Regularization Methods for Constrained Mechanical Multibody Systems*

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Abstract

The equations of motion of multibody systems with holonomic constraints are of index 3 and therefore not directly solvable by standard ODE or DAE methods. Until now, a number of regularization methods have been proposed to treat these systems [1, 18, 15, 13], but as they are based on different points of view they have never been compared with respect to their physical properties, invariance under diffeormorphisms, and convergence behaviour.

In this paper we show that these methods are closely related. Especially, the approach in [1] can be seen to be identical with the linearized form of [15, 13], which are almost identical. These methods are invariant under coordinate transformations, but this is not the case for [16, 17]. The methods [1, 17] can be easily extended to the slightly more general case of index 3 systems in Hessenberg form. Convergence properties of the methods are discussed in the framework of singular perturbation theory.

Zusammenfassung. Die Bewegungsgleichugen holonomer Starrkörpersysteme besitzen den Index 3 und sind infolgedessen nicht mit Standardverfahren für gewöhnliche Differentialgleichungen oder Algebro-Differentialgleichungen lösbar. Gegenwärtig sind eine Reihe von Regularisierungsmethoden vorgeschlagen worden, diese Systeme zu approximieren [1, 18, 15, 13]. Da die Methoden von unterschiedlichsten Standpunkten aus vorgeschlagen wurden, gibt es bisher noch keinen Versuch, sie hinsichtlich ihrer physikalischen Eigenschaften, möglicher Invarianz unter Diffeomorphismen und Konvergenzverhalten zu vergleichen.

Im vorliegenden Artikel wird gezeigt, daß diese Methoden eng verbunden sind. Insbesondere erweist sich der Zugang in [1] als identisch mit den Linearisierungen

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der Vorschlägen in [15, 13], die wiederum fast identisch sind. Diese Methoden sind invariant unter Koordinatentransformationen, während dies für [16, 17] nicht gilt. Die Methoden können leicht auf den allgemeineren Fall von Index-3-Systemen in Hessenberg-Form erweitert werden. Konvergenzeigenschaften der Methoden werden im Rahmen der Theorie singulärer Störungen gezeigt.

Keywords. Regularization methods, constraint mechanical multibody systems, stabilization of constraints, singular perturbations, extrapolation methods

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1 Introduction

In this paper the equations of motion of mechanical systems modelled by multibody systems are considered. These are systems of rigid or elastic bodies connected by force elements such as springs and dampers or joints. As the former lead to known forces, the latter result in algebraic constraint equations and lead to unknown constraint forces.

Since during the last decade the need for automatic multibody simulators in industry (simulation of robots, vehicles, mechanisms) increased, much interest has been spent in the numerical treatment of differential-algebraic equations describing the motion:

$$M(q)\ddot{q} = F(q,\dot{q},t) + G^T(q)\lambda \tag{1.1a}$$

$$0 = g(q) \tag{1.1b}$$

with the symmetric positive-definite mass matrix M, the generalized coordinates q, the generalized velocities $\dot{q}$, the forces F (applied forces as well as Coriolis, centrifugal and gravitational forces). g are holonomic constraints[1], the constraint matrix $G = \frac{\partial g}{\partial q}$ is supposed to have full rank. The term $G^T\lambda$ is the constraint force, λ the Lagrange multiplier.

Differentiation of the constraints on position level leads to the constraints on velocity level

$$\dot{g} = 0 = G(q)\dot{q}, \tag{1.2}$$

and the constraints on acceleration level

$$\ddot{g} = 0 = G(q)\ddot{q} + G_q(q)(\dot{q},\dot{q}), \tag{1.3}$$

where the subscript is used to indicate a partial derivative.
Solving (1.1a) for $\ddot{q}$, substituting this in (1.3), the resulting equation can be solved for λ because M is symmetric and positive-definite and G has full rank[2]:

$$\lambda = -(GM^{-1}G^T)^{-1}(GM^{-1}F + G_q(\dot{q},\dot{q})). \tag{1.4}$$

Substituting λ into (1.1a) results in

$$M(q)\ddot{q} = (I - G^T(GM^{-1}G^T)^{-1}GM^{-1})F - G^T(GM^{-1}G^T)^{-1}G_q(\dot{q},\dot{q}). \tag{1.5}$$

[1] The methods can be easily extended to the case of nonholonomic constraints.

[2] Arguments dropped for ease of notation.

As in [6], we will call this equation the underlying ODE of the system[3].

Since three differentiation steps are necessary to obtain a differential equation for λ, the index of (1.1) is three.

Higher index systems, i.e. equations with an index greater than or equal to 2, are known to include differentiation problems: The solution of an index k system depends on derivatives of the right-hand side up to order $k-1$. This leads to the definition of the perturbation index in [10]. This index definition is based on analyzing the dependence of the solution on perturbations of the right-hand side of the DAE. Roughly speaking, the system has index k if its solution depends on derivatives of the perturbation up to order $k-1$. Perturbations occur during the numerical integration e.g. from discretization, truncation and roundoff errors. This is the reason why the numerical treatment of higher index systems causes numerical difficulties when treated by standard ODE methods.

Therefore some sort of index reduction process is advisable. After an index reduction by differentiation of constraints as shown above, the index-reduced systems (1.1a), (1.3) or (1.5) can be numerically integrated by well-known numerical methods (e.g. BDF, Runge-Kutta or extrapolation methods, for an overview see [3, 9, 11]). Unfortunately, the numerical solution of the index-reduced system does not fulfil the original constraints (1.1b), (1.2) and, furthermore, because of error propagation, a drift-off from these constraints occurs.

Another difficulty with index reduction by differentiation is that the stability behaviour may completely be changed by this process. For the case of linear constant coefficient DAEs it has been shown that additional zero-eigenvalues with Jordan-blocks of order $k-1$ are introduced for index k systems, which lead to instability. An instructive example of the nonlinear case can be found in [21].

A survey of alternative approaches [8, 19, 26, 5] to treat these systems with index reduction by differentiation and using some sort of projection to fulfil the original constraints is given in [6]. In that paper a classification for projection methods into coordinate projection methods and derivative projection methods is given. Those methods are not investigated here. Further approaches can be found in [27, 7].

From an analytical point of view, higher index systems are ill-posed problems in the sense of Hadamard in some naturally given topologies [13]. The problem of solving $Tx = q, \quad T : X \to Y$ is well-posed if the existence and uniqueness of the solution are guaranteed and the solution depends continuously on the data. This last point is not fulfilled in case of higher index systems, since derivatives are involved. This observation is the basis for regularization methods [13].

Regularization methods can also be considered as another way of index reduction.

In the following section we describe various regularization methods for multibody system equations. The famous stabilization approach of Baumgarte [1], which is motivated from control theory, can be interpreted as a regularization, too. The same is true for the approach of Lötstedt [17], which is based on introducing additional springs and dampers in order to fulfil the constraints. These approaches will be extended to

[3] In various other papers the underlying ODE includes a differential equation for λ, too.

index 3 systems in Hessenberg-form:

$$
\begin{aligned}
\dot{v} &= f(u,v,w,t) && (1.6a)\\
\dot{u} &= h(u,v,t) && (1.6b)\\
0 &= g(u,t) && (1.6c)
\end{aligned}
$$

with $g_u h_v f_w$ being nonsingular in an open neighbourhood of the solution.

Two regularization methods proposed by Knorrenschild [15] and Hanke [13] are considered directly for (1.6). All these methods have many similarities, but no effort has been made to compare them with respect to physical interpretation, transformation invariances and convergence results. This will be done in this paper.

Another well-known method for parametrizing higher index systems is the *pencil regularization* [4, 2]. This method does not fit completely into the former methods since it yields ordinary differential equations immediately. Therefore, it will not be considered here, we refer to [13] for this topic. Other possibilities have recently been considered in [14].

2 Regularization Methods for Mechanical Systems

In this section various methods that can be interpreted as regularization methods are described.

Baumgarte's Approach. The oldest method that can be interpreted as a regularization was introduced by Baumgarte [1]. He introduced stabilizing control terms into the index-1-equation (1.3), i.e. he chose a linear combination of $\ddot{g}$ (1.3), $\dot{g}$ (1.2), g (1.1b) instead of (1.3):

$$\ddot{g} + 2\alpha\dot{g} + \beta^2 g = 0.$$

α and β are chosen such that $g \equiv 0$ is a stable solution of this equation: $\alpha > 0$. Often $\beta = \alpha$ is chosen, which corresponds to the aperiodic limit case. This yields

$$
\begin{aligned}
M\ddot{q} &= F + G^T\lambda && (2.1a)\\
0 &= G\ddot{q} + G_q(\dot{q},\dot{q}) + 2\alpha G\dot{q} + \beta^2 g. && (2.1b)
\end{aligned}
$$

Generalizing this method to index 3 Hessenberg systems (1.6) leads to

$$
\begin{aligned}
\dot{v} &= f(u,v,w,t) && (2.2a)\\
\dot{u} &= h(u,v,t) && (2.2b)\\
0 &= g_{uu}(h,h) + 2g_{ut}h + g_u(h_v f + h_u h + h_t) + g_{tt} + 2\alpha(g_u h + g_t) + \beta^2 g. && (2.2c)
\end{aligned}
$$

Obviously, the partial derivative of the algebraic constraint with respect to the algebraic variable w yields $g_u h_v f_w$ such that (2.2) is an index 1 system.

One difficulty with the Baumgarte approach is the choice of the parameters α, β. This question was discussed in [28], but has not been sufficiently cleared until now.

Choosing α, β too large results in stiff ODEs and a great amount of computing time. Note that these systems are not stiff in the sense that the stepsize is restricted by stability requirements, but by accuracy requirements such that stiff integrators are not the way out. The smaller the parameters become, the smaller the stabilizing effect.

Lötstedt's Approach. The next approach considered here was introduced by Lötstedt [16, 17, 18] for constrained mechanical systems and, in a more general form, in [18] for index-2-systems. He introduces additional springs and dampers in order to fulfil the algebraic constraint, which results in

$$M\ddot{q} = F - G^T(Kg + DGv). \tag{2.3}$$

The spring and damper parameters K, D are chosen such that no oscillations occur. This approach is motivated as a penalty technique applied to Hamilton's principle: Let L be the Lagrangian of the system. Hamilton's principle is the constrained optimization problem

$$\begin{aligned} \int_{t_0}^{t_1} L(q, \dot{q}, t)dt &\rightarrow \text{extremum} \\ g(q) &= 0. \end{aligned}$$

This problem is replaced by the unconstrained optimization problem with the penalty functional

$$\int_{t_0}^{t_1} (L(q, \dot{q}, t) - \frac{1}{2}\varepsilon^{-1}\kappa g(q)^2)dt,$$

which leads to the Euler-Lagrange-equations

$$M(q)\ddot{q} = F - \varepsilon^{-1}\kappa G^T g.$$

Since the damping term introduces dissipative forces, this term cannot be interpreted in the above manner.

Another interpretation of Lötstedt's approach is shortly discussed in [16] and based on Gauss' principle of least constraints.

Lötstedt's method can be regarded as a combination of Baumgarte's method with singular perturbations: In a first step, the algebraic constraint is replaced by

$$0 = \dot{g} + \kappa g \quad \Longleftrightarrow \quad 0 = G\dot{q} + \kappa g$$

such that $g \equiv 0$ is a stable solution again (i.e. $\kappa > 0$). Regularizing the resulting index 2 system as in [18] yields:

$$\varepsilon\lambda = -(G\dot{q} + \kappa g).$$

Solving this for λ and substituting into the differential equation implies

$$M\ddot{q} = F - \frac{1}{\varepsilon}G^T(G\dot{q} + \kappa g),$$

which is exactly (2.3) with $K = \varepsilon^{-1}\kappa I$ and $D = \varepsilon^{-1}I$.

Lötstedt's approach can be generalized to the case of index 3 systems in Hessenberg form:

$$
\begin{aligned}
\dot{v} &= f(u,v,w,t) && (2.4a)\\
\dot{u} &= h(u,v,t) && (2.4b)\\
\varepsilon w &= -(g_u h + g_t + \kappa g). && (2.4c)
\end{aligned}
$$

As the partial derivative of the algebraic constraint with respect to w yields εI, this is an index 1 system.

Knorrenschild's approach. A third approach was proposed by Knorrenschild [15]. As he gives regularizations reducing the index by one, one has to apply his procedure twice. Since his method is not directly proposed for mechanical systems, the starting point is an index 3 Hessenberg system. In a first step (1.6c) is replaced by

$$
0 = g(u + \varepsilon \dot{u}, t) = g(u + \varepsilon h(u,v,t), t) \tag{2.5}
$$

and, in a second step, the resulting index 2 system is parametrized in a similar manner, i.e. (2.5) is replaced by

$$
0 = g(u + \mu \dot{u} + \varepsilon h(u + \mu \dot{u}, v + \mu \dot{v}, t), t),
$$

which results in

$$
\begin{aligned}
\dot{v} &= f(u,v,w,t)\\
\dot{u} &= h(u,v,t)\\
0 &= g(u + \mu h(u,v,t) + \varepsilon h(u + \mu h(u,v,t), v + \mu f(u,v,w,t), t), t).
\end{aligned}
$$

This, again, is an index 1 system.

Applying this to constrained mechanical systems provides

$$
\begin{aligned}
M\ddot{q} &= F + G^T \lambda && (2.6a)\\
0 &= g(q + (\varepsilon + \mu)v + \mu\varepsilon M^{-1}(F + G^T\lambda)). && (2.6b)
\end{aligned}
$$

Hanke's Approach. The last approach considered here was introduced in [12, 13]. It was motivated by regularization methods (in the sense of Tikhonov) for general index 2 equations proposed in [20]. Parameters are introduced in order to arrive at an index 1 problem:

$$
\begin{aligned}
\dot{v} &= f(u,v,w,t) && (2.7a)\\
\dot{u} &= h(u, v + \mu \dot{v}, t) && (2.7b)\\
0 &= g(u + \varepsilon \dot{u}, t), && (2.7c)
\end{aligned}
$$

which leads to

$$0 = g(u + \varepsilon h(u, v + \mu f(u, v, w, t), t), t) \tag{2.8}$$

as an algebraic equation. In the original paper $\varepsilon = \mu$ was selected, but for some reasons it makes sense to choose $\varepsilon \neq \mu$ (see Section 3 below).

Applying this approach to constrained mechanical systems yields

$$\begin{aligned} \dot{q} &= v + \mu\dot{v} && \text{(2.9a)} \\ M\dot{v} &= F + G^T\lambda && \text{(2.9b)} \\ 0 &= g(q + \varepsilon v + \mu\varepsilon M^{-1}(F + G^T\lambda)). && \text{(2.9c)} \end{aligned}$$

3 Properties of Different Parametrizations Applied to Mechanical Systems

In this section, the different approaches introduced above in order to stabilize the algebraic constraints in the index reduction process are compared. It will be shown that the forces tangential to the manifold are the same, the methods differ only in orthogonal forces. The methods proposed in [15, 13] differ from [1] only in higher order terms of the parameters ε, μ. All these methods are invariant under diffeomorphisms in the coordinate space and scalings of g, this is not the case for [16, 17].

In the following the matrix product

$$P = M^{-1}G^T(GM^{-1}G^T)^{-1}G. \tag{3.1}$$

plays an important role.

Lemma 3.1 *Let P be given by (3.1). Then*

1. *$I - P$ is a projection onto the nullspace of G.*
2. *P is an orthogonal projection with respect to the scalar product*

$$< x, y >_M := x^T My.$$

3. *P is invariant with respect to smooth coordinate changes, i.e. if $T : U_{\bar{q}} \to U_q$ is a diffeomorhism and $\bar{G}(\bar{q}) = \frac{\partial}{\partial\bar{q}}g(T(\bar{q}))$, then $P = M^{-1}\bar{G}^T(\bar{G}M^{-1}\bar{G})^{-1}\bar{G}$.*
   P is also invariant under scalings of g.

The proof is obvious.

Remark 3.1 *The invariance of P with respect to coordinate changes is a remarkable property. It is well-known that the Lagrangian calculus is independent of the special choice of the generalized coordinates q. More precisely, the motion of a system is independent of diffeormorphisms of the generalized coordinates. P has this property, too, which leads to the invariance of the equations of motion described now.*

Proposition 3.1 *For the unperturbed system as well as for all parametrizations it holds that*

$$(I - M^{-1}G^T(GM^{-1}G^T)^{-1}G)\dot{v} = (I - M^{-1}G^T(GM^{-1}G^T)^{-1}G)M^{-1}f \tag{3.2}$$

or, equivalently,

$$(I - P)\dot{v} = (I - P)M^{-1}f.$$

Proof: Multiply the equation describing the dynamical behaviour by the terms in parantheses. □

Lemma 3.1 yields that $I - P$ is a projection onto the tangent space of the manifold

$$\mathcal{M} = \{q|g(q) = 0\}.$$

That means that (3.2) describes the dynamics of the system restricted to the manifold. Only those components of the forces contribute to a change of absolute value of the velocity that are parallel to the manifold. In this sense, additional accelerations perpendicular to the constraint manifold are a consequence of the curvature of this manifold. This can be seen from the next proposition:

Proposition 3.2 *For the constrained mechanical system it holds that*

$$P\ddot{q} = -M^{-1}G^T(GM^{-1}G^T)^{-1}G_q(\dot{q},\dot{q}) \tag{3.3}$$

For the parametrized systems, the analogous properties are summarized in the following proposition.

Proposition 3.3

1. *For (2.1) (Baumgarte's method), it holds that*

$$P\ddot{q} = M^{-1}G^T(GM^{-1}G^T)^{-1}G\ddot{q} = -M^{-1}G^T(GM^{-1}G^T)^{-1}(G_q(\dot{q},\dot{q}) + 2\alpha G\dot{q} + \beta^2 g) \tag{3.4}$$

2. *For (2.3) (Lötstedt's method), it holds that*

$$P\ddot{q} = \underbrace{M^{-1}G^T(GM^{-1}G^T)^{-1}G}_{P}M^{-1}F - \varepsilon^{-1}M^{-1}G^T(G\dot{q} + \kappa g)$$

3. *For (2.6) (Knorrenschild's method), it holds that*

$$P\ddot{q} = -M^{-1}G^T(GM^{-1}G^T)^{-1}\left(\frac{(\mu+\varepsilon)^2}{2\varepsilon\mu}G_q(\dot{q},\dot{q}) + \frac{\mu+\varepsilon}{\varepsilon\mu}G\dot{q} + \frac{1}{\varepsilon\mu}g\right) + \mathcal{R} \tag{3.5}$$

with

$$\mathcal{R} = \mathcal{O}\left((\mu+\varepsilon)\|\dot{q}\|\|\ddot{q}\| + \mu\varepsilon\|\ddot{q}\|^2 + \frac{(\mu+\varepsilon)^2}{\varepsilon\mu}(\|\dot{q}\|^3 + \|\ddot{q}\|^3)\right).$$

4. For (2.9) (Hanke's method), it holds that

$$P\dot{v} = -M^{-1}G^T(GM^{-1}G^T)^{-1}\left(\frac{\varepsilon}{2\mu}G_q(v,v) + \frac{1}{\mu}Gv + \frac{1}{\varepsilon\mu}g\right) + \mathcal{R} \tag{3.6}$$

with

$$\mathcal{R} = \mathcal{O}\left(\varepsilon\|v\|\|\dot{v}\| + \varepsilon\mu\|\dot{v}\|^2 + \frac{\varepsilon^2}{\mu}\|v+\varepsilon\dot{v}\|^3\right)$$

Proof: Solving the algebraic equation for λ (after the linearization of the constraints if necessary), inserting this into the differential equation and premultiplying by the projector yields the result. □

Obviously, Lötstedt's method is not independent with respect to coordinate changes as the others are.

A nice property of Baumgarte's approach is that $g = 0$ is a first integral in contrast to the others.

In the linearizations, Knorrenschild's and Hanke's method are almost identical. The close relationship between these methods and [1] can be seen by comparing (3.4) and (3.5),(3.6) respectively. They only differ by $\mathcal{R}$, which is of higher order in ε, μ if $\varepsilon = \mathcal{O}(\mu), \mu = \mathcal{O}(\varepsilon)$.

Compared with (3.3) the parameters of (3.6) should satisfy $\varepsilon = 2\mu$. Comparing (3.3) and (3.5) would lead to $(\varepsilon + \mu)^2 = 2\varepsilon\mu$, which would yield $\varepsilon = \mu = 0$. Hence, in this case, a "canonical" choice of these parameters cannot be derived.

4 Convergence properties

In this section we characterize convergence properties of the different parametrizations. For the sake of simplicity the consideration will be restricted to initial value problems in autonomous equations. In an interval $[0, T]$, consider the general index 3 problem in Hessenberg form

$$\dot{v} = f(u,v,w) \tag{4.1a}$$
$$\dot{u} = h(u,v) \tag{4.1b}$$
$$0 = g(u) \tag{4.1c}$$

with $g_u h_v f_w$ nonsingular in a neighbourhood of the solution.

Choice of the initial conditions. It is well-known that the determination of consistent initial values for (4.1) to be solvable is a severe problem. Obviously, it makes no sense to state initial values for w explicitly. Even initial values for u, v cannot be chosen freely. Instead, they must fulfil

$$0 = g(u(0)) \tag{4.2a}$$
$$0 = g_u(u(0))h(u(0), v(0)). \tag{4.2b}$$

In general, conditions can only be given for the so-called state variables (see [6] for a definition). Roughly speaking, that means to divide $(u^T, v^T)^T$ into independent and dependent coordinates, where the latter can be computed from the former by the use of (4.2) or its equivalent for arbitrary t. This statement can be formulated more precisely as follows. Let $u(t) \in I\!R^n$, $v(t) \in I\!R^k$, $w(t) \in I\!R^l$. Consider initial conditions

$$R(u(0), v(0)) = 0 \tag{4.3}$$

with

(AIC) $R : I\!R^n \times I\!R^k \to I\!R^r, \quad r = n + k - 2l,$

(4.2),(4.3) possess a solution $(u^{(0)}, v^{(0)})$ such that

$$V = \begin{pmatrix} R_{u(0)} & R_{v(0)} \\ g_u & 0 \\ g_{uu}h + g_u h_u & g_u h_v \end{pmatrix}_{|(u^{(0)}, v^{(0)})} \quad \text{is nonsingular.}$$

With these assumptions the solvability of (4.2), (4.3) in a neighbourhood of $(u^{(0)}, v^{(0)})$ can be assured by the implicit function theorem. [AIC] is in agreement with what one should expect for constrained mechanical systems: In case of linear constraints we have

$$V = \begin{pmatrix} R_{q(0)} & R_{\dot q(0)} \\ G & 0 \\ 0 & G \end{pmatrix}.$$

$V \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = 0$ leads to $Px_1 = 0$, $Px_2 = 0$ such that initial conditions can only be chosen for $(I - P)q$ and $(I - P)\dot q$, i.e. the state variables. The problem how to obtain (4.3) such that (AIC) holds will not be discussed further.

Motivation: Linear case. The parametrizations lead to stiff problems, where the stiffness is controlled by a small parameter (or two small parameters). The appropriate tool for analyzing the convergence behaviour if these parameters tend to 0 is the theory of singular perturbations [29, 22]. In order to motivate the following investigations consider the simple constant coefficient problem

$$\varepsilon \dot y = Ay + b \tag{4.4}$$

with a nonsingular square matrix A and a constant vector b. $\varepsilon \to 0$ results the reduced problem

$$0 = Ay + b$$

with the solution

$$\bar y_0 = -A^{-1} b.$$

Let Φ denote a fundamental matrix of $\dot y = Ay$. Then

$$y_\varepsilon(t) = \Phi(t/\varepsilon)c + \bar y_0$$

is the general solution of the singularly perturbed problem (4.4). $\Phi(t)$ consists of functions $p(t)e^{\lambda t}$ with polynomials p and eigenvalues λ of A. Therefore, adding initial conditions $y_\varepsilon(0) = y^0$, $y_\varepsilon(t)$ will converge towards the solution $\bar{y}_0$ of the reduced problem iff for all eigenvalues λ of A

$$\mathrm{Re}(\lambda) < 0.$$

The convergence is not regular since, depending on y^0, a short region of width $\mathcal{O}(\varepsilon)$ occurs near the initial point where $y_\varepsilon(t)$ differs significantly from $\bar{y}_0$. Such a behaviour is called a *boundary layer*.

The behaviour discussed above on a simple example carries over to more general problems. The following theorem states the situation more precisely.

Theorem 4.1 *[29] Consider the initial value problem*

$$\dot{z} = f(z, y, t, \varepsilon), \quad \varepsilon\dot{y} = g(z, y, t, \varepsilon) \tag{4.5}$$

with $z(0) = z_\varepsilon^0$, $y(0) = y_\varepsilon^0$ for $0 < \varepsilon < \varepsilon_*$.[4] *Suppose*

1. *The functions f, g are sufficiently smooth.*
2. *$f, g, y_\varepsilon^0, z_\varepsilon^0$ have asymptotic expansions with respect to ε , i.e.*

$$\begin{aligned} f(z,y,t,\varepsilon) &= \sum_{j=0}^{N} f_j(z,y,t)\varepsilon^j + \mathcal{O}(\varepsilon^{N+1}), \quad y_\varepsilon^0 = \sum_{j=0}^{N} y_j^0\varepsilon^j + \mathcal{O}(\varepsilon^{N+1}) \\ g(z,y,t,\varepsilon) &= \sum_{j=0}^{N} g_j(z,y,t)\varepsilon^j + \mathcal{O}(\varepsilon^{N+1}), \quad z_\varepsilon^0 = \sum_{j=0}^{N} z_j^0\varepsilon^j + \mathcal{O}(\varepsilon^{N+1}) \end{aligned}$$

   for some $N > 0$.
3. *The initial value problem*

$$\dot{z} = f(z, y, t, 0), \quad 0 = g(z, y, t, 0) \tag{4.6}$$

   with $z(0) = z_0^0$ has a solution $(z_0(t), y_0(t))$.
4. *$W(t) := g_y(z_0(t), y_0(t), t, 0)$ has only eigenvalues $\lambda_i(t)$ such that*

$$Re(\lambda_i(t)) \leq -\sigma < 0 \quad \forall t$$

   for some constant $\sigma > 0$.
5. *y_0^0 belongs to the domain of attraction of the attraction point $y_0(0)$ of the equation $\dot{\tilde{y}} = g(z_0^0, \tilde{y}, 0, 0)$, i.e. solving $\dot{\tilde{y}} = g(z_0^0, \tilde{y}, 0, 0)$, $\tilde{y}(0) = y_0^0$ leads to $\tilde{y}(t) \overset{t\to\infty}{\longrightarrow} y_0(0)$.*

Then, for sufficiently small $\varepsilon_* > 0$, (4.5) has exactly one solution $(z_\varepsilon, y_\varepsilon)$ in a neighbourhood of (z_0, y_0). Furthermore, the asymptotic expansions

$$z_\varepsilon(t) = \sum_{j=0}^{N}(z_j(t) + \bar{z}_j(\tau))\varepsilon^j + \mathcal{O}(\varepsilon^{N+1}), \quad y_\varepsilon(t) = \sum_{j=0}^{N}(y_j(t) + \bar{y}_j(\tau))\varepsilon^j + \mathcal{O}(\varepsilon^{N+1})$$

hold, where $\tau = t/\varepsilon$, $|\bar{z}_j(\tau)|, |\bar{y}_j(\tau)| \leq Ce^{-\rho\tau}$ with $\sigma \geq \rho > 0$ and $\bar{z}_0(\tau) \equiv 0$. Moreover, $\bar{y}_0(\tau) \equiv 0$ iff $y_0^0 = y_0(0)$.

[4]Subscripts are used to denote the regularization parameters and superscripts to denote initial values.

Convergence results, sketch of the proof. Condition 4. of the theorem implies the nonsingularity of the Jacobian g_y. Thus, (4.6) is a semi-explicit index 1 system. Therefore, a straightforward application of Theorem 4.1 to the parametrizations is not possible since the reduced system is just (4.1), which has index 3. Such a problem is called a *singular singularly perturbed problem* and causes severe difficulties [23, 30]. The way out is a transformation of the parametrizations into standard form governed by Theorem 4.1.

The necessary considerations are examplified using Hanke's parametrization. As the proofs are rather technical, we only summarize the essential steps and refer the reader to [12] for details.

1. Suppose

   (AS) (4.1), (4.2), (4.3) have a solution $(u_0(t), v_0(t), w_0(t))$.

2. (AIC) guarantees that (4.3) contains only initial conditions on the state variables. This is necessary in order to fulfil the consistency equations. In contrast, the parametrization (2.8) is an index 1 problem calling for a complete set of initial values for $u_0(0), v_0(0)$. The idea is to complete (2.7) by (4.2) and (4.3), yielding

$$u_\varepsilon(0) = u_0(0) \tag{4.7a}$$
$$v_\varepsilon(0) = v_0(0) \tag{4.7b}$$

   by (AIC). Now, $w_\varepsilon(0)$ is the solution x_ε of

$$g(u_0(0) + \varepsilon h(u_0(0), v_0(0) + \mu f(u_0(0), v_0(0), x_\varepsilon))) = 0. \tag{4.8}$$

   For simplicity, let $2\varepsilon = \mu$. This choice is not crucial as long as $0 < c_1 \leq \frac{\varepsilon}{\mu} \leq c_2$ for $\varepsilon \to 0$ with some constants c_1, c_2. Since x_ε will play the role of y_ε in (4.5), its initial value $x_\varepsilon(0)$ must have an asymptotic expansion of order N. This holds if

   (ACE) g is sufficiently smooth and

$$\begin{aligned} g_u(u_0(0)) \cdot h_v(u_0(0), v_0(0)) f(u_0(0), v_0(0), x) = \\ -g_{uu}(h(u_0(0), v_0(0)), h(u_0(0), v_0(0))) \end{aligned} \tag{4.9}$$

   has a solution x_0 sufficiently close to $w_0(0)$.

   Note that, in general, $x_0 \neq w_0(0)$, since $w_0(0)$ does not solve (ACE), but

$$\begin{aligned} g_u(u_0(0)) h_v(u_0(0), v_0(0)) f(u_0(0), v_0(0), w_0(0)) = \\ -g_{uu}(u_0(0))(h(u_0(0), v_0(0)), h(u_0(0), v_0(0))) \\ -g_u(u_0(0)) h_u(u_0(0), v_0(0) h(u_0(0), v_0(0))) \end{aligned} \tag{4.10}$$

   i.e. (4.1c) twice differentiated.

3. Now transform the system (4.1) and its parametrized form (2.8), respectively. In order to obtain an index 1 system use twofold differentiation of the constraint in (4.1). In (2.8), one differentiation of the constraint leads to

$$\varepsilon^2 \dot{w} = K(u, v, w, \varepsilon) \tag{4.11}$$

with the limit

$$K(u, v, w, 0) = -[g_u(u) h_v(u, v) f_w(u, v, w)]^{-1} g_u(u) h(u, v),$$

for $\varepsilon \to 0$, such that the formal limit of (4.11) is equivalent to the first total derivative of $g(u) = 0$. Since

$$K_w(u_0, v_0, w_0, 0) \equiv 0,$$

assumption (4.) of the theorem cannot hold. Computing $K_w(u, v, w, \varepsilon)$ one obtains

$$K_w(u, v, w, \varepsilon) = \varepsilon \tilde{K}(u, v, w, \varepsilon) \text{ iff } f_{ww}(u, v, w) \equiv 0$$

with some smooth function $\tilde{K}$. Therefore, assume

(AP) $f_{ww}(u, v, w) \equiv 0$, i.e. w appears only linearly in f.

For mechanical systems this is no restriction since w represents the Lagrange multiplier λ. Having done so, differentiate (4.11) once again and substitute $\varepsilon \dot{w} = z$. Now the relevant matrix W can be computed to be

$$\begin{pmatrix} 0 & I \\ -I & -2I \end{pmatrix}$$

having only the eigenvalue -1.

Now, by Theorem 3.1,

$$u_\varepsilon(t) = \sum_{j=0}^{N} (u_j(t) + \bar{u}_j(\tau)) \varepsilon^j + \mathcal{O}(\varepsilon^{N+1})$$

and corresponding expressions hold true for $v_\varepsilon(t)$, $w_\varepsilon(t)$, where $\tau = t/\varepsilon$, $|\bar{u}_j(\tau)|$, $|\bar{v}_j(\tau)|$, $|\bar{w}_j(\tau)| \le C e^{-\rho\tau}$, $\rho > 0$ and $\bar{v}_0 = 0, \bar{u}_0 = 0$. The coefficients u_0, v_0, w_0 are the solutions of the original index 3 problem.

For Knorrenschild's parametrization (2.5), almost identical results can be derived. Instead of (4.9) the first term x_0 of the asymptotic expansion of $w_\varepsilon(0)$ solves a slightly modified equation. Namely, having $\varepsilon = \mu$, (4.9) is replaced by

$$\begin{aligned} g_u(u_0(0) h_v(u_0(0), v_0(0)) f(u_0(0), v_0(0), x) = \\ -2 g_{uu}(u_0(0))(h(u_0(0), v_0(0), h(u_0(0), v_0(0))) \\ -g_u(u_0(0)) h_u(u_0(0), v_0(0)) h(u_0(0), v_0(0)). \end{aligned} \tag{4.12}$$

There is no choice of parameters $\varepsilon = \varepsilon(\mu)$ such that the resulting equation is identical to (4.10). An asymptotic expansion of the form (3) still holds, but with different coefficients $u_j, v_j, w_j, \bar{u}_j, \bar{v}_j, \bar{w}_j$.

In his paper [15] Knorrenschild proposes another choice of initial conditions in order to avoid the boundary layer. Assuming $u_0(0), v_0(0), w_0(0)$ to be known or easily accessible, $(u_\varepsilon(0), v_\varepsilon(0), w_\varepsilon(0))$ is determined by

$$\begin{aligned} w_\varepsilon(0) &= w_0(0) && (4.13a)\\ v_\varepsilon(0) + \varepsilon f(u_\varepsilon(0), v_\varepsilon(0), w_\varepsilon(0)) &= v_0(0) && (4.13b)\\ u_\varepsilon(0) + \varepsilon h(u_\varepsilon(0), v_\varepsilon(0)) &= u_0(0). && (4.13c) \end{aligned}$$

It is easy to see that, for sufficiently small $\varepsilon > 0$, $u_\varepsilon(0), v_\varepsilon(0)$ are uniquely determined by (4.13) and have asymptotic expansions. Theorem 4.1 implies the existence of asymptotic expansions again.

Baumgarte's approach has the same properties with respect to asymptotic expansions. Choose $\alpha = \beta = \varepsilon^{-1}$ for convenience. Taking (4.2), (4.3) and the algebraic relation of (2.2) into account one obtains

$$u_\varepsilon(0) = u_0(0), \quad v_\varepsilon(0) = v_0(0), \quad w_\varepsilon(0) = w_0(0)$$

such that no initial layers appear. The convergence proof can be carried out along the same lines as shown above for Hanke's method. Again (AIC), (AS), and (AP) have to be true.

For Lötstedt's variant (2.4) convergence was shown in [18]. In the author's terminology, the results can be stated as follows: Suppose that (AIC), (AS), (AP) hold. Then w_ε is determined by

$$\varepsilon w_\varepsilon(0) = -(g_u(u_0(0))h(u_0(0), v_0(0)) + \kappa g(u_0(0))) \equiv 0.$$

In that case, the matrix $W(t)$ of Theorem 3.1 is

$$W(t) = -g_v(v_0)h_u(u_0, v_0)f_w(u_0, v_0, w_0). \tag{4.14}$$

Asymptotic expansions can be assured if

(AL) the eigenvalues $\lambda(t)$ of (4.14) fulfil $\mathrm{Re}\lambda(t) \leq -\sigma < 0$.

At first glance, (AL) seems to be a severe restriction since it depends essentially on the sign of g. For constrained mechanical systems, (4.14) yields

$$W(t) = -GM^{-1}G^T$$

such that (AL) is fulfilled because M is symmetric and positive-definite. Since $w_0(0) \neq 0$ in general, w_ε has an initial layer near $t = 0$. Remark that the convergence does not depend on κ and its sign!

The nonautonomous case. A last topic must be addressed. As it is possible to carry over (2.4) and (2.2) to nonautonomous systems, this is not so for (2.9) and (2.5) [13]. Consider (2.9) for example. A straightforward extension for nonautonomous systems would lead to

$$\begin{aligned}\dot{v} &= f(u, v, w, t)\\ \dot{u} &= h(u, v + \varepsilon\dot{v}, t)\\ 0 &= g(u + \varepsilon\dot{u}, t)\end{aligned}$$

In this case $w_\varepsilon(0)$ does not have an asymptotic expansion in powers of ε unless $g_t(u_0(0), 0) = 0$ such that the subsequent considerations do not apply.

Formally taking t as a new dependent variable fulfilling $\dot{t} = 1, t(0) = 0$, (1.6) reduces to an autonomous system. The application of (2.9) yields

$$\dot{v} = f(u, v, w, t) \tag{4.15a}$$

$$\dot{u} = h(u, v + \varepsilon\dot{v}, t + \varepsilon) \tag{4.15b}$$

$$0 = g(u + \varepsilon\dot{u}, t + \varepsilon) \tag{4.15c}$$

which leads to an advanced argument. In this case $g_t(u(0), 0) = 0$ is not necessary such that (4.15) seems to be the preferable parametrization. Since $u(t) + \varepsilon\dot{u} \approx u(t + \varepsilon)$, the last equation is an approximation of $0 = g(v(t + \varepsilon), t + \varepsilon)$. Assuming $g(u(t), t) = 0$, (4.15c) can be viewed as the approximation

$$\frac{d}{dt}g(u(t), t) \approx \frac{1}{\varepsilon}(g(u(t + \varepsilon), t + \varepsilon) - g(u(t), t).$$

Hence, this idea is closely related to a proposition in [24], p.38.

If $u_0(0), v_0(0), w_0(0)$ are assumed to be known, one can avoid advanced arguments using Knorrenschild's idea [15].

5 Numerical Example

Last but not least there remains the problem of numerically solving the regularized equations. At present a number of methods and codes for solving initial value problems for index 1 DAEs are known. These codes are not constructed to solve stiff problems, but they are successfully applicable to problems without or with mild boundary layers. Having in mind the use of such "standard" codes the regularization parameter cannot be very small. Since the interest is restricted to the solution for $\varepsilon \to 0$, a straightforward use would lead to rough approximations with limited expense. The way out is suggested by the results of the previous sections: Having at hand asymptotic expansions, extrapolation procedures can be used.

The idea of the Richardson extrapolation is well-known in numerical analysis. Assuming that some quantity Q is a smooth function of a parameter ε, some values $Q(\varepsilon_0), \ldots, Q(\varepsilon_n)$ are computed. An estimation of $Q(0)$ is obtained via an interpolation function (usually a polynomial or a rational function) interpolating the known

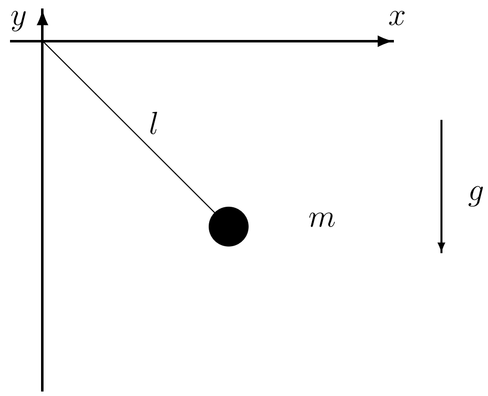

Figure 1: The mathematical pendulum

values. This technique is simple to implement. A justification of such a process can be given using asymptotic expansions. In terms of asymptotic expansions, this extrapolation eliminates the lower order terms in ε. Thus one obtains solutions which converge with the orders 1,2,... in ε. Since the solutions of the regularized DAEs do not depend smoothly on the parameter near the initial layer, extrapolation is not appropriate there.

As a simple example consider the mathematical pendulum (Fig. 1). The Euler-Lagrange equations in Cartesian coordinates are

$$\begin{aligned} m\ddot{x} &= -x\lambda \\ m\ddot{y} &= -mg - y\lambda \\ x^2 + y^2 &= l^2 \end{aligned} \tag{5.1}$$

where m is the mass, l is the length of the rod, and g is the gravitational constant. λ describes the inner forces due to the constraint. For simplicity, let $m = 1$ and $l = 1$. In our computations we have chosen $g = 13.750371636041$, which leads to the period 2. In order to obtain a system in standard form, introduce $p = \dot{x}$, $q = \dot{y}$ such that (5.1) becomes

$$\begin{aligned} \dot{x} &= p \\ \dot{y} &= q \\ \dot{p} &= -x\lambda \\ \dot{q} &= -g - y\lambda \\ x^2 + y^2 &= 1 \ . \end{aligned} \tag{5.2}$$

(5.2) was solved on $[0, 1]$ with horizontal initial position. The exact solution cannot be expressed analytically. Only the period can be obtained via incomplete elliptic integrals. Instead, a solution computed by means of the program DASSL [25] with a high precision (10^{-12}) for the index 1 formulation of the pendulum equation was used

Table 1: (x, y), Tolerance 10^{-8}

initial layer region									
ε	e_0	α_0	e_1	α_1	e_2	α_2	e_3	α_3	e_4
1.00(-1)	6.76(-2)								
5.00(-2)	3.41(-2)	2.0	5.02(-3)						
2.50(-2)	1.71(-2)	2.0	1.14(-3)	4.4	1.61(-4)				
1.25(-2)	8.55(-3)	2.0	2.97(-4)	3.8	1.78(-5)	9.0	4.33(-5)		
6.25(-3)	4.28(-3)	2.0	8.08(-5)	3.7	8.69(-6)	2.1	7.39(-6)	5.9	5.00(-6)

smooth region									
ε	e_0	α_0	e_1	α_1	e_2	α_2	e_3	α_3	e_4
1.00(-1)	7.19(-1)								
5.00(-2)	4.76(-1)	1.5	2.33(-1)						
2.50(-2)	2.81(-1)	1.7	8.64(-2)	2.7	3.75(-2)				
1.25(-2)	1.55(-1)	1.8	2.79(-2)	3.1	8.45(-3)	4.4	5.23(-3)		
6.25(-3)	8.14(-2)	1.9	8.13(-3)	3.4	1.74(-3)	4.9	7.96(-4)	6.6	5.01(-4)

as a reference solution at 10 equally spaced points in $[0, 1]$. In order to distinguish the boundary layer from the smooth part, $[0, 0.1]$ was considered as the "initial layer region" and $[0.2, 1]$ as the "smooth region".

Table 1 contains typical results.[5] In (2.9), $\varepsilon = 2\mu$ was chosen. Starting with the relatively large parameter $\varepsilon = 0.1$ the parameter was halved in each step. The resulting index 1 DAE was solved using DASSL with a tolerance of 10^{-8}. e_i is the maximum relative error of the extrapolated solution of the i-th extrapolation step in the initial layer and the smooth regions, respectively. The theoretical values α_i should approach 2.0, 4.0, 8.0, 16.0.

The results indicate that in some components no boundary layer is present. Since the initial layer appears in higher order derivatives, extrapolation behaves irregularly. This effect is due to our choice of the initial values.

6 Conclusion

In this paper various regularization methods [1, 18, 15, 13] for constrained mechanical systems are investigated. It turns out that they are very similar: This is obviously the case for [15, 13], and it can be shown that [1] can be interpreted as a linearization of these approaches. [16, 17, 18] differ from these approaches in that they are not invariant under coordinate transformations. Convergence of the different methods and the existence of asymptotic expansions is shown in the framework of [13].

Although no attempt is made to compare these methods with respect to their numerical behaviour, all of them will lead to stiff equations causing a high amount of

[5] The notation $a.b(c)$ means $a.b \times 10^c$.

Table 2: (p, q), Tolerance 10^{-8}

initial layer region									
ε	e_0	α_0	e_1	α_1	e_2	α_2	e_3	α_3	e_4
1.00(-1)	2.04(-2)								
5.00(-2)	6.90(-3)	3.0	6.66(-3)						
2.50(-2)	2.17(-3)	3.2	2.55(-3)	2.6	1.19(-3)				
1.25(-2)	6.14(-4)	3.5	9.45(-4)	2.7	4.08(-4)	2.9	2.96(-4)		
6.25(-3)	1.61(-4)	3.8	2.92(-4)	3.2	7.53(-5)	5.4	2.77(-5)	10.7	9.84(-6)

smooth region									
ε	e_0	α_0	e_1	α_1	e_2	α_2	e_3	α_3	e_4
1.00(-1)	4.25(-1)								
5.00(-2)	2.57(-1)	1.6	9.02(-2)						
2.50(-2)	1.46(-1)	1.8	4.08(-3)	2.2	2.44(-2)				
1.25(-2)	7.90(-2)	1.9	1.48(-2)	2.8	6.14(-3)	4.0	3.68(-3)		
6.25(-3)	4.12(-2)	1.9	4.61(-3)	3.2	1.22(-3)	5.1	6.21(-4)	5.9	4.17(-4)

Table 3: λ, Tolerance 10^{-8}

initial layer region									
ε	e_0	α_0	e_1	α_1	e_2	α_2	e_3	α_3	e_4
1.00(-1)	3.87(-2)								
5.00(-2)	1.25(-2)	3.1	1.38(-2)						
2.50(-2)	3.48(-3)	3.6	5.50(-3)	2.5	2.75(-3)				
1.25(-2)	8.67(-4)	4.0	1.75(-3)	3.2	4.94(-4)	5.6	1.72(-4)		
6.25(-3)	2.06(-4)	4.2	4.54(-4)	3.8	2.33(-5)	21.2	4.40(-5)	3.9	5.85(-5)

smooth region									
ε	e_0	α_0	e_1	α_1	e_2	α_2	e_3	α_3	e_4
1.00(-1)	2.85(-1)								
5.00(-2)	1.76(-1)	1.6	6.80(-2)						
2.50(-2)	1.00(-1)	1.8	3.02(-2)	2.2	1.84(-2)				
1.25(-2)	5.51(-2)	1.8	1.08(-2)	2.8	4.27(-3)	4.3	2.25(-3)		
6.25(-3)	2.91(-2)	1.9	3.28(-3)	3.3	7.91(-4)	5.4	3.04(-4)	7.4	1.77(-4)

computing effort. As a way out of this trouble the asymptotic expansions can be used for extrapolating $\varepsilon \to 0$ [13]. The question how they can be used to give error estimates for the difference between the solutions of the perturbed and unperturbed systems is still under investigation.

Another way out is the integration of the underlying ODE (1.5) or index-reduced DAE together with some stabilizing projection [6]. This will not introduce extra stiffness into the equations. In this case the constraint equations are not fulfilled asymptotically, i.e. for $t \to \infty$, but without time delay.

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