

Remark. If in addition a state constraint $g(y(t)) \geq 0$ of index $k+1$ (order k) is active along some subinterval $[t_a, t_b]$, then index reduction analogously leads to IVP invariants $\hat{g}^0, \ldots, \hat{g}^{k-1}$, plus an algebraic condition $\hat{g}^k \equiv 0$ that determines u^*.

3. Initial value problems with invariants. The numerical solution of IVP is a core task for multiple shooting codes to solve boundary value problems. If these IVP are solved exactly, invariants are preserved. Due to discretization errors the so called drift phenomenon can be observed as it is widely discussed mainly in the multibody community (cf., e.g., [1,2,5,12,16,17]). Again we consider semi-explicit DAE of the form (1), which may have IVP invariants according to our definition. In initial value problems, a valuable technique to improve the solution accuracy in the presence of invariants is the projection of the numerical solution onto the invariant manifold. In this section this technique is investigated and incorporated in the numerical computation of derivative matrices.

3.1. Invariant conservation by projection. The basic algorithm for the numerical solution of IVP for DAE with invariants using projection is (in the time step t_{k-1} to t_k):

1. discretize and solve the given DAE system; obtain the trajectory value $\tilde{y}^k$
2. project to satisfy the invariant, i.e. solve the optimization problem

$$\begin{aligned} &\min_{y^k} \|y^k - \tilde{y}^k\|_w^2 \\ \text{s. t.} \quad & h(t_k, y^k; t^0, \xi) = 0, \qquad \xi = y(t^0), \end{aligned}$$

where $\|\cdot\|_w$ denotes a *weighted* norm derived from a scalar product. This optimization subproblem may be solved by a generalized Gauß-Newton iteration [10].

A careful convergence analysis shows that in many cases one iteration is sufficiently accurate to project $\tilde{y}^k$ onto the invariant manifold. For ease of notation we will only consider this special case in the present paper (for a more thorough discussion see [2,16]). This first iteration may be written in terms of the Moore-Penrose pseudoinverse,

$$y^k := \tilde{y}^k - \left[\frac{\partial h}{\partial y}(t_k, \tilde{y}^k; t^0, \xi)\right]^+ h(t_k, \tilde{y}^k; t^0, \xi).$$

If the scalar product—i.e., the scaling—used for the projection and the local error criterion are compatible, then the following equation is valid up to first order (for details cf. [16,2]):

$$\|\tilde{y}^k - y(t_k)\|_w^2 \doteq \|\tilde{y}^k - y^k\|_w^2 + \|y^k - y(t_k)\|_w^2.$$

(Here $y(t)$ denotes the exact solution.) Hence the projected numerical solution y^k not only satisfies the constraints more accurately, it is also more accurate in general.

3.2. Internal Numerical Differentiation for DAE. In order to solve boundary value problems, not only trajectory values are needed but also their derivatives with respect to initial values and parameters.

LEMMA 2. *The derivative of the solution of the relaxed DAE (1a) with respect to the initial values y^0, the Wronskian*

$$W(t, t^0) := \begin{pmatrix} W_1(t, t^0) \\ W_2(t, t^0) \end{pmatrix} := \frac{\partial}{\partial y^0} y(t; t^0, y^0),$$

satisfies the variational DAE

$$\begin{aligned} \dot{W}_1 &= f_y W, \qquad W(t^0, t^0) = I, \\ 0 &= \hat{g}_y W + \hat{g}_{y^0}. \end{aligned}$$

Proof. This follows from the construction of the relaxed algebraic equation $\hat{g}$ according to definition (2a). ∎

When computing the derivatives of the solution of a DAE with respect to initial values and possibly parameters, one observes that this solution itself is the result of an intricate adaptive discretization algorithm in the course of the integration. Two different ways are considered.

(1) The differentiation of the whole numerical integration procedure (either by forward differences or analytically as, for instance, by automatic differentiation), which we call external numerical differentiation (END).

END treats the numerical solution procedure for an initial value problem as a black box process. Therefore, its derivative approximations are severely influenced by adaptive components, which may also cause nondifferentiabilities and discontinuities of the numerical solution. The latter result from step size and order selection, pivoting in linear system solutions, Newton-type iteration steps due to projections, implicit schemes, switching point location etc. Hence, the results of END are in general meaningless or highly inaccurate, at least for less stringent tolerances.

(2) In contrast, the principle of Internal Numerical Differentiation (IND) is to compute the derivative only of the discretization scheme approximating the DAE initial value problem (again either by forward differences or analytically). This approximate scheme is generated by an adaptive procedure. The resulting adaptive components of the numerical integration procedure, however, are not differentiated.

The adaptive procedure (and the discretization) must be chosen such that the discretization scheme approximates with the desired accuracy not only the solution but also its derivatives. It should also be chosen such that the derivative calculation is as efficient as possible. Since the exact derivative of an approximate problem solution is computed, IND is stable in the sense of backward analysis and yields useful derivatives even for coarse approximation accuracies. Step and order selection are not differentiated, iterative procedures are reformulated and reinterpreted to allow for application of the implicit function theorem. Since intermediate coefficients, matrices, decompositions etc. are used both for the computation of the solution and its derivatives, high computational savings may be gained. Details for various integration methods are given, e.g., in [9,10]).

3.3. IND for linearly implicit DAE in multibody systems. Relaxed index reduced multibody systems in descriptor form may be written as linearly implicit DAE of index 1,

$$B(y_1)\begin{pmatrix}\dot{y}_1\\ y_2\end{pmatrix} = f(y_1;t,t^0,y^0), \quad B(y_1) \text{ non-singular.}$$

In order to compute the derivatives of the solution with respect to the initial values by external differentiation one would have to compute B^{-1} many times. This would be expensive and also lead to instabilities due to pivoting, roundoff errors, etc. A possible way to generate a stable, efficient and accurate way of IND by forward differences may be derived observing three IVP, which lead to analytically but not numerically equivalent derivative calculations.

LEMMA 3. *The following three initial value problems for linearly implicit DAE of index 1 have the same variational DAE:*

(a) $B(y_1)\begin{pmatrix}\dot{y}_1\\ y_2\end{pmatrix} = f(y_1;t,t^0,y^0), \quad y(t^0) = y^0$

(b) $B(y_1)\begin{pmatrix}\dot{\eta}_1\\ \eta_2\end{pmatrix} = f(\eta_1;t,t^0,\eta^0) + [B(y_1) - B(\eta_1)]\begin{pmatrix}\dot{y}_1\\ y_2\end{pmatrix},$

$\eta(t^0) = \eta^0 = y^0$, $y =$ *solution of (a)*

(c) $B(y_1)\begin{pmatrix}\dot{\delta}_1\\ \delta_2\end{pmatrix} = [f(y_1+\delta_1;t,t^0,y^0+\delta^0) - f(y_1;t,t^0,y_1^0)] + [B(y_1) - B(y_1+\delta_1)]\begin{pmatrix}\dot{y}_1\\ y_2\end{pmatrix},$

$\delta(t^0) = \delta^0 = 0$, $y =$ *solution of (a)*

These three different formulations can be used to generate an appropriate variational scheme for a given discretization of the DAE. Thus, e.g., for a Runge-Kutta or polynomial extrapolation method one may obtain the following algorithm for the computation of the Wronskian by a finite difference approximation in integration step k:

(1) compute all stages of the discretized nominal trajectory $\tilde{y}^{k+1}$ by DAE (a),

(2) compute a varied step η_i^{k+1} from $\eta_i^k := \tilde{y}^{k+1} + \varepsilon_i e_i$ by DAE (b) using the same discretization scheme and replacing $y_1, \dot{y}_1$ and y_2 by the results of (a) in all stages.

(3) calculate $\tilde{W}^{k+1} e_i = (\eta_i^{k+1} - \tilde{y}^{k+1})/\varepsilon_i$ and from this $W^{k+1} = \tilde{W}^{k+1} W^{k+1}$.

Analogously, it is possible to use DAE (c) to compute directional derivatives of the discrete solution of the DAE (a) directly, which is less prone to roundoff. Both variants (b) and (c) offer the advantage that repeated factorizations of the matrix B are avoided. For multistep methods as described in [2,16] the situation is slightly more complicated. In case of automatic differentiation the differences in square brackets in (b) and (c) may be replaced by directional derivatives.

3.4. IND for DAE with invariants. The application of the principle of Internal Numerical Differentiation for DAE of index 1 with invariants, which are solved by invariant projection, is based on the following theorem.

THEOREM 1. *If the solution of DAE (1a) satisfies an initial value problem invariant $h(t, y; t^0, y^0) \equiv 0$, then its Wronskian satisfies the IVP invariant*

$$h_y(t, y; t^0, y^0) W(t, t^0) + h_{y^0}(t, y; t^0, y^0) \equiv 0.$$

Proof. Differentiate h. □

Since one needs h_y for both the projections onto $\{y \in \mathbb{R}^n \mid h(t, y; t^0, y^0) = 0\}$ and onto $\{W \in \mathbb{R}^{n\times n} \mid h_y(t, y; y^0) W(t, t^0) + h_{y^0}(t, y; t^0, y^0) = 0\}$ for the derivative, both operations may be coupled. The following algorithm for one-step integration methods generalizes the principle of Internal Numerical Differentiation to the projection onto invariants.

Start:

input initial values t^0, $\xi = y^0$

Integration step: $t_k \mapsto t_{k+1}$

(1) compute y^{k+1} as the result of one integration step of the DAE (1a)

(2) compute $\tilde{W}^{k+1}$ with the same integration scheme as y^{k+1} (or consistent alternatives for linearly implicit DAE) as the derivative of the one step scheme

(3) multiply $W^{k+1} = \tilde{W}^{k+1} \hat{W}^k$

(4) compute $H_{k+1} := h_y(t^{k+1}, y^{k+1}; t^0, \xi)$

(5) project:

$\hat{y}^{k+1} = y^{k+1} - H_{k+1}^+ h(t^{k+1}, y^{k+1}; t^0, \xi)$

$\hat{W}^{k+1} = W^{k+1} - H_{k+1}^+ [H_{k+1} W^{k+1} + h_\xi]$

In this way the knowledge of an initial value problem invariant can be used to stabilize the computation of both the solution and its derivatives by IND.

4. Boundary value problems. There are two main numerical solution methods for boundary value problems in ODE and DAE: multiple shooting and collocation. Their basic properties are briefly summarized.

4.1. Multiple shooting for DAE. First we recall the multiple shooting method for ODE. It is based on the solution of initial value problems on the subintervals of an appropriately chosen mesh

$$\pi : t_0 = \tau_1 < \ldots < \tau_{m-1} < \tau_m = t_f. \tag{19}$$

The state variables on every subinterval are replaced by the computed solution $y^\pi(t; y^j)$ of the initial value problems

$$\begin{aligned} \dot{y}^\pi(t) &= f(t, y^\pi(t)), \quad t \in [\tau_j, \tau_{j+1}], \\ y^\pi(\tau_j) &= y^j. \end{aligned}$$

Thus, the ODE boundary value problem is transformed to the finite dimensional nonlinear system of equations

$$c_j := y^\pi(\tau_{j+1}; y^j) - y^{j+1} = 0, \quad j = 1, \ldots, m-1 \qquad \text{(continuity conditions)} \tag{20}$$

$$r_2(y^1, \ldots, y^m) = 0 \qquad \text{(boundary conditions)} \tag{21}$$

This method can be generalized to index 1 DAE of the form (1) if one uses only $y_1^1, \ldots, y_1^m$ as the independent variables and regards the DAE in principle as the ODE $\dot{y}_1 = f(y_1, y_2(y_1))$. In this case the local initial value problems are well defined for all initial values y_1. However, the initial values for y_2 must then always be kept consistent, which is advisable only in the case when algebraic variables appear linearly in the algebraic constraint. In highly nonlinear algebraic equations which appear, e.g., in chemical applications, or in parameter estimation problems when parameters in the algebraic conditions are unknown, it may be unwise or even impossible to always require algebraic variables consistent with the algebraic constraints, especially when the complexity of generating and maintaining consistent algebraic variables is high. Therefore our multiple shooting method for DAE boundary value problems is based on the relaxed formulation (1a), permitting local initial values which are inconsistent with the original index 1 condition during the iteration,

$$\begin{aligned} \dot{y}_1^\pi(t) &= f(t, y_1^\pi(t), y_2^\pi(t)), \quad t \in [\tau_j, \tau_{j+1}], \\ 0 &= g(y_1^\pi(t), y_2^\pi(t)) - g(y_1^j, y_2^j). \\ y_1^\pi(\tau_j) &= y_1^j \end{aligned}$$

The algebraic variables y_2^j are determined by (interior point) conditions at all nodes,

$$g(y_1^j, y_2^j) = 0,$$

whereas continuity conditions are specified for the differential variables y_1^j only. Hierarchical invariants resulting from index reduction are used in the integration of the local initial value problems, as described in the previous sections.

4.2. Collocation for DAE. An alternative to multiple shooting is collocation. Collocation is based on the approximation of the solution of the ODE by a piecewise polynomial of degree k on a mesh. One requires that the approximative solution satisfies the ODE on a subdivision of this mesh, the collocation points. These are defined by linear transformation of a given set of points $0 \le \rho_1 < \cdots < \rho_k \le 1$ into the mesh intervals, $t_{jl} = t_j + \rho_l(\tau_{j+1} - \tau_j)$, $l = 1, \ldots, k$. Additionally, the approximate solution has to be continuous at the mesh points and has to satisfy the boundary conditions. Again, this method transforms the ODE boundary value problem to a finite dimensional nonlinear system of equations,

$$
\begin{aligned}
\dot{y}^\pi(t_{jl}; y^j, z^j) &= f(t_{jl}, y^\pi(t_{jl}; y^j, z^j)), && \text{(collocation conditions)}\\
y^\pi(\tau_{j+1}; y^j, z^j) - y^{j+1} &= 0, \quad j = 1, \ldots, m-1 && \text{(continuity conditions)}\\
r_2(y^1, \ldots, y^m) &= 0 && \text{(boundary conditions)}
\end{aligned}
$$

where z^j are local collocation variables, and y^π denotes now the local polynomial solution within the mesh subintervals. The solution of this system of equations can also be regarded as the solution of a multiple shooting method, in which the local integration is performed by a one step integration of an implicit Runge-Kutta method.

The generalization to DAE (1) can be done in two ways. One way is to use only the differential variables as independent variables and to reduce the DAE again to the ODE $\dot{y}_1 = f(y_1, y_2(y_1))$. For DAE which are nonlinear with respect to the algebraic variables this is not efficient since it involves internal iterations within the collocation scheme. For such DAE it is preferable to satisfy the algebraic constraint only at the solution of the BVP, i.e., to replace the collocation conditions at each collocation point by the conditions

$$
\left.
\begin{aligned}
\dot{y}_1^\pi(t_{jl}; y^j, z^j) &= f(t_{jl}, y_1^\pi(t_{jl}; y^j, z^j), y_2^{jl}),\\
0 &= g(y_1^\pi(t_{jl}; y^j, z^j), y_2^{jl}),
\end{aligned}
\right\} \quad j = 1, \ldots, m-1, \quad l = 1, \ldots, k,
$$

and to solve these conditions iteratively in the same way as the collocation conditions in the ODE case. Continuity conditions are again only specified for the differential variables.

5. Elimination of continuity conditions. The following considerations are based on the assumption that it is desirable to exploit the explicit knowledge of boundary value problem invariants. The requirements of satisfying the DAE and the invariants formally overdetermine the solution of the BVP. Both multiple shooting and collocation are based on a finite dimensional discretization of the solution of the DAE boundary value problem. Both have in common the explicit requirement of the continuity condition

$$y_1^\pi(\tau_{j+1}; y^j[, z_j]) - y_1^{j+1} = 0$$

This common feature will be used in the multistage least squares approach below.

5.1. A multistage least squares approach. The linearized discretized system of boundary, continuity, and possibly collocation conditions may be ill-conditioned due to error propagation introduced by the continuity conditions. This may be the case especially in coupled nonlinear systems with both rapidly increasing and rapidly decreasing components which lack sufficient dichotomy properties. Thus, it appears desirable to exploit the explicit knowledge about some solution components which is present in the BVP invariants, and to require continuity only of those components within the invariant subspace.

The decision above, to rank the invariant condition higher than the formally equivalent components of continuity conditions, naturally leads to the requirement

$$h(t, y^*(t)) \equiv 0,$$

or weaker, for appropriate nodes τ_j,

$$h(\tau_j, y^*(\tau_j)) = 0. \tag{22}$$

Remark. Note that the only type of invariants treated throughout this section are BVP invariants, which do not depend explicitly on the initial values.

For the sake of clarity of the presentation we assume in the following that the invariants do not depend on the algebraic variables, which is of course true for hierarchical invariants resulting from index reduction. The more general case that algebraic variables also appear in the BVP invariants can be treated numerically in various ways that are all interpretable in the multistage least-squares framework described below. For instance, the use of the algebraic index 1 conditions to eliminate the algebraic variables from the invariants can be viewed as using another type of generalized inverse for the invariant projection. On the other hand, applying orthogonal transformations to the composite Jacobian of both invariants and algebraic conditions leads to a Moore-Penrose inverse and an invariant projection in the full (y_1, y_2)-space. In this case we have to formally include continuity conditions for the algebraic variables.

Together with the continuity conditions, conditions (22) are formally overdetermined yet redundant, at least at the solution trajectory of the BVP. For overdetermined systems a multistage least squares approach was introduced in [10,33,11], which can be outlined as follows.

- Choose a ranking of the conditions (rank 1, rank 2, ...)
- satisfy conditions of rank k as well as possible using the degrees of freedom left by conditions of rank $1, \ldots, k-1$

A general form of a nonlinear multistage least squares problem is

$$\begin{array}{rll} & \|f_k(x)\|_2^2 = \min\limits_{x \in X_k} & (k) \\ \text{subject to} & \|f_{k-1}(x)\|_2^2 = \min\limits_{x \in X_{k-1}} & (k-1) \\ & \vdots & \\ \text{subject to} & \|f_1(x)\|_2^2 = \min\limits_{x \in X_1} & (1) \end{array}$$

where $X_1 = \mathbb{R}^m$ and $X_i = \{x \in X_{i-1} \mid \|f_i(x)\|_2^2 = \min\}$ for $i = 2, \ldots, k$.

This problem class includes overdetermined least squares problems with equality constraints. The nonlinear problem is solved iteratively by a generalized Gauß-Newton method, $x^{l+1} = x^l + \alpha^l \Delta x^l$, where Δx^l solves the linearized problem

$$\begin{array}{rll} & \|J_k \Delta x + f_k\|_2^2 = \min\limits_{\Delta x \in Y_k} & (k) \\ \text{subject to} & \|J_{k-1} \Delta x + f_{k-1}\|_2^2 = \min\limits_{\Delta x \in Y_{k-1}} & (k-1) \\ & \vdots & \\ \text{subject to} & \|J_1 \Delta x + f_1\|_2^2 = \min\limits_{\Delta x \in Y_1} & (1) \end{array}$$

Here $f_i = f_i(x^l)$, $J_i = \partial f_i(x^l)/\partial x$, and Y_i are the tangential spaces to the manifolds X_i at x^l. Abbreviating $J^T = (J_k^T, \ldots, J_1^T)$ and $f^T = (f_k^T, \ldots, f_1^T)$, the linear system can be rewritten as

$$J \Delta x^l + f \cong 0.$$

According to [10,33] there is a generalized inverse J^+ (satisfying $J^+ J J^+ = J^+$) such that $\Delta x^l = -J^+ f$. Therefore the convergence theory for generalized Gauß-Newton methods applies (cf. [10,33]).

For the practical realization of the multistage approach one has to be more specific about the ranking. The ranking proposed here is:

rank 1: boundary value problem invariants
rank 2: continuity and multipoint boundary conditions, recursively nested,
rank 3: least squares conditions (in parameter estimation problems)

This ranking results in a reformulation of the local continuity conditions. At nodes τ_j, where BVP invariants are to be satisfied, the following local least squares problems have to be solved:

$$
\begin{aligned}
&\|y_1^\pi(\tau_j; y^{j-1}[, z^{j-1}]) - y_1^j\|_2^2 = \min_{y_1^j} \\
&\text{s.t.} \quad h(\tau_j; y_1^j) = 0.
\end{aligned} \tag{23}
$$

This formulation is equivalent to the orthogonal projection of the continuity conditions onto the invariant manifold.

In the case of collocation, the linearization of the collocation and consistency conditions

$$
\begin{aligned}
\dot{y}_1^\pi(t_{j-1,l}; y^{j-1}, z^{j-1}) - f(t_{j-1,l}, y^\pi(t_{j-1,l}; y^{j-1}, z^{j-1}), y_2^{j-1,l}) &= 0 \\
g(y^\pi(t_{j-1,l}; y^{j-1}, z^{j-1}), y_2^{j-1,l}) &= 0
\end{aligned}
$$

is used as pre-condensation; it eliminates z^{j-1} to yield exactly the same problem structure as in multiple shooting (cf. [3]).

Linearizing (23) at y^{j-1} leads to the local linear least squares problems

$$
\begin{aligned}
&\|W_1^j \Delta y^{j-1} - \Delta y_1^j + c_j\|_2^2 = \min_{\Delta y_1^j} \\
&\text{s.t.} \quad H_j \Delta y_1^j + h_j = 0,
\end{aligned} \tag{24}
$$

where

$$
\begin{aligned}
H_j &:= \partial h(t_j; y_1^j)/\partial y_1, \\
h_j &:= h(t_j, y^j),
\end{aligned}
$$

and c_j denotes $y_1^\pi(t_j; y^{j-1}[, z^{j-1}]) - y_1^j$. Using an orthogonal factorization of the matrix H_j^T,

$$
H_j^T = (Y_j, Z_j)\begin{pmatrix} L_j^T \\ 0 \end{pmatrix} := Q_j \begin{pmatrix} L_j^T \\ 0 \end{pmatrix}, \qquad Q_j^T Q_j = I,
$$

one obtains a linear system which is equivalent to (24)

$$
\begin{aligned}
Z_j^T W_1^j \Delta y^{j-1} - Z_j^T \Delta y_1^j + Z_j^T c_j &= 0, \\
H_j \Delta y_1^j + h_j &= 0.
\end{aligned}
$$

This system replaces the usual continuity conditions at each node. Transforming the state variables such that

$$
\Delta y_1^j = Y_j \boldsymbol{d}_Y^j + Z_j \boldsymbol{d}_Z^j
$$

yields partial solution,

$$
\boldsymbol{d}_Y^j = -L_j^{-1} h_j,
$$

and one obtains the projected continuity conditions

$$Z_j^T W_1^j Z_{j-1} \boldsymbol{d}_Z^{j-1} - \boldsymbol{d}_Z^j = -Z_j^T c_j + Z_j^T W_1^j Y_{j-1} L_{j-1}^{-1} h_{j-1}.$$

Since in this way some of the variables are eliminated from the system a priori, the condition number for the system of invariants and projected continuity conditions may be expected to be better than the original one, which is investigated in the next section and confirmed by the numerical applications.

Applying the convergence theory in [10] it can be shown that the iterative scheme is linearly convergent with a convergence rate $\kappa = \mathcal{O}(\text{local discretization error})$.

Remark. Ascher and Petzold [4] suggest a related approach based on a projected collocation method for two-point BVP for DAE of higher index, which is not derived from the multistage optimization principle. A generalization to parameter identification problems is not considered.

5.2. The influence of invariant projection on the matrix conditioning. In the case of differential equations with rapidly decreasing and increasing components but poor dichotomy properties, extremely ill-conditioned boundary value problems may arise. This situation must be expected, e.g., in practical applications of optimal control, where the canonical system of state and adjoint equations (13,15) exhibits strongly increasing and decreasing components. Dichotomy, however, does often not exist since the control is determined by the algebraic equations $(16, 16')$ or, in the singular control case, by (18), and thus introduces a strong coupling between states and adjoints (see, e.g., [32]). For investigations of the relation of dichotomy properties and the conditioning of boundary value problems we refer to [22] in the ODE case and to [28] in the DAE case. Here we are concerned with the conditioning of the discrete boundary value problem, i.e., the conditioning of the shooting matrix.

In the following we consider a model problem with an order k invariant $h^k(t, y(t))$ according to definition 1, which leads to a hierarchy of order l invariants $h^l(t, y(t)) = (d/dt)^{k-l} h^k(t, y(t))$, $l \in \{0, \ldots, k\}$. The combined invariant $h = (h^0, \ldots, h^k) = 0$ is assumed to be nondegenerate (i.e., $\partial h(t, y)/\partial y$ has full rank) in a neighborhood of the solution trajectory; we enforce it by an initial condition

$$h(t_0, y(t_0)) = 0. \tag{25}$$

We further assume multipoint boundary conditions which together with (25) and the multiple shooting continuity conditions have a non-singular Jacobian in a neighborhood of the solution (which is therefore unique). Now we compare the conditioning of the Jacobian for a multiple shooting system using continuity conditions for all state variables to that of a system which enforces the BVP invariant $h = 0$ by projection at all nodes as proposed in the multistage approach above. For the sake of brevity we restrict the analysis to ODE with a hierarchy of invariants. Choosing the shooting mesh according to (19), with discretization variables $y^1, \ldots, y^m$, this yields the shooting system (20,21) augmented by (25), i.e., $h(\tau_1, y^1) = 0$ in the discrete variables. This explicit initial condition for invariants (25) is just a means to simplify the presentation here. In the general case boundary conditions (21) implicitly include conditions on the invariants.

In the following we will use the orthogonal splitting into "vertical" subspaces $\mathrm{im}(Y_j)$ and "horizontal" subspaces $\mathrm{im}(Z_j) = \ker(H_j)$ to examine the influence of invariant projection on the shooting matrix

$$\bar{A} := \begin{pmatrix} H_1 & 0 & \dots & 0 & 0 \\ B_1 & B_2 & \dots & B_{m-1} & B_m \\ G_1 & -I & & & \\ & G_2 & -I & & \\ & & \ddots & \ddots & \\ & & & G_{m-1} & -I \end{pmatrix}.$$

Here $G_j := W^{j+1}(\tau_{j+1}, \tau_j) \equiv W_1^{j+1}(\tau_{j+1}, \tau_j)$ (cf. Lemma 2) are the ODE Wronskian matrices and $B_j := \partial r_2 / \partial y^j$ are the derivatives of boundary conditions r_2. By multiplication with $\operatorname{diag}(Q_1, I, \dots, I)$ from the right we obtain the orthogonally transformed matrix

$$A := \begin{pmatrix} L_1 & 0 & 0 & \dots & 0 & 0 \\ B_1^Y & B_1^Z & B_2 & \dots & B_{m-1} & B_m \\ G_1^Y & G_1^Z & -I & & & \\ & & G_2 & -I & & \\ & & & \ddots & \ddots & \\ & & & & G_{m-1} & -I \end{pmatrix},$$

which has the same condition as $\bar{A}$. Now define matrices

$$\begin{aligned} \tilde{H}_1 &:= (L_1\ 0), & H &:= \operatorname{diag}(\tilde{H}_1, H_2, \dots, H_m) = LY^T, \\ & & L &:= \operatorname{diag}(L_1, L_2, \dots, L_m), \\ \tilde{Y}_1 &:= (I\ 0), & Y &:= \operatorname{diag}(\tilde{Y}_1, Y_1, \dots, Y_m), \\ \tilde{Z}_1 &:= (0\ I), & Z &:= \operatorname{diag}(\tilde{Z}_1, Z_2, \dots, Z_m). \end{aligned}$$

The following lemma shows that $Y^T A Z = 0$, so that the orthogonally transformed shooting matrix $(Y\ Z)^T A (Y\ Z)$ has the decoupled form

$$\left(\begin{array}{cccc|cccc} L_1 & & & & & & & \\ G_1^{YY} & -I & & & & & & \\ & \ddots & \ddots & & & & & \\ & & G_{m-1}^{YY} & -I & & & & \\ \hline B_1^Y & \dots & B_{m-1}^Y & B_m^Y & B_1^Z & \dots & B_{m-1}^Z & B_m^Z \\ G_1^{ZY} & & & & G_1^{ZZ} & -I & & \\ & \ddots & & & & \ddots & \ddots & \\ & & G_{m-1}^{ZY} & & & & G_{m-1}^{ZZ} & -I \end{array}\right), \qquad \begin{aligned} B_j^Y &:= B_j Y_j, \\ B_j^Z &:= B_j Z_j, \\ G_j^{YY} &:= Y_{j+1}^T G_j Y_j \\ &= L_{j+1}^{-1} L_j, \\ G_j^{ZY} &:= Z_{j+1}^T G_j Y_j, \\ G_j^{ZZ} &:= Z_{j+1}^T G_j Z_j, \end{aligned}$$

LEMMA 4. *Consider the linearized MPBVP along a solution trajectory. Then the horizontal space* $\ker(H) = \operatorname{im}(Z)$ *is an invariant subspace of* A, *i.e.,* $\operatorname{im}(AZ) \subset \operatorname{im}(Z)$.

Proof. A direct, block-wise calculation of AZ shows that the assertion follows from $\operatorname{im}(G_j Z_j) \subset \operatorname{im}(Z_{j+1}) = \ker(H_{j+1})$ for $j \in \{1, \dots, m-1\}$. We consider a single interval $I_j = [\tau_j, \tau_{j+1}]$ and proceed by induction over the order of the invariant.

(a) Consider an IVP invariant h^0 of order zero, satisfying

$$0 \equiv h(t, y(t; \tau_j, y^j); \tau_j, y^j) := h^0(t, y(t; \tau_j, y^j)) - h^0(\tau_j, y^j)$$

along the DAE solution $y(t;\tau_j,y^j)$. Since $y(\tau_{j+1};\tau_j,y^j)=y^{j+1}$, we have from theorem 1

$$0 \equiv h_y^0(\tau_{j+1},y^{j+1})G_j - h_y^0(\tau_j,y^j) = H_{j+1}^0 G_j - H_j^0.$$

This yields $H_{j+1}^0 G_j Z_j = H_j^0 Z_j = 0$, and hence $\mathrm{im}(G_j Z_j) \subset \ker(H_{j+1}^0)$.

(b) Now consider a hierarchy of invariants $h^0,\ldots,h^k$ of respective orders $0,\ldots,k$, satisfying

$$0 \equiv h^k(t,y(t;\tau_j,y^j)) - h^k(\tau_j,y^j) - \sum_{l=1}^{k-1} \beta^l(t-\tau_j)h^l(\tau_j,y^j)$$

with suitable functions β^l. Denoting $H_j^l := h_y^l(\tau_j,y^j)$, $H_j = h_y(\tau_j,y^j)$ is composed row-wise from blocks $\{H_j^l\}_{l=0}^k$. Theorem 1 yields

$$0 \equiv H_{j+1}^k G_j - H_j^k - \sum_{l=1}^{k-1} \beta^l(\tau_{j+1}-\tau_j)H_j^l.$$

Since $\ker(H_j) = \bigcap_{l=0}^k \ker(H_j^l)$, one obtains $H_{j+1}^k G_j Z_j = H_j^k Z_j + \sum \beta^l H_j^l Z_j = 0$ and hence $\mathrm{im}(G_j Z_j) \subset \ker(H_{j+1}^k)$. By induction, we also have $\mathrm{im}(G_j Z_j) \subset \ker(H_{j+1}^l)$ for all $l<k$. Thus, $\mathrm{im}(G_j Z_j) \subset \ker(H_{j+1}) = \mathrm{im}(Z_{j+1})$, which concludes the proof. □

Ill-conditioning of the multiple shooting type matrix $A^{YY} := Y^T A Y$ is a possible reason for numerical instabilities in the solution of the full system. It is well-known that the propagated error does not grow if A^{YY} can be interpreted as a discretization of differential equations with decreasing components, or, in other words, that the matrix products $G_j^{YY}\ldots G_1^{YY} = L_{j+1}^{-1}L_1$ do not grow with j. One way of ensuring this is to use Baumgarte stabilization. More generally, the subsystem can also be stably solved if the differential equations exhibit dichotomy and the invariant is enforced by an appropriate boundary condition instead of the initial condition.

In the critical cases considered in this paper it is not very likely that such dichotomy properties exist and that appropriate boundary conditions are specified. Rather, one would even expect the invariant conditions to be imposed on the initial values (or, e.g., on entry points of singular arcs) in order to reduce the degrees of freedom as described in [11]. However, invariant projection according to the multistage least squares approach (cf. (23,24), with $y^j \equiv y_1^j$) means replacing A^{YY} by the equivalent block-diagonal system

$$L = \begin{pmatrix} L_1 & & \\ & \ddots & \\ & & L_m \end{pmatrix}.$$

This system decouples the determination of the vertical components at different multiple shooting nodes and thus eliminates error propagation due to the continuity conditions. Of course, the expected improvement in the conditioning of the subsytem depends on the well-conditioning of the matrices H_j or L_j, respectively, i.e., a proper formulation of the invariants. The following theorem shows that the remaining system $A^{ZZ} = Z^T A Z$, which operates only on the invariant subspace, has indeed a reduced condition number as compared to the full original system A. Numerical evidence given in the applications below strongly supports this theoretical result.

THEOREM 2. *Consider the linearized MPBVP along a solution trajectory. Then* $\mathrm{cond}_2(Z^T A Z) \le \mathrm{cond}_2(A)$.

Proof. According to lemma 4, the solution property of the trajectory implies that the horizontal space $\ker(H) = \operatorname{im}(Z)$ is an invariant subspace of A. Lemma 5 will show that projection onto an invariant subspace reduces the condition number of a matrix, which concludes the proof of the theorem. $\square$

Remark. Note that the non-singularity of the original shooting matrix $\bar{A}$ and of the block-diagonal matrix L imply the equivalence of the original BVP formulation with the formulation modified by the invariant projection. (This equivalence is taken for granted throughout this paper.) Both formulations have locally unique solutions, and these are identical since the solution of the original BVP satisfies the invariants.

LEMMA 5. *Consider the linear equations*

$$Ax = a \quad in\ \mathbb{R}^n \qquad and \qquad Z^T AZz = Z^T a \quad in\ \mathbb{R}^k, \quad 0 < k \le n,$$

where A is non-singular and Z is an isometry of $\mathbb{R}^k$ with an invariant subspace of A. Then

$$\operatorname{cond}_2(Z^T AZ) \le \operatorname{cond}_2(A).$$

Proof. Since Z is isometric we have $Z^T Z = \mathrm{id}$, and ZZ^T is the orthogonal projection onto $\operatorname{im}(Z)$. Therefore the invariant subspace property $\operatorname{im}(AZ) \subset \operatorname{im}(Z)$ implies $(Z^T AZ)^T (Z^T AZ) = Z^T A^T (ZZ^T) AZ = Z^T (A^T A) Z = (AZ)^T (AZ) > 0$. Hence it suffices to prove the assertion for the symmetric, positive definite matrix $S = A^T A$, since

$$\operatorname{cond}_2(A) = \frac{\sigma_{\max}(A)}{\sigma_{\min}(A)} = \sqrt{\frac{\lambda_{\max}(S)}{\lambda_{\min}(S)}} = \sqrt{\operatorname{cond}_2(S)}.$$

(Here $\sigma_{\max} > \sigma_{\min} > 0$ and $\lambda_{\max} > \lambda_{\min} > 0$ are the maximal and minimal singular values and eigenvalues, respectively.) Now denote by $S(k)$, $S(n)$, $S^*(k) \subset S(n)$ the unit spheres in $\mathbb{R}^k$, $\mathbb{R}^n$, and in the k-dimensional subspace $\operatorname{im}(Z) \subset \mathbb{R}^n$, respectively. Then we have

$$\lambda_{\max}(S) = \max_{x \in S(n)} x^T Sx \ge \max_{x = Zz \in S^*(k)} x^T Sx = \max_{z \in S(k)} z^T Z^T SZz = \lambda_{\max}(Z^T SZ),$$

and similarly $\lambda_{\min}(S) \le \lambda_{\min}(Z^T SZ)$. $\square$

5.3. Reducing the number of directional derivatives in multiple shooting. The presence of invariants indicates that the number of variables, and hence free initial values, in a DAE system is larger than the actual degrees of freedom. This is obviously true for mechanical systems in descriptor form, but also holds for optimal control problems. Therefore, the question arises whether invariants can be used to reduce the computational work for derivative generation.

It was already shown in [33,10] that any multipoint boundary condition (including BVP invariants such as velocity and position constraints at the initial point) may be used to reduce the number of necessary directional derivatives to the number of degrees of freedom.

This situation is basically unchanged if BVP invariants are replacing the continuity conditions at interior shooting nodes. The computation of the subspaces, however, is now based on the invariants rather than the continuity conditions. In brief, neglecting additional multipoint conditions, one directly computes the projected matrix and vector

$$Z_j^T W_1^j Z_{j-1}, \qquad Z_j^T W_1^j Y_{j-1} L_{j-1}^{-1} h_{j-1},$$

i.e., the directional derivatives of

$$Z_j^T y_1^\pi(\tau_j; y^{j-1})$$

with respect to the subspace spanned by the vector $Y_{j-1}L_{j-1}^{-1}h_{j-1}$ and the columns of Z_{j-1}. When the number n of variables is large as compared to the actual degrees of freedom, k, very substantial reductions in the computational cost are achieved. For industrial robots, e.g., with only one degree of freedom per joint the number of state variables may be up to six times the number of degrees of freedom. Effective implementations to realize these savings are by means of variational or adjoint discretization schemes as described in [10], or analogously the forward or reverse mode in automatic differentiation [19].

Two fundamental results may be recalled and summarized, which can be found in [33,11,10] and are easily proved.

a) In a multibody system in descriptor form, the invariants on velocity and position constraints reduce the degrees of freedom in the system to two times the number of kinematic degrees of freedom, plus the degrees of freedom resulting from unknown parameters (e.g., in parameter estimation). This result holds with and without BVP invariant projection, and with or without relaxed formulation of the invariants.

b) In an optimal control problem as described in section 2, the maximum number of degrees of freedom in the associated multipoint BVP that comprises the necessary conditions is always equal to the degrees of freedom present in the state variables and free system parameters. This complexity result holds basically independent of the formulation of the associated multipoint BVP chosen from the many possible.

6. Numerical applications. The algorithmic features above were implemented in the multiple shooting code PARFIT [9] and the collocation code COLFIT [34]. The effectivity of the enhanced software packages is demonstrated in the following numerical applications. All numerical computations were performed in double precision IEEE arithmetic on a workstation.

6.1. Parameter identification for the slider crank mechanism. The planar slider crank mechanism is a simple model for a cylinder system in an engine. This mechanism is widely used as a test example for numerical integrators of initial value problems in multibody dynamics since it has strong "drift properties" [2]. Here it is used to demonstrate the effectivity of our approach for parameter estimation in mechanical systems in descriptor form.

The dynamical system is modeled in descriptor form as a DAE of index 3 according to [1]. The parameterization chosen here is indicated in Figure 1.

It coincides with the coordinate choice III in [1]. Differential variables are the positions of the points $Q = (p_1, p_2)$ and $P = (p_3, 0)$. The geometric constraints for these coordinates are

$$0 = g(p) := \begin{pmatrix} r^2 - p_1^2 - p_2^2 \\ l^2 - (p_3 - p_1)^2 - p_2^2 \end{pmatrix} \qquad \begin{array}{l} \text{(radius of the crank)} \\ \text{(length of the connecting rod)} \end{array}$$

Therefore the whole system possesses one degree of freedom only. The geometric constraints are differentiated two times in order to reduce the index to 1. The differential part of the system is then given by

$$M\ddot{p} = \begin{pmatrix} c_1 & 0 & c_2 \\ 0 & c_1 & 0 \\ c_2 & 0 & c_3 \end{pmatrix} \ddot{p} = \frac{n_1}{r^2} \begin{pmatrix} -p_2 \\ p_1 \\ 0 \end{pmatrix} - \begin{pmatrix} 0 \\ m\gamma(l - l_1)/l \\ 0 \end{pmatrix} - G(p)^T \lambda$$

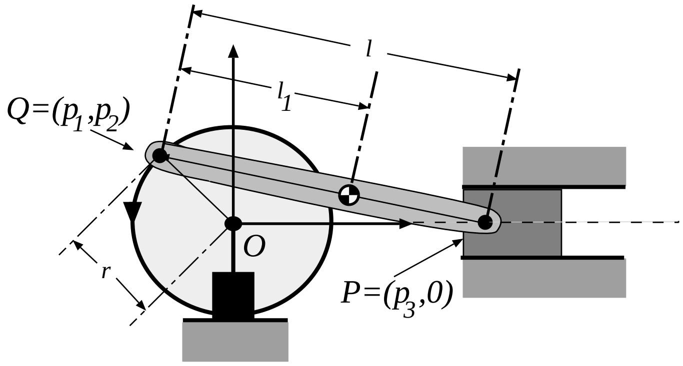


FIG. 1. *Planar Model of a Slider-Crank Mechanism*

where

$$c_1 := \frac{J_1}{r^2} + \frac{m(l-l_1)^2 + J_2}{l^2}, \quad c_2 := \frac{m(l-l_1)l_1 + J_2}{l^2}, \quad c_3 := \frac{ml_1^2 + J_2}{l^2}$$

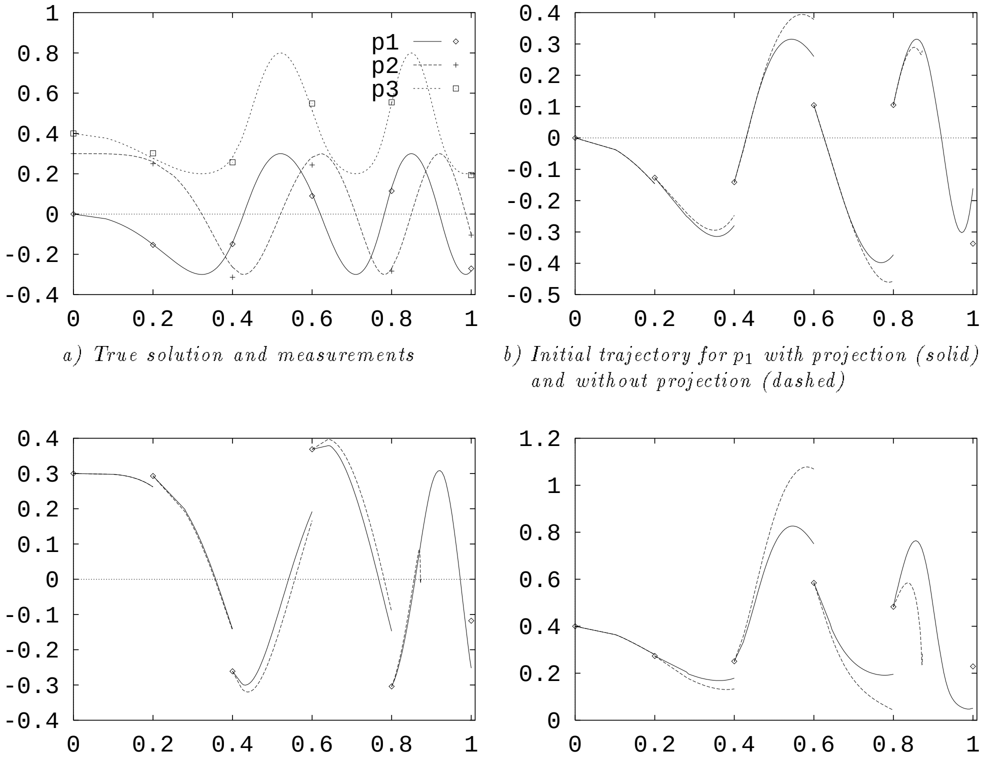
Here M is the mass matrix (which is independent of p_i), and $G(p)$ is the constraint matrix, i.e., the derivative of $g(p)$. The parameters $\gamma, n_1, l, l_1, r, J_1, J_2$ denote the gravity constant, the force which rotates the crank about the origin O, the lengths and the radius as shown in Figure 1, and the inertias of the crank and the connecting rod, respectively. The parameter m defines the mass of the connecting rod, which is to be estimated in this application. The values chosen for these parameters are $m = 1.0$, $\gamma = 13.75$, $n_1 = 1.0$, $l = 0.5$, $l_1 = 0.25$, $r = 0.3$, $J_1 = 1.0$,$J_2 = 1.0$. For further details of the model see [1].

The differential equations above together with the index 1 conditions are used as the model equations describing the dynamics of the system. The functions g and $\dot{g}$ are used both as boundary value problem invariants, and (in relaxed formulation, see equation (9)) as invariants of the local initial value problems.

The task considered here is to identify the mass m from given measurements of the state (p_1, p_2, p_3) at times $t_i = 0, 1, \ldots, 5$. A highly exact trajectory is produced using a special purpose ADAMS-method with high integration accuracy (cf. [12]). These data are then perturbed by Gaussian noise with a standard deviation of $\sigma = 10\%$ in order to produce artificial measurements. The first plot (a) in Figure 2 shows the measurements and the exact trajectories. The parameter m is initially guessed with the value $m^0 = 0.5$, which intentionally does not coincide with the true value $m = 1$.

In order to investigate the usefulness of the exploitation of invariants, two different versions of the multiple shooting code PARFIT [9] are applied. To the knowledge of the authors no other multiple shooting code is available, which is capable of treating parameter identification problems in DAE and could serve as another candidate for comparison. Both versions of PARFIT—referred to as version 1 and version 2 in the sequel—use an extrapolation method based on the midpoint rule for the solution of local initial value problems. This integrator is equipped with the internal numerical differentiation technique as discussed in section 3.3. PARFIT version 2 additionally exploits the arising IVP and BVP invariants for the position and the velocity level, as discussed in section 3. The integration tolerance used in either case is 10^{-5}. The Gauß-Newton iteration is stopped when a scaled norm of the Gauß-Newton increment drops below 10^{-3}.

Plots (b–d) in Figure 2 compare the initial trajectory of PARFIT version 1 (solid



a) True solution and measurements

b) Initial trajectory for p_1 with projection (solid) and without projection (dashed)

c) Initial trajectory for p_2 with projection (solid) and without projection (dashed)

d) Initial trajectory for p_3 with projection (solid) and without projection (dashed)

FIG. 2. *Measurements and initial trajectories*

TABLE 1
Comparison of minimal and maximal singular values $\sigma_{\min}, \sigma_{\max}$, and the resulting condition number $\text{cond} = \sigma_{\max}/\sigma_{\min}$.

PARFIT	$\sigma_{\min}$	$\sigma_{\max}$	cond
version 1	$7.92 \cdot 10^{-2}$	$1.71 \cdot 10^{3}$	$2.16 \cdot 10^{4}$
version 2	1.27	$1.03 \cdot 10^{2}$	$8.15 \cdot 10^{1}$

line) and PARFIT version 2 (dashed line), where the integration in each multiple shooting interval is started at the artificial measurements.

Due to the noise of the initial guess the starting values for each multiple shooting interval do not satisfy the higher index constraints on position and velocity level. Without exploitation of the invariants this results in a strong drift behavior, which version 1 of PARFIT cannot cope with. The last multiple shooting interval cannot be integrated completely, and the Gauß-Newton iteration cannot be started. Version 2 of PARFIT is able to use the measurements as initial values, it converges safely after 12 iterations. The final parameter estimate is $m = 0.9765$.

In a second experiment we use as measurement data the exact data, produced as described above, without any perturbation. Again we use $m^0 = 0.5$ as initial guess for the parameter. In this case the exact parameter can be identified after 17 iterations using version 1 of PARFIT, and after 7 iterations using version 2 of PARFIT. Here the expected improvement in the condition number of the multiple shooting matrix can be observed. In order to investigate the stabilizing effect of the projection onto invariants, we compare the condition numbers of the submatrix corresponding to the continuity conditions resp. projected continuity conditions for the two versions of PARFIT. The submatrix of linearized boundary and least-squares conditions, which is not modified by the projection, is not considered. For test purposes the condition number is computed by a singular value decomposition at the solution of the parameter identification problem (for both versions of PARFIT). Table 1 lists the computed results.

6.2. Periodic optimal cruise of a motor glider aircraft. In the following we will apply the proposed techniques to a challenging optimal control problem, the periodic cruise of a motor glider aircraft with high aerodynamic efficiency $(C_L/C_D)_{\max}$. This problem is characterized by highly nonlinear system dynamics with rapidly increasing and rapidly decreasing components. Hence, extremely large error propagation of initial value perturbations occurs, which result in a very small convergence domain for the multiple shooting algorithm. Additionally, ill-conditioned multi-point boundary conditions drastically decrease the accuracy of the Newton increments (cf. [32]).

The goal of optimization is to minimize the fuel consumption $m_f(x_{\mathrm{cyc}})$ over the (horizontal) length x_{cyc} of a period,

$$\frac{m_f(x_{\mathrm{cyc}})}{x_{\mathrm{cyc}}} = \min .$$

The dynamic equations for altitude h, flight path angle γ, speed V, and fuel consumption m_f are given by the ordinary differential equations

$$\begin{aligned} \frac{dh}{dx} &= \tan\gamma, & \frac{dV}{dx} &= \frac{T - D - mg\sin\gamma}{mV\cos\gamma}, \\ \frac{d\gamma}{dx} &= \frac{L - mg\cos\gamma}{mV^2\cos\gamma}, & \frac{dm_f}{dx} &= \frac{\dot{m}_f}{V\cos\gamma}, \end{aligned}$$

where x is the horizontal range. Lift and drag forces are modeled as

$$L = \frac{1}{2}\rho S V^2 C_L, \qquad D = \frac{1}{2}\rho S V^2 C_D,$$

where ρ is the air density, S is the wing area, and

$$C_D = C_{D_0} + K C_L^2 .$$

Fuel consumption characteristics are described by

$$\dot{m}_f = \sigma(V) T(h, V, \delta),$$

where the thrust model accounts for the effects of altitude, speed and throttle setting,

$$T(h, V, \delta) = T_{\max}(h, V)\delta .$$

The atmospheric model which describes air density and thrust dependence on altitude agrees with the ICAO Standard Atmosphere.

We neglect the loss of mass due to fuel consumption during one period, hence the total mass m of the aircraft is considered constant. The initial condition for the fuel consumed is

$$m_f(0) = 0;$$

periodicity conditions for the remaining state variables are

$$h(x_{\text{cyc}}) = h(0), \qquad \gamma(x_{\text{cyc}}) = \gamma(0), \qquad V(x_{\text{cyc}}) = V(0).$$

Control variables are the lift coefficient C_L and the throttle setting δ which are subject to box constraints

$$C_{L_{\min}} \le C_L \le C_{L_{\max}}, \qquad 0 \le \delta \le 1.$$

It can be seen that the Hamiltonian is regular with respect to the lift coefficient, whereas it is singular of order 1 with respect to the throttle setting. The solution trajectories exhibit two very short singular arcs which are located around the lower and upper turning points, and rather long climbing and gliding phases which are traversed at full thrust, $\delta \equiv 1$, and with the motor switched off, $\delta \equiv 0$, respectively.

In [31] flight mechanics aspects of the problem are studied and numerical solutions with a singular control for the throttle setting are presented. Investigations in [32] show that a numerical solution of the problem becomes extremely hard with decreasing wing loading and with increasing aerodynamic efficiency. By an improved algorithmic treatment with PARFIT and reformulation of the BVP results were obtained in [32] for motor gliders with aerodynamic efficiencies up to $(C_L/C_D)_{\max} = 33$. In addition to this, a singular feedback control based on Baumgarte's approach was applied in [30] in order to stabilize the system on the singular arcs, and compute numerical results for aerodynamic efficiencies up to $(C_L/C_D)_{\max} = 40$. The algorithmic developments of the present paper allow aerodynamic efficiencies beyond $(C_L/C_D)_{\max} = 60$, thus demonstrating the efficacy of the exploitation of invariants for this practical example.

Although the motor glider dynamics are given by an ODE rather than a higher index DAE, the autonomous nature of the optimal control problem and the presence of singular arcs offer exploitation of several invariants according to the theoretical results in section 2.

(a) During bang-bang phases ($\delta \equiv 0$ or $\delta \equiv 1$), the Hamiltonian is an IVP invariant on each shooting interval and may be used for projection when solving the IVP on that subinterval.

(b) During a singular phase $[t_a, t_b]$ two invariants derived from the switching function may be used for projection, e.g.,

$$\text{(b1)} \qquad S^0(\lambda, y) - S^0_0 - (t - t_a)S^1_0 \equiv 0,$$
$$\text{(b2)} \qquad S^1(\lambda, y) - S^1_0 \equiv 0,$$

where $S^i_0 = S^i(\lambda(t_a), y(t_a))$ are the initial values on entry to the singular arc. Alternatively, the damped version ($\alpha > 0$) as described in section 2 may be applied (non-stiff Baumgarte). The Hamiltonian need not be constant along $[t_a, t_b]$ as long as S^0_0, S^1_0 are inconsistent.

(c) Furthermore, the Hamiltonian is a BVP invariant. Hence, at the solution its level must coincide at each node with some (unknown) value $\bar{H}$, which may be introduced into the BVP as a system parameter. Additional but not independent BVP invariants are given on the singular arcs by S^0, S^1, both of which must vanish along the exact solution.

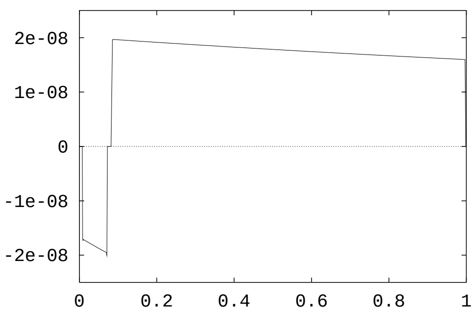


FIG. 3. *Switching function* S.

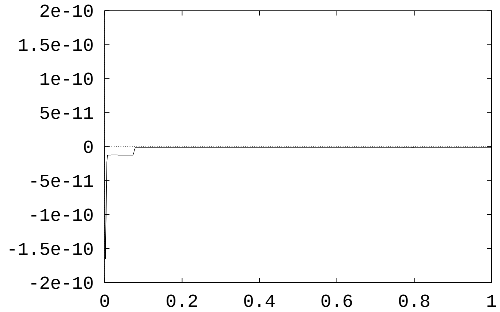


FIG. 4. *Deviation of Hamiltonian*, ΔH.

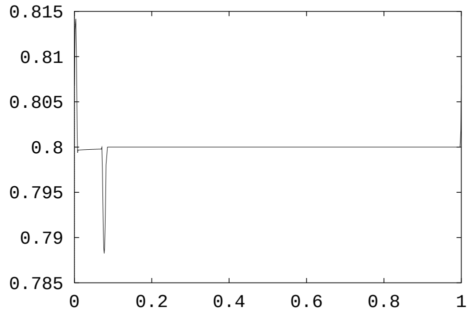


FIG. 5. *Lift coefficient* C_L.

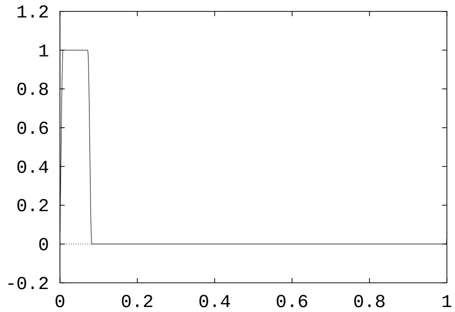


FIG. 6. *Throttle setting* δ.

Numerical computations were performed with the enhanced version of PARFIT that incorporates the algorithmic developments due to this paper. The following two simple measures proved to be sufficient to stabilize the numerical computation for aerodynamic efficiency values up to $(C_L/C_D)_{\max} = 60$ (which is already far beyond today's technical standards). On bang-bang arcs, projection onto the constant Hamiltonian was applied during integration and internal differentiation (i.e., exploitation of IVP invariants). On singular arcs, only replacement of continuity conditions by requiring $S^0 = 0$ at each multiple shooting node in the interior of the singular arcs was applied (i.e., exploitation of BVP invariants).

Some characteristic quantities of the solution at $(C_L/C_D)_{\max} = 1/0.0165$ are illustrated in Figs. (3–6), namely the histories of the switching function, of the deviation ΔH of the Hamiltonian from its initial level, and of the control functions C_L and δ. The range is normalized to $x_{\mathrm{cyc}} = 1$ in all the figures.

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