Regularization Methods for Higher Index Differential-Algebraic Equations

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1 Introduction

In recent time, great interest has been spent in the numerical solution of differential-algebraic equations (dae's). This notion is adopted to describe dynamical systems subject to balance invariants and singular differential equations. Consider an ordinary differential equation

$$F(x', x, t) = 0 \tag{1.1}$$

with $t \in [0, 1]$. If the Jacobian $F_{x'}(y, x, t) := \frac{\partial}{\partial x'} F(y, x, t)$ is nonsingular for all (y, x, t), (1.1) is equivalent to an explicit ordinary differential equation at least locally by the Implicit Function Theorem. So-called *differential-algebraic equations* arise if $F_{x'}(y, x, t)$ is singular *for all* (y, x, t). Sometimes such systems are referred to as differential equations on manifolds, semistate equations, generalized state space systems, or descriptor systems. Such problems arise in a variety of applications, e. g., electrical networks, constraint mechanical systems of rigid bodies, chemical reaction kinetics, and control theory. Later on we will use the notion of a dae in a narrower sense (see the following section for more precise definitions), nevertheless, a broad class of applications will be covered by our notion.

In many cases, (1.1) has the simpler (so-called *semiexplicit*) form

$$u' = f(u, v, t) \tag{1.2a}$$

$$0 = g(u, v, t) \ . \tag{1.2b}$$

If $g_v(u, v, t)$ remains nonsingular for all (u, v, t), (1.2b) can be solved for v (at least locally) by the Implicit Function Theorem. So (1.2) can be transformed into the state space form

$$u' = \phi(u, t) \tag{1.3a}$$

$$v = \psi(u, t) \ . \tag{1.3b}$$

Following [GM86] , dae's (1.1) which can be transformed (at least theoretically) into the state space form (1.3) are called *transferable*. The theory and practice of numerical methods for solving (1.3) is well developed. Obviously, it is not a good idea to use the transformation from (1.1) to (1.3) explicitly even if it is known in advance (which is the case for linear problems, see below). On the one hand, in many cases this transformation is very expensive to perform. On the other hand, the structure of the original problem (e. g. sparseness) gets lost. However, it is possible to modify numerical methods which work well for (1.3) such that they are successfully applicable to transferable dae's (1.1) directly. Unfortunately, many important problems do not belong to the class of transferable dae's. For nontransferable dae's, well-known ode methods often lead to disastrous numerical results. In order to classify dae's in this respect it is common to use the notion of an index. The index 1 is assigned to transferable dae's. Higher index problems are dae's with an index greater than 1. Consider (1.2) with (1.2b) not depending on v, i. e.,

$$u' = f(u,v,t) \tag{1.4a}$$
$$0 = g(u,t) \ . \tag{1.4b}$$

Equation (1.4) is not transferable. What about the behaviour of solutions of (1.2) and (1.4), respectively, with respect to perturbations of the right-hand side? Introduce

$$0 = g(u,v,t) + \delta(t) \tag{1.5}$$
$$0 = g(u,t) + \delta(t) \ . \tag{1.6}$$

Assuming $g_v(u,v,t)$ to be nonsingular in (1.2b), the system (1.2a), (1.5) is equivalent to

$$\begin{aligned} u' &= \overline{\phi}(u,t,\delta) \\ v &= \overline{\psi}(u,t,\delta) \end{aligned}$$

with $\overline{\phi}, \overline{\psi}$ being smooth functions of its arguments. On the other hand, assume $g_u(u,t)f_v(u,v,t)$ to be nonsingular and (1.4a), (1.6) to be solvable. Then δ is necessarily differentiable and

$$0 = g_u(u,t)u' + g_t(u,t) + \delta' = g_u(u,t)f(u,v,t) + g_t(u,t) + \delta' \ .$$

By the Implicit Function Theorem, the latter equation is solvable for v such that (1.4a), (1.6) is equivalent to

$$\begin{aligned} u' &= \Phi(u,t,\delta') \\ v &= \Psi(u,t,\delta') \ , \end{aligned}$$

thus the solution depends on the *derivative* of the perturbation. Such an equation is said to possess the index 2. In general, the solution of dae's with index k depends on $k-1$ derivatives of perturbations of the right-hand side of (1.1) [HLR89]. In other words, higher index equations contain differentiation problems. Such problems are known to be *ill-posed* in some naturally given topologies [Gro84]. Having accepted this point of view it is not surprising that usual ode methods fail (more precisely, they become unstable) when they are applied to higher index equations: Integration methods are applied to differentiation problems.

What is to be done in such a situation? Three questions should be answered:

1. Can we avoid to handle higher index problems?
2. Can we do with unstable methods? That means, are there finite difference methods with *weak* instabilities such that convergence of sufficient order is secured and error control and automatic grid selection are possible?
3. Are there alternative ways to treat higher index problems?

The answer of the first question leads to reduction methods. By algebraic and analytic manipulations, a higher index equation is transformed into an equivalent lower index dae or even into an ordinary differential equation. If this can be done, a great variety of reliable and efficient codes are applicable to solving the problem numerically. Unfortunately, these methods have some drawbacks. It is very hard to design a computer implementation of the reduction process. In special cases, computer algebra methods seem to be appropriate. Moreover, the structure of the original system will be destroyed. But what is even worse, analytic properties will be changed dramatically. Consider e. g. (1.4) with the index 2 condition $g_u f_v$ being regularly fulfilled. The most simple (and, so far most often used) way to reduce the index is simply differentiation of (1.4b) with respect to t, which provides

$$0 = g_u(u,t)f(u,v,t) + g_t(u,t) \ . \tag{1.7}$$

Together with the initial condition $0 = g(u(t_0), t_0)$ for some fixed $t_0 \in [0,1]$, (1.7) is equivalent to (1.4b). The system (1.4a), (1.7) has the form (1.2) and fulfils the transferability condition. Hence, the index is lowered by one by differentiating the algebraic constraints. Solving the index-reduced system numerically, (1.4b) will no longer be fulfilled due to the truncation error of the discretization method. This so-called *drift-off* of the numerical solution leads to states without physical interpretation. Moreover, the stability behaviour of the reduced system can be completely changed. See [FL89] for an impressing example. Meanwhile, more refined reduction methods have been constructed, improving the simple process described above. A more detailed elaboration can be found in the paper of Griepentrog in this issue.

In recent time, considerable progress in answering question 2 has been made. For initial value problems for index 2 systems (1.4), backward differentiation formulae [LP86, BE88, Mar90b], Runge-Kutta methods [HLR89], and extrapolation methods [Lub89] have been investigated. All these methods lead to instabilities, but these instabilities are very weak such that they can be dealt with. Even error estimation can be carried out, but in a somewhat restricted way. The "bad" component v (which contains the differentiation) is proposed to be excluded from the error control [PL86], or the the error estimation for v should be weighted by the local stepsize [HLR89]. For boundary value problems, recently [AP90] and [Han] proposed, independently of each other, an algorithm basing on

Runge-Kutta methods. Up to now these are the only direct methods for index 2 boundary value problems.

For general systems (1.1) with index 2, the situation is essentially worse. A simple linear example [GP84] shows that even the backward Euler method (i. e. the simplest bdf, and also the simplest Radau IIA Runge-Kutta method) becomes exponentially unstable. This impressing example suggests that it is probably impossible to construct ode methods even for linear time-varying index 2 problems.

In the index 3 case, results about weak instability and convergence for semiexplicit systems in the so-called *Hessenberg form* [Cla88] are proved for Runge-Kutta methods [HLR89], whereas the statements about the backward differentiation formulae are rather discouraging [BE88, Mar89b].

The aim of the present paper can be shortly formulated: The answer to question 3 is "yes, there are", i. e.,there are algorithms to solve index 2 and index 3 dae's numerically, which are at least competitive to the above mentioned approaches. The underlying idea is simple though very unusual in the context of ordinary differential equations: Higher index dae's are *ill-posed* problems, therefore, treat them as such! That means, use some *regularization* procedure. At first glance this approach might appear a rather heavy gun. This is true in so far as standard regularization techniques, e. g., Tikhonov regularization [EHN90] or least-squares collocation [Han88], are concerned. Instead we propose special parameterizations that are closely connected with the special structure of dae's and the source of their ill-posedness.

Section 2 contains the introduction of two parameterizations for general linear time-varying index 2 systems, namely, one given by März [Mar86] and the so-called pencil regularization by Campbell [Cam82] and Boyarincev [Boy80]. Let us mention that other parameterizations proposed by various authors [Bau72, Lot85, Kno88] are closely related. A forthcoming paper will be concerned with an analysis of the relations of all these methods. The pencil regularization is motivated by the fact that, for linear constant coefficient dae's, the underlying matrix pencil must be regular if initial value problems shall possess unique solutions. If this is the case, a simple perturbation leads to implicit dae's. Boyarincev [Boy] had another motivation: The pencil regularization is related to a regularization of certain partial differential equations whose discretizations are just dae's. Unfortunately, for time varying higher index systems, the time dependent matrix pencil is no longer regular in general such that the pencil regularization fails. Therefore, this method is only considered for a time independent nullspace of $F_{x'}(y, x, t)$. März introduced her parameterization in order to approximate index 2 systems by transferable ones. This aim is reached using a more subtle perturbation taking into account the special geometric structure of dae's. While März proposed her method from a purely theoretical point of view, it turned out that it has a nice interpretation in terms of electrical circuit theory [Kno88]. The method can be interpreted, for some higher index dae's describing electrical networks, as adding small circuit elements to such a circuit in order to fulfil a so-called "transversality" condition which in turn can be interpreted as an index 1 condition [CMI80, MCKI81]. Using appropriate Hilbert spaces it will be shown that these parameterizations lead to regularization procedures in the sense of Tikhonov.[1]

As a by-product of these results it appears that the parameterizations yield singular perturbation problems for dae's. Therefore, in Sect. 3 we analyze their behaviour by means of asymptotic expansions. Some convergence results about the pencil regularization for very special linear dae's are known. In [Cob82], for constant coefficient systems with arbitrary index, convergence in distributions is proved. [Cam83] contains a convergence proof for systems that are in a certain sense conveniently transferable into a special canonical form (see also [Cam84]). A similar result can be found in [Boy80]. We present our results which solve the convergence problem for both parameterizations in the general index 2 case. In the spirit of März' approach a parameterization is proposed for general time varying index 3 systems. Analogous results to the index 2 case are derived though we do not obtain convergence in any case. Since the conditions for applying the pencil regularization are probably very stringent, we do not consider it.

For nonlinear problems, a simple generalization is not possible. In Sect. 4 this is done for nonlinear index 2 and 3 systems in Hessenberg form. We show that März' approach (and a closely related one by Knorrenschild) leads to asymptotic expansions of the boundary layer type. Doing so the results of [Kno88] are simplified and generalized. Moreover, we prove analogous results for the pencil regularization for the first time.

The linear and nonlinear singular perturbation problems must be solved numerically. Experience from the ode case says that it is easier by orders of magnitude to solve the reduced problem rather than the singular perturbed problem with a very small parameter. However, we take the opposite direction: The higher index dae (reduced problem) is approximated by singularly perturbed transferable dae's. In order to overcome the inherent loss of efficiency of numerical methods we construct extrapolation procedures using the derived asymptotic expansions. Section 5 contains the numerical algorithm as well as some examples.

2 Regularization for Linear Index 2 Dae's

Consider ordinary differential equations

$$A(t)x'(t) + B(t)x(t) = q(t) \ , \tag{2.1}$$

for $t \in [0,1]$, subject to the boundary conditions

$$D_0 x(0) + D_1 x(1) = \gamma \ . \tag{2.2}$$

Here, $A(t)$ and $B(t)$ are $m \times m$-matrices depending continuously on $t \in [0,1]$. In the notation we will follow [GM86, Mar89a, Mar89c], see also the paper of Hansen in this volume. (2.1) is called a *normal dae* if $A(t)$ is smooth, i. e. there exists a continuously differentiable matrix function Q such that $Q(t)$ projects

[1] Recall that the pencil regularization is only considered for a constant nullspace.

R^m onto the nullspace $\mathcal{N}(A(t))$ of $A(t)$ for every $t \in [0,1]$. Remark that, for a normal dae, rank $A(t)$ is constant on $[0,1]$.

Having $P = I - Q$, (2.1) is obviously equivalent to

$$A(Px)' + (B - AP')x = q. \tag{2.3}$$

Here and in the following we omit the argument t if no confusion can arise. These equation represent the fact that only some components of x (namely Px) are determined by differential relations while others are simply given by algebraic equations. When dealing with solutions, this fact should be taken into account. It is, therefore, natural to introduce the following definition.

Definition. (i) A function $x \in C[0,1]^m$ is called a *solution of (2.1)* if $Px \in C^1[0,1]^m$ and it fulfils (2.3) for all $t \in [0,1]$.
(ii) A function $x \in L^2(0,1)^m$ is called a *generalized solution of (2.1)* if $Px \in H^1(0,1)^m$ and it fulfils (2.3) almost everywhere on $[0,1]$, where $H^1(0,1)^m$ denotes the usual Sobolev space [Ada75].

Obviously, every solution is a generalized solution.

In order to isolate different classes of dae's from the general form (2.1) it is convenient to introduce the notion of an index. Recently, there have been many different definitions of an index in common use, leading to different notions. Fortunately, in many applications they coincide. We will use the definitions given by Griepentrog&März, which appear to be very useful in theoretical investigations of dae's. Their definition slightly generalizes the definition of the *global index* [GP84].

For (2.3), we introduce the following notations:

$$\begin{array}{lll}
A_0 = A, & B_0 = B - AP', & \\
A_1 = A_0 + B_0 Q, & B_1 = B_0 P, & \tilde{B}_1 = (B_0 - A_1(PP_1)')P, \\
A_2 = A_1 + B_1 Q_1, & & \\
\tilde{A}_2 = A_1 + \tilde{B}_1 Q_1, \; \tilde{B}_2 = \tilde{B}_1 P_1, & & \\
A_3 = \tilde{A}_2 + \tilde{B}_2 Q_2. & &
\end{array}$$

Here, $Q_1(t)$ denotes a projection onto $\mathcal{N}(A_1(t))$, and $Q_2(t)$ is a projection onto $\mathcal{N}(\tilde{A}_2(t))$, $P_i = I - Q_i$. Working with $\tilde{B}_1$ we suppose PP_1 to be continuously differentiable.

Definition. (i) Equation (2.1) is called *transferable* if $A_1(t)$ is nonsingular for every $t \in [0,1]$.
(ii) Equation (2.1) is called *tractable with index 2* if $A_1(t)$ is singular, but $A_2(t)$ is nonsingular for every $t \in [0,1]$.
(iii) Equation (2.1) is called *tractable with index 3* if $A_1(t)$ and $\tilde{A}_2(t)$ are both singular, but $A_3(t)$ is nonsingular for every $t \in [0,1]$.

Remark. (i) The definition is independent of the special choice of the projector functions Q, Q_1, Q_2.
(ii) If PP_1 is continuously differentiable, $A_2(t)$ is singular if and only if $\tilde{A}_2(t)$ is

so.
(iii) If (2.1) is tractable with index 2, Q_1 can be chosen such that $Q_1Q = 0$. Analogously, if (2.1) is tractable with index 3 and some smoothness conditions are fulfilled, Q_1 and Q_2 can be chosen such that $Q_2Q_1 = 0, Q_2Q = 0, Q_1Q = 0$.

Example. A very important special case of dae's are semiexplicit systems. The following three types arise in applications frequently:

$$u' = B_{11}u + B_{12}v + q_1 \tag{2.4a}$$
$$0 = B_{21}u + B_{22}v + q_2 \tag{2.4b}$$

and

$$u' = B_{11}u + B_{12}v + q_1 \tag{2.5a}$$
$$0 = B_{21}u + q_2 \tag{2.5b}$$

and

$$u' = B_{11}u + B_{12}v + B_{13}w + q_1 \tag{2.6a}$$
$$v' = B_{21}u + B_{22}v + q_2 \tag{2.6b}$$
$$0 = B_{32}v + q_3 \ . \tag{2.6c}$$

Recently Clark [Cla88] referred to such systems as systems in Hessenberg form. Assume
(i) B_{22} to be nonsingular in (2.4),
(ii) $B_{21}B_{12}$ to be nonsingular in (2.5),
(iii) $B_{32}B_{21}B_{13}$ to be nonsingular in (2.6).
Then (2.4), (2.5), (2.6) are transferable, tractable with index 2, and tractable with index 3, respectively. Note that (1.2) and (1.4) are the nonlinear counterparts of (2.4) and (2.5), respectively.

Before we can start the regularization, we must state precisely in which sense higher index dae's are ill-posed. Following Hadamard, the problem of solving $Tx = q$ ($T : X \to Y$ with some given metric spaces X, Y) is called *well-posed* iff
(i) it has a solution for every right-hand side $q \in Y$ (i. e. T is surjective),
(ii) this solution is unique (i. e. T is injective), and
(iii) the solution depends continuously on the data (i. e. T^{-1} is continuous).
Otherwise, the problem is called *ill-posed.* For dae's being transferable or tractable with index 2, 3, (ii) is no serious restriction. As will be seen later, the solution space of the homogeneous equation has finite dimension. Adding appropriate boundary conditions, T will be injective. The most essential problem is (iii), which is closely connected with (i). (iii) depends essentially on the topologies of X and Y. In principle, T^{-1} is continuous in any case if Y is equipped with the discrete metric. Obviously, this makes no sense. In general, with each equation (T), a family of "naturally given" spaces and norms is coupled. (Say, how do you feel about measuring the error in the data. For instance, in order to handle

errors on a computer some discrete $C-$ or L^2-norm will do.) For our dae (2.1), (2.2), the operator T has the form

$$Tx = \begin{pmatrix} A(Px)' + (B - AP')x \\ D_0x(0) + D_1x(1) \end{pmatrix}. \tag{2.7}$$

According to our definition of a generalized solution, the space X should be

$$C_A^1[0,1] = \{x \in C[0,1]^m | Px \in C^1[0,1]^m\} \tag{2.8}$$
$$H_A^1(0,1) = \{x \in L^2(0,1)^m | Px \in H^1(0,1)^m\} \tag{2.9}$$

with the norms

$$\|x\|_{\infty,A} = \|x\|_\infty + \|(Px)'\|_\infty$$
$$\|x\|_{1,A}^2 = \|x\|^2 + \|(Px)'\| \ .$$

Here, $\|\cdot\|$ denotes the norm of $L^2(0,1)^m$ and $\|\cdot\|_\infty$ denotes the norm of $C[0,1]^m$. Neither the sets $C_A^1[0,1], H_A^1(0,1)$ nor their topologies depend on the special choice of the projector Q [GM86, Han89]. Finally, since Y should contain the range $\mathcal{R}(T)$ of T, $Y = C[0,1]^m \times M$ and $Y = L^2(0,1)^m \times M$, respectively, where $M = \mathcal{R}(D_0, D_1)$. In the special case of an ode we have $P = I$ and we arrive at the usual settings with $M = R^m$. Before stating an existence and uniqueness theorem for transferable dae's some words about the admissible boundary conditions are necessary. Consider the transferable dae (2.4). Due to the nonsingularity of B_{22}, it is equivalent to the system

$$u' = (B_{11} - B_{12}B_{22}^{-1}B_{21})u + q_1 - B_{12}B_{22}^{-1}q_2 \tag{2.10a}$$
$$v = -B_{22}^{-1}B_{21}u - B_{22}^{-1}q_2 \ . \tag{2.10b}$$

Once (2.10a) is solved, v is given by the algebraic relation (2.10b). Hence, boundary conditions are only allowed for u, but not for v. In general, boundary conditions should be given for Px in (2.2), only.

Theorem 1 [GM86]. *Let (2.1) be transferable. Let $D_0 = D_0P(0)$, $D_1 = D_1P(1)$, and* rank $\begin{pmatrix} D_0 & D_1 \\ Q(0) & 0 \end{pmatrix} = m$. *Suppose that the homogeneous boundary value problem*

$$z'(PA_1^{-1}B_0 - P')z = 0$$
$$D_0z(0) + D_1z(1) = 0, Qz(0) = 0$$

has only the trivial solution. Then the boundary value problem (2.1), (2.2) has, for every $q \in L^2(0,1)^m$ and every $\gamma \in M = \mathcal{R}(D_0, D_1)$, exactly one generalized solution. This solution depends continuously on the data.

Remark. The same assertion is true if $L^2(0,1)^m$ is replaced by $C[0,1]^m$ and (2.9) by (2.8), i. e. a solution.

The proof of Theorem 1 can be given by splitting techniques using A_1, P, Q, see the paper of Hansen. As a result, every transferable dae can be transformed into the state space form with a differential equation for Px and an algebraic relation for Qx.

What about index 2 dae's? Such equations contain differentiation problems for some components of the right-hand side. Hence, the range of T is a dense nonclosed subset of Y. But this is equivalent to the discontinuity of T^{-1}. Therefore, index 2 equations are ill-posed in the X, Y-setting — a fact calling for regularization. More precisely, by splitting techniques one can show that a dae (2.1) tractable with index 2 is equivalent to [Han90c]

$$y = PQ_1A_2^{-1}q \tag{2.11a}$$
$$z' + (PP_1A_2^{-1}B_0P - (PP_1)')z - (PP_1)'y = PP_1A_2^{-1}q \tag{2.11b}$$
$$r = QP_1A_2^{-1}q - QP_1A_2^{-1}B_0z + (QP_1P)'z - QP_1Py' \tag{2.11c}$$
$$(I - PP_1)z(0) = 0 \tag{2.11d}$$

where $y = PQ_1x, z = PP_1x, r = Qx$. Here we assumed Q_1 to be the canonical projection $Q_1 = Q_{1,s} := Q_1A_2^{-1}B_0P$. (2.11) gives rise to a number of conclusions.

Remark. (i) $z = PP_1x$ is the only component given by a differential equation. Therefore, boundary conditions are only applicable to PP_1x. Hence, we suppose $D_0 = D_0PP_1(0), D_1 = D_1PP_1(1)$ to hold.
(ii) y and z play the same role as Qx and Px, respectively, in case of a transferable dae. The "bad" behaviour of (2.1) is due to the nullspace component r.
(iii) The following theorem holds. The same remark as that following Theorem 1 applies.

Theorem 2 [Han90c]. *Let (2.1) be tractable with index 2. Let $D_0 = D_0PP_1(0), D_1 = D_1PP_1(1)$, and* rank $\begin{pmatrix} D_0 & D_1 \\ I - PP_1(0) & 0 \end{pmatrix} = m$. *Suppose that the homogeneous boundary value problem*

$$z' + (PP_1A_2^{-1}B_0P - (PP_1)')z = 0$$
$$D_0z(0) + D_1z(1) = 0, (I - PP_1)z(0) = 0$$

has only the trivial solution. Then the boundary value problem (2.1), (2.2) has a generalized solution if and only if $q \in L^2(0,1)^m$ such that $PQ_1A_2^{-1}q \in H^1(0,1)^m$ and $\gamma \in M = \mathcal{R}(D_0, D_1)$. This solution is unique.

Corollary 3. *Under the hypotheses of Theorem 2, T^{-1} exists and is unbounded.*

The crucial point from the point of view of applications is the fact that the data (q, γ) are usually only known up to a certain noise level $\delta = (\delta_1, \delta_2)$, say

$$||q^\delta - q|| \le \delta_1, |\gamma^\delta - \gamma| \le \delta_2 \ . \tag{2.12}$$

This noise may be due to, e. g., model inaccuracy or even discretization effects. Even if the problem $Tx = (q^\delta, \gamma^\delta)$ is solvable, say by x^δ, it does not hold that

$x^\delta \to x$ for $\delta \to 0$. The following question arises: Does there exist a family $\{T_\varepsilon | \varepsilon > 0\}$[2] of operators $T_\varepsilon : X \to Y$ (and how to construct it) with the properties:
(i) The problems $T_\varepsilon = (q, \gamma)$ are well-posed.
(ii) For every $(q, \gamma) \in \mathcal{R}(T)$, there exists a parameter choice strategy $\varepsilon = \varepsilon(\delta)$ with $\varepsilon(\delta) \to 0$ for $\delta \to 0$ such that

$$\sup\{\|T^{-1}_{\varepsilon(\delta)}(q^\delta, \gamma^\delta) - T^{-1}(q, \gamma)\|_X \,|\, \|q^\delta - q\| \le \delta_1, |\gamma^\delta - \gamma| \le \delta_2\} \stackrel{\delta \to 0}{\longrightarrow} 0 \ .$$

Such a family together with the parameter choice strategy is called a *regularization algorithm*. The construction of T_ε and $\varepsilon(\delta)$ is usually divided into two steps. Firstly, a family $\{T_\varepsilon | \varepsilon > 0\}$ is constructed such that, for all $(q, \delta) \in \mathcal{R}(t)$, $T_\varepsilon^{-1}(q, \delta) \to T^{-1}(q, \delta)$. After an estimation of the convergence velocity and the growth of $\|T_\varepsilon^{-1}\|$[3] $\varepsilon = \varepsilon(\delta)$ can be chosen. Most of all, Tikhonov regularization [Gro84] or other standard regularization methods are used when solving ill-posed problems. This is possible for dae's, too [Han88, EHN90]. However, this is a rather heavy gun. Therefore, we are looking for parameterizations which are closer related to the special structure of dae's. One such possibility, the *pencil regularization*, was given independently by Boyarincev [Boy80] and Campbell [Cam82]. For this, (2.1) is replaced by

$$(A + \varepsilon B)x' + Bx = q \ . \tag{2.13}$$

This parameterization aims at ordinary differential equations. For transferable dae's or constant coefficient dae's, the matrix pencil (A, B) is nonsingular [GM86] such that this goal is reached. Unfortunately, this is no longer true for time varying coefficients.

Example. The dae (2.1) with the coefficients

$$A(t) = \begin{pmatrix} 0 & 0 \\ 1 & -t \end{pmatrix}, B(t) = \begin{pmatrix} 1 & -t \\ 0 & 0 \end{pmatrix}, t \in [0, 1]$$

is tractable with index 2. Obviously, for all ε, $A + \varepsilon B$ is singular. Even more, the parametrized equation is tractable with index 2 having, therefore, the same ill-posedness as the original problem.

Nevertheless, for a time independent nullspace $\mathcal{N}(A(t))$, the pencil regularization can be successfully applied. A further parameterization of (2.1) was proposed by März [Mar86]. She considered the equation

$$(A + \varepsilon BP)x' + (B + \varepsilon BPP')x = q \ . \tag{2.14}$$

2 In the literature, the regularization parameter is usually called α. For reasons that will be clear later, we prefer ε.
3 By the Banach-Steinhaus theorem and the unboundedness of T^{-1}, $\|T_\varepsilon^{-1}\|$ grows unboundedly.

In a more convenient notation it simply reads

$$(A + \varepsilon B_1)(Px)' + B_0 x = q \tag{2.15}$$

showing that only the equations containing the Px-component are perturbed. März aimed at obtaining transferable dae's. This was a good idea since, by Theorem 1, such dae's are well-posed provided that appropriate boundary conditions are given. Heuristically, it seems evident that the dae is less changed if it is transformed into a transferable dae rather than an ode. Using the same methods as in (2.11) it can be shown that (2.15) is equivalent to

$$\begin{aligned}
&\varepsilon y' + (I - \varepsilon(PQ_1)')y - \varepsilon(PQ_1)'PP_1 z = PQ_1 A_2^{-1} q && (2.16a)\\
&(I + \varepsilon PP_1 A_2^{-1} B_0 P)z' + \\
&\qquad (PP_1 A_2^{-1} B_0 P - (PP_1)' + \varepsilon PP_1 A_2^{-1} B_0 P (PQ_1)')z + \\
&\qquad (\varepsilon PP_1 A_2^{-1} B_0 P (PQ_1)' - (PP_1)')y = PP_1 A_2^{-1} q && (2.16b)\\
&r = QP_1 A_2^{-1} q - QP_1 A_2^{-1} B_0 z + (QP_1 P)' z - QP_1 P y' \\
&\qquad -\varepsilon QP_1 A_2^{-1} B_0 P (z' + y') && (2.16c)\\
&(I - PP_1)z(0) = 0 && (2.16d)\\
&(I - PQ_1)y(0) = 0 && (2.16e)
\end{aligned}$$

where $y = PQ_1 x, z = PP_1 x, r = Qx$. This representation shows immediately that, for sufficiently small $\varepsilon > 0$, (2.15) is transferable since (2.16a), (2.16b) is a system of ode's for $Px = y + z$ and (2.16c) is the algebraic relation for $Qx = r$. Equation (2.16) and Theorem 1 imply immediately

Theorem 4 [Han90c]. *Let the assumptions of Theorem 2 be fulfilled and*

$$T_\varepsilon x = \begin{pmatrix} (A + \varepsilon B_1)(Px)' + B_0 x \\ D_0 x(0) + D_1 x(1) \\ PQ_1 x(0) \end{pmatrix}.$$

Then, for sufficiently small $\varepsilon > 0$, the problem $T_\varepsilon x = (q, \gamma, \beta)$ has exactly one solution x_ε for all $q \in L^2(0,1)^m, \gamma \in M$ and $\beta \in \mathcal{R}(PQ_1(0))$. This solution depends continuously on the data.

For a given index 2 boundary value problem, after parameterization we have the freedom to choose $PQ_1 x(0)$. Since $PQ_1 x(0) = PQ_1 A_2^{-1} q(0)$ because of (2.11a), we consider the convergence of the solutions x_ε of the problem

$$T_\varepsilon x = (q, \gamma, PQ_1 A_2^{-1} q(0)) \tag{2.17}$$

towards the solution x of $Tx = (q, \gamma)$. Introducing appropriate notations, (2.16a), (2.16b) read

$$\begin{aligned}
\varepsilon y' &= U_{11}(\varepsilon) y + \varepsilon V_{12} z + q_1 && (2.18a)\\
(I + \varepsilon C) z' &= U_{21}(\varepsilon) y + U_{22}(\varepsilon) z + q_2 && (2.18b)
\end{aligned}$$

whereas (2.11a), (2.11b) are

$$0 = -y + q_1 \tag{2.19a}$$
$$z' = U_{21}(0)y + U_{22}(0)z + q_2 \ , \tag{2.19b}$$

the latter system being the reduced system of the singular perturbation problem (2.18)[4]. The boundary conditions are $D_0z(0) + D_1z(1) = \gamma$ for (2.18) and (2.19), and additionally $y(0) = q_1(0)$ for (2.18). We must investigate the convergence properties of solutions of (2.18) towards that of (2.19). It is a standard result from singular perturbation theory that, since (2.18a) is a stable differential equation for y and initial values $y(0)$ are given, pointwise convergence should be secured provided that sufficiently smooth data are given [VB73]. However, we are interested, firstly, in convergence in $L^2(0,1)^m$ and, secondly, for nonsmooth data q_1, q_2. It is a rather technical and sophisticated proof to show that this assertion holds true. In a first step the convergence of some convolution operators is shown via their Fourier transforms. Then the stability estimates

$$\|y_\varepsilon\| \le c(\varepsilon|\gamma| + \varepsilon^{1/2}|\beta| + \|q_1\| + \varepsilon\|q_2\|) \tag{2.20a}$$
$$\|z_\varepsilon\| \le c(|\gamma| + \varepsilon^{1/2}|\beta| + +\|q_1\| + \|q_2\|) \tag{2.20b}$$

with β replacing $PQ_1A_2^{-1}q(0)$ are established. Now it is easy to derive the estimate $\|Px_\varepsilon - Px\| = O(\varepsilon)$. Using (2.18), (2.19) one obtains furthermore $\|(Px_\varepsilon)' - (Px)'\| = o(1)$ and $\|Qx_\varepsilon - Qx\| = o(1)$ such that $\|x_\varepsilon - x\|_{1,A} = o(1)$. If more smoothness is known, even $\|x_\varepsilon - x\|_{1,A} = O(\varepsilon^{1/2})$ holds. Note that we obtain, for the differential components Px, the best order of convergence we could expect, namely ε. In applications Px often represents the state variables, whereas Qx is some kind of a Lagrange multiplier. If we are only interested in the state variables, fast convergence occurs.

If we are given perturbed data $(q^\delta, \gamma^\delta, \beta^\delta)$ such that

$$\|q^\delta - q\| \le \delta_1, |\gamma^\delta - \gamma| \le \delta_2, |\beta^\delta - PQ_1A_2^{-1}q(0)| \le \delta_3 \ , \tag{2.21}$$

(2.20) and the estimate $\|x_\varepsilon^\delta - x\| \le \|x_\varepsilon^\delta - x_\varepsilon\|_{1,A} + \|x_\varepsilon - x\|_{1,A}$ lead to parameter choice strategies $\varepsilon = \varepsilon(\delta)$. In case of smoother data, orders of convergence with respect to the noise level can be derived. For the best choice, they yield $\|x_\varepsilon^\delta - x\|_{1,A} = O(\delta_1^{1/3} + \delta_2 + \delta_3^{1/2})$.

It is nice to remark that, if $(q,\gamma) \notin \mathcal{R}(T)$, then $\{x_\varepsilon\}$ does not contain any weakly convergent subsequence. This behaviour is very close to that of Tikhonov regularization and related methods. We summarize the results.

Theorem 5 [Han90c]. *Let the assumptions of Theorem 4 be fulfilled. Let $\varepsilon > 0$ be sufficiently small. Denote by x_ε and x_ε^δ the solutions of $T_\varepsilon x = (q, \gamma, PQ_1A_2^{-1}q(0))$ and $T_\varepsilon x = (q^\delta, \gamma^\delta, \beta^\delta)$, respectively, where $\delta = (\delta_1, \delta_2, \delta_3)$ and (2.21) holds. Then:*
(i) Let $(q, \gamma) \in \mathcal{R}(T)$.

[4] Readers who are not familiar with singular perturbation theory can skip the following paragraphs up to Theorem 5. More about singular perturbations can be found in the following section.

a)$\|x_\varepsilon - x\|_{1,A} \to 0$ *for* $\varepsilon \to 0$. *If* $\lim_{\delta\to 0}\varepsilon(\delta) = 0$, $\lim_{\delta\to 0}\frac{\delta_1}{\varepsilon(\delta)} = 0$ *and* $\lim_{\delta\to 0}\frac{\delta_3^2}{\varepsilon(\delta)} = 0$, *then* $\|x^\delta_{\varepsilon(\delta)} - x\|_{1,A} \to 0$ *for* $\varepsilon \to 0$.
b) If $PQ_1, PP_1 \in C^2[0,1]^{m\times m}$ *and* $PQ_1A_2^{-1}q \in H^2(0,1)^m$, *then* $\|x_\varepsilon - x\|_{1,A} = O(\varepsilon^{1/2})$. *Moreover, if* $\varepsilon \sim \max(\delta_1^{2/3}, \delta_3)$, *then* $\|x^\delta_{\varepsilon(\delta)} - x\|_{1,A} = O(\delta_1^{1/3} + \delta_2 + \delta_3^{1/2})$.
(ii) Let $(q,\gamma) \notin \mathcal{R}(T)$. *Then* $\|x_\varepsilon\| \to \infty$ *for* $\varepsilon \to 0$.

Let us now consider the pencil regularization (2.13) for a constant nullspace $\mathcal{N}(A(t))$. In this case, (2.13) is equivalent to (2.16) with (2.16c) replaced by

$$\varepsilon\tilde{r}' + (I - \varepsilon(PQ_1)')\tilde{r} = r_\varepsilon \tag{2.22}$$

and r_ε given by (2.16c). This is again a stable singularly perturbed equation. Choosing the boundary conditions $D_0x(0)+D_1x(1) = \gamma$, $PQ_1x(0) = PQ_1A_2^{-1}q(0)$ and, additionally, the initial condition $r(0) = Qx(0) = r_0$, for some fixed r_0, leads to results analogous to those for März parameterization.

In the present section we have investigated the convergence properties of the parameterizations (2.13) and (2.14) in the sense of regularization methods. Therefore, we preferred to use the Hilbert space $H^1_A(0,1)$ as the underlying function space. The analysis showed that we really met singular perturbation problems. In this context the convergence behaviour of the regularized solutions should be further characterized by means of asymptotic methods. The results obtained so far are of more or less theoretical interest. They do not answer the question of how to solve the regularized problem $T_\varepsilon x = (q,\gamma,\delta)$. For designing numerical methods, deeper insight into the structure of the equations is necessary. This will be done in the next section.

3 Characterizing Regularization Methods by Means of Asymptotic Expansions

In the last section we introduced two parameterizations for linear dae's being tractable with index 2. First convergence results were given. In the present section we will further characterize the relation between the sought solution of the higher index equation and its regularized approximations by means of asymptotic expansions with respect to the regularization parameter. In the second part we introduce a parametrization for linear index 3 dae's and give sufficient conditions for their convergence. In contrast to the index 2 case where März' parametrization leads to convergence in any case, this is no longer true for dae's being tractable with index 3.

Definition. Let$X$ be a Banach space and $x : (0,\varepsilon_0] \to X$ a family of elements of X. We say that X has an *asymptotic expansion in powers of* ε *of the order* N if there is a polynomial $y : (0,\varepsilon_0] \to X$ of degree less than or equal to N such that $x(\varepsilon) = y(\varepsilon) + O(\varepsilon^{N+1})$ for $\varepsilon \to 0$. In signs: $x \simeq y$.

Remark. (i) The approximating polynomial y is unique.
(ii) If x is analytical in 0, it has asymptotic expansions of any order.
(iii) If x has asymptotic expansions of any order, a formal series can be written down. In general, this series neither converges nor, if it does nevertheless, is equal to x.

Consider a family of linear equations

$$T_\varepsilon x = y_\varepsilon \tag{3.1}$$

with linear bounded T_ε. Let us assume that both T_ε and y_ε have asymptotic expansions of order N:

$$T_\varepsilon \simeq \sum_{j=0}^{N} T_j \varepsilon^j \tag{3.2a}$$

$$y_\varepsilon \simeq \sum_{j=0}^{N} y_j \varepsilon^j \quad . \tag{3.2b}$$

One should expect that $x = x_\varepsilon$ has also such an expansion. Inserting a formal expansion for x into (3.1) and using (3.2) provides

$$T_0x_0 + \varepsilon(T_0x_1 + T_1x_0) + \varepsilon^2(T_0x_2 + T_1x_1 + T_2x_0) + \cdots + O(\varepsilon^{N+1}) = \sum_{j=0}^{N} y_j\varepsilon^j + O(\varepsilon^{N+1}) \tag{3.3}$$

Since asymptotic expansions are unique, comparing equal powers of ε yields the system

$$T_0x_0 = y_0 \tag{3.4a}$$

$$T_0x_j = \sum_{k=1}^{j} T_k x_{j-k} + y_j, \quad j = 1, \ldots, N \ . \tag{3.4b}$$

The first order approximation (3.4a) is called the *reduced problem.* If T_0 is continuously invertible, the coefficients of x_j are uniquely determined by (3.4). Denoting

$$x_\varepsilon^N = \sum_{j=0}^{N} x_j \varepsilon^j \tag{3.5}$$

we obtain

$$T_\varepsilon x_\varepsilon^N = y_\varepsilon + O(\varepsilon^{N+1}) \tag{3.6}$$

by construction. Subtracting the exact solution x_ε (which exists because of (3.2a), the bijectivity of T_0, and Banach's lemma) yields

$$T_\varepsilon(x_\varepsilon^N - x_\varepsilon) = O(\varepsilon^{N+1}).$$

Applying again Banach's lemma implies the desired result $x \simeq x_\varepsilon^N$.

The most important assumption for the latter result is the bijectivity of T_0. Such a problem (3.1) is called a *regular perturbation problem*. Roughly speaking, for regular perturbation problems, the solution has an asymptotic expansion in powers of ε of the same type as the operator and the data. If T_0 is not continuously invertible, we have a *singular perturbation problem*. As we will see later, in a lot of such problems (3.4) is still uniquely solvable such that (3.6) holds for (3.5). However, now one needs further assumptions in order to obtain $x \simeq x_\varepsilon^N$ via a stability argument.

Let us return to ill-posed problems and their regularizations. It is reasonable to assume that the regularized operator T_ε has something to do with the original one T, say, e. g., $T_\varepsilon x \to Tx$ for all $x \in X$. At least every practically relevant regularization algorithm known to the author has this property. By (3.2a), $T_\varepsilon \to T_0$ such that $T = T_0$ with discontinuous T^{-1}. Hence, we have a singular perturbation problem. This can easily be seen for our parameterizations in (2.18) and (2.19). Whereas (2.18) is, for every fixed $\varepsilon \neq 0$, well-posed in $X = C^1[0,1]^{2m}$ and $Y = C[0,1]^{2m} \times R^{2m}$, (2.18) is not so.[5]

After the general consideration let us return to our special singular perturbation problems. Our aim is the characterization of the convergence of x_ε towards x for $\varepsilon \to 0$. In the following the norm is always $\|\cdot\|_\infty$.

Example. Consider the constant coefficient system $\varepsilon y' = Ay + b$ with $b \in R^m$ together with its reduced problem $0 = Ay + b$. We assume A to be nonsingular. Let Φ denote a fundamental matrix of $y' = Ay$. Then $y_\varepsilon(t) = \Phi(t/\varepsilon)c + \overline{y}_0$ is the general solution of the singularly perturbed system with $\overline{y}_0 = A^{-1}b$ being the solution of the reduced problem. $\Phi(t)$ consists of functions $p(t)e^{\lambda t}$ with polynomials p and eigenvalues λ of A. This representation shows that an asymptotic expansion in the sense of the definition cannot be expected. Instead, depending on the sign of the real part $\Re(\lambda)$ of λ and ε, and the boundary conditions, at least short regions near the boundaries occur where y_ε differs significantly from $\overline{y}_0$, and this transition behaves, for $\varepsilon > 0$, like $O(\exp(\Re(\lambda)t/\varepsilon)$ for $\Re(\lambda) < 0$ and $O(\exp(\Re(\lambda)(1-t)/\varepsilon)$ for $\Re(\lambda) > 0$. Such a behaviour is called a boundary layer. In order that this becomes true, decaying components of Φ must be controlled by initial conditions and increasing components of Φ by end conditions provided that such a dichotomy is present in the problem.

After these preparations we suppose that the hypotheses and conclusions of the following theorem, which will be used extensively later on, are clear. For further use in the next section, which is devoted to nonlinear problems, we give the nonlinear version. Essentially, this is Theorem 4.1 of [VB73].

Theorem 6. *Consider the boundary value problem*

$$z' = f(z, y, \cdot, \varepsilon) \tag{3.7a}$$

[5] Equation (2.19) is a transferable dae of the form (2.4). Our statement is no contradiction to Theorem 1 since (2.19) is well-posed with $X = C[0,1]^m \times C^1[0,1]^m$ and $Y = C[0,1]^{2m} \times R^m$, but not in the (X,Y)-setting for (2.18).

$$\varepsilon y' = g(z, y, \cdot, \varepsilon) \tag{3.7b}$$
$$h(z(0), z(1)) = 0 \tag{3.7c}$$
$$y(0) = y_\varepsilon^0 \tag{3.7d}$$

with $t \in [0,1]$ for $0 < \varepsilon \le \varepsilon_*$. Suppose
(i) The functions f, g, h are sufficiently smooth.
(ii) f, g, y_ε^0 have asymptotic expansions with respect to ε.
(iii) The boundary value problem

$$\begin{aligned} z' &= f(z, y, \cdot, 0) \\ 0 &= g(z, y, \cdot, 0) \\ h(z(0), z(1)) &= 0 \end{aligned}$$

has a solution (z_0, y_0).
(iv) $W(t) = g_y(z_0(t), y_0(t), t, 0)$ has only eigenvalues $\lambda_i(t)$ such that $\Re(\lambda_i(t)) \le -\sigma < 0$ for all $t \in [0,1]$.
(v) The equation of the first variation

$$\begin{aligned} z' &= f_z(\phi_0)z + f_y(\phi_0)y \\ 0 &= g_z(\phi_0)z + g_y(\phi_0)y \end{aligned}$$

$$h_{z(0)}(z_0(0), z_0(1))z(0) + h_{z(1)}(z_0(0), z_0(1))z(1) = 0$$

has the trivial solution, only, where $\phi_0 = (z_0, y_0, \cdot, 0)$.
(vi) $y_0^0 = \lim_{\varepsilon \to 0} y_\varepsilon^0$ belongs to the domain of attraction of the attraction point $y_0(0)$ of the equation $\tilde{y}' = g(z_0(0), \tilde{y}, 0)$.
Then, for sufficiently small $\varepsilon_* > 0$, (3.7) has exactly one solution $(z_\varepsilon, y_\varepsilon)$ in a neighbourhood of (z_0, y_0). The asymptotic expansions

$$\begin{aligned} z_\varepsilon(t) &\simeq \sum_{j=0}^{N} (z_j(t) + \overline{z}_j(\tau))\varepsilon^j \\ y_\varepsilon(t) &\simeq \sum_{j=0}^{N} (y_j(t) + \overline{y}_j(\tau))\varepsilon^j \end{aligned}$$

hold, where $\tau = t/\varepsilon, |\overline{z}_j(\tau)|, |\overline{y}_j(\tau)| \le C\exp(-\alpha\tau)$ with $-\sigma \le -\alpha < 0$ and $\overline{z}_0(\tau) \equiv 0$. Moreover, $\overline{y}_0(\tau) \equiv 0$ if and only if $y_0^0 = y_0(0)$.

Remark. (i) Because of assumption (iv) there is only a boundary layer near the left-hand boundary $t = 0$.
(ii) The asymptotic representations of z_ε and y_ε contain a regular part according to Definition represented by z_j and y_j and a boundary layer correction represented by $\overline{z}_j$ and $\overline{y}_j$. The regular expansion is valid pointwise for every $t > 0$ and uniformly on every closed subinterval not containing the left-hand boundary.

From now on we assume that all functions and projections involved are sufficiently smooth. Applying Theorem 6 to März' parameterization (2.14) is now straightforward. A comparison of the systems (2.18) and (2.19) shows that the relevant matrix $W(t)$ of assumption (iv) is identical to $-I$ having only the eigenvalue -1. Therefore, additional *initial* conditions must be given for $y = PQ_1x$, say $PQ_1x(0) = y^0$. Then the asymptotic expansions hold true. Moreover, $\overline{y}_0(\tau) \equiv 0$ if and only if $y^0 = PQ_1x_0(0)$. This is the exact initial condition we already used in Sect. 2. Usually, it is very hard to compute these additional initial conditions. Having asymptotic expansions of $z_\varepsilon, y_\varepsilon$ we insert them into (2.16c), thus giving an expansion of r_ε. Summarizing we obtain

Theorem 7 [Han90a]. *Let the hypotheses of Theorem 2 be fulfilled. Let x_ε be the solution of (2.15), (2.2) and $PQ_1x(0) = y^0$. Then the asymptotic expansion*

$$x_\varepsilon(t) \simeq \overline{x}_{-1}(\tau)\varepsilon^{-1} + \sum_{j=0}^{N}(x_j(t) + \overline{x}_j(\tau))\varepsilon^j$$

holds. Here, $\tau = t/\varepsilon, |\overline{x}_j(\tau)| \leq C\exp(-\alpha\tau), j = -1, 1, 0, \ldots, N, \alpha > 0$ and $P\overline{x}_{-1} = 0$. Moreover, $\overline{x}_{-1}(\tau) \equiv 0$ if and only if $y^0 = PQ_1x_0(0)$.

Remark. In a transferable dae, the nullspace component Qx is only implicitly given by algebraic relations. Therefore, $Qx(0)$ is given by $Px(0)$ and the dae. The first term $\overline{x}_{-1}\varepsilon^{-1}$ corresponds to an *unbounded* boundary layer in Qx.

Example. In the semiexplicit index 2 equation (2.5) we have simply

$$PQ_1 = \begin{pmatrix} R & 0 \\ 0 & 0 \end{pmatrix}$$

with the projection $R = B_{12}(B_{21}B_{12})^{-1}B_{21}$. Hence, the equation $PQ_1x(0) = PQ_1A_2^{-1}q(0)$ simply reads

$$B_{21}u(0) = -q_2(0) \ , \tag{3.8}$$

which is (2.5b) for $t = 0$. Hence, in order to avoid the unbounded boundary layer one should choose the additional initial condition (3.8) besides (2.2).

Corollary 8. *Theorem 7 is true for the pencil regularization (2.13), too, provided that an additional initial condition $Qx(0) = r^0$ is chosen.*

Proof. $Qx = \tilde{r}$ fulfils (2.22) with r_ε having the asymptotic expansion

$$r_\varepsilon(t) \simeq \overline{r}_{-1}(\tau)\varepsilon^{-1} + \sum_{j=0}^{N}(r_j(t) + \overline{r}_j(\tau))\varepsilon^j \ . \tag{3.9}$$

This representation suggest to look for a similar expansion of $\tilde{r}_\varepsilon$:

$$\tilde{r}_\varepsilon(t) \simeq \overline{\overline{r}}_{-1}(\tau)\varepsilon^{-1} + \sum_{j=0}^{N}(r_j(t) + \overline{\overline{r}}_j(\tau))\varepsilon^j \ . \tag{3.10}$$

Since $\tilde{r}_\varepsilon(0) = r^0$, for (3.10) to hold, $\overline{\tilde{r}}_{-1}(0) = 0$ has to be true. Now, inserting (3.9) and (3.10) into (2.22) and equating equal powers of ε yields, in the boundary layer,

$$\varepsilon^{-1} : \overline{r}_{-1}(\tau) = \overline{\tilde{r}}'_{-1}(\tau) + \overline{\tilde{r}}_{-1}(\tau) \tag{3.11a}$$

$$\varepsilon^{j} : \overline{r}_{j}(\tau) = \overline{\tilde{r}}'_{j}(\tau) + \overline{\tilde{r}}_{j}(\tau) - (PQ_1)'(0)\overline{\tilde{r}}_{j-1}(\tau), \quad j = 0, 1, \cdots \tag{3.11b}$$

and for the regular part

$$\varepsilon^0 : r_0 = \tilde{r}_0 \tag{3.12a}$$

$$\varepsilon^j : r_j = \tilde{r}'_{j-1} + \tilde{r}_j - (PQ_1)'\tilde{r}_0, \quad j = 1, 2, \cdots \tag{3.12b}$$

Equation (3.11a) together with $\overline{\tilde{r}}_{-1}(0) = 0$ yields $\overline{\tilde{r}}_{-1}$ such that $|\overline{\tilde{r}}_{-1}(\tau)| \leq Ce^{-\alpha t}$. Equation (3.12a) yields $\tilde{r}_0$. Applying the initial condition $\tilde{r}(0) = r^0$ we obtain $\overline{\tilde{r}}_0(0) = r^0 - \tilde{r}_0(0)$. Equation (3.11b) provides $\overline{\tilde{r}}_0$ now. Having determined these coefficients, $\tilde{r}^0 = \overline{\tilde{r}}_{-1}\varepsilon^{-1} + \overline{\tilde{r}}_0 + \tilde{r}_0$ fulfils

$$\varepsilon(\tilde{r}^0)' + (I + \varepsilon(PQ_1)')\tilde{r}^0 = r_\varepsilon + O(\varepsilon)$$

such that the usual stability argument proves (3.10) for $N = 0$. The proof is completed by successive computation of higher order approximations using (3.11) and (3.12). □

In a very short way we will give the respective results for dae's being tractable with index 3. Unfortunately, the things are essentially more complex than in the index 2 case. We do not investigate the pencil regularization here. First of all let us mention that März' parameterization (2.15) does not work for general index 3 dae's.

Example. Let $m = 3$,

$$A(t) = \begin{pmatrix} 0 & 1 & 0 \\ 0 & \alpha t & 1 \\ 0 & 0 & 0 \end{pmatrix}, \quad B(t) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1+\alpha & 0 \\ 0 & \alpha t & 1 \end{pmatrix}, \quad \alpha \in R. \tag{3.13}$$

With these matrices, (2.1) is tractable with index 3 for every fixed α. We obtain

$$A + \varepsilon B_1 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & \alpha t + \varepsilon(1+\alpha) & 1 \\ 0 & \varepsilon\alpha t & \varepsilon \end{pmatrix}.$$

Computing $A_{1\varepsilon}$ it is easy to show that (2.15) is transferable if and only if $\alpha \neq -1$. If $\alpha = -1$, (2.15) is tractable with index 2 on every subinterval of R not containing 0.

In [Han90a] we proposed to use

$$(A + \varepsilon \tilde{B}_1)(Px)' + B_0 x = q \ , \tag{3.14}$$

instead. According to the definition of dae's being tractable with index 3 let $Q_{2,s} = Q_2 A_3^{-1} \tilde{B}_2$. $Q_{2,s}$ is a projection onto $\mathcal{N}(\tilde{A}_2)$. Choose Q_1 such that $Q_1 Q = 0$ and $Q_2 = Q_{2,s}$. Then the analogue of (.11) is

$$\begin{aligned}
& z' + (PP_1P_2A_3^{-1}\tilde{B}_1 - (PP_1P_2)')z - (PP_1P_2)'y = \\
& \qquad PP_1P_2A_3^{-1}q && \text{(3.15a)}\\
& y = PP_1Q_2A_3^{-1}q && \text{(3.15b)}\\
& r = PQ_1P_2A_3^{-1}q + PQ_1Q_2(y'+z') - PQ_1P_2A_3^{-1}\tilde{B}_1 z && \text{(3.15c)}\\
& s = QP_1P_2A_3^{-1}q + QQ_1(r'+y'+z') - QP_1P_2(y'+z') && \text{(3.15d)}\\
& (I - PP_1P_2(0))z(0) = 0 && \text{(3.15e)}
\end{aligned}$$

where $z = PP_1P_2x$, $y = PP_1Q_2x$, $r = PQ_1x$, $s = Qx$. Again it is easy to see that some components of q must be twice continuously differentiable in order that (2.1) has a solution. The "bad" behaviour of the index 3 problem is due to the nullspace component $s = Qx$. In a manner similar to Theorem 2 it is now easy to establish an existence and uniquness theorem. Instead of doing so we state the following assumption.

Assumption (LP3). (i) Equation (2.1) is tractable with index 3, $Q_1 Q = 0$, $Q_2 \equiv Q_{2,s} = Q_2 A_3^{-1}\tilde{B}_2$.
(ii) In (2.2) $D_0 = D_0 PP_1P_2(0)$, $D_1 = D_1 PP_1P_2(1)$, rank $\begin{pmatrix} D_0 & D_1 \\ I - PP_1P_2(0) & 0 \end{pmatrix} = m$.
(iii) Equations (2.1), (2.2) have a unique solution x_0.

Equation (3.14) can now be expanded to the system

$$\begin{pmatrix} \varepsilon y' \\ z' \\ Dy' + \varepsilon r \end{pmatrix} = \begin{pmatrix} U_{11}(\varepsilon) & & \\ & \ddots & \\ & & U_{33}(\varepsilon) \end{pmatrix} \begin{pmatrix} y \\ z \\ r \end{pmatrix} + \begin{pmatrix} f(\varepsilon) \\ g(\varepsilon) \\ h(\varepsilon) \end{pmatrix} \tag{3.16}$$

with cofficients and right-hand sides being analytic with respect to ε whose reduced version is just (3.15a), (3.15b), (3.15c). Moreover, $D = PQ_1Q_2$ does not vanish. In order to obtain a system in the standard singularly perturbed form (3.7) the first equation of (3.16) should be differentiated. After some algebraic manipulations a system of the form (3.7) arises where the matrix W of Theorem 6(iv) is given by

$$W = \begin{pmatrix} -I + (PP_1Q_2A_3^{-1}\tilde{B}_1)'PQ_1Q_2 & -(PP_1Q_2A_3^{-1}\tilde{B}_1)'PQ_1 \\ PQ_1Q_2 & -I \end{pmatrix} . \tag{3.17}$$

The eigenvalues of W determine the convergence behaviour of the solutions of (3.14) provided that appropriate boundary conditions are given. Unfortunately, the eigenvalues of W may vary almost arbitrarily.

Example. Let A, B be given by (3.13). It holds

$$W = \begin{pmatrix} -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & -\alpha^2 t & -(1+\alpha) & 0 & \alpha & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & -\alpha t & -1 & 0 & -1 & 0 \\ 0 & (\alpha t)^2 & -\alpha t^2 & 0 & 0 & -1 \end{pmatrix} .$$

The eigenvalues of W are -1 (fourfold) and the zeros of $\lambda^2+(2+\alpha)\lambda+1+2\alpha = 0$. The real parts of these eigenvalues can have an arbitrary sign in dependence on α.

In order to get an idea of the most desired properties of the parameterization recall that we need that (3.14) works at least for semiexplicit systems (2.6). After some tedious calculations one obtains for (2.6)

$$W = \begin{pmatrix} -I & W_1 & 0 & W_3 & 0 & 0 \\ 0 & -I & 0 & 0 & 0 & 0 \\ 0 & 0 & -I & 0 & 0 & 0 \\ 0 & W_2 & 0 & -I & 0 & 0 \\ 0 & 0 & 0 & 0 & -I & 0 \\ 0 & 0 & 0 & 0 & 0 & -I \end{pmatrix}$$

with some matrix functions W_1, W_2, W_3. W has the eigenvalues -1 only. Therefore, it is reasonable to *require* that the eigenvalues $\lambda_i(t)$ of (3.17) fulfil

$$\Re(\lambda_i(t)) \le -\sigma < 0, t \in [0,1] \ . \tag{3.18}$$

Theorem 9. *Let (LP3) and (3.18) hold true. Then (3.14), (2.2) together with the additional initial conditions*

$$PP_1Q_2x(0) = PP_1Q_2A_3^{-1}q(0), \tag{3.19a}$$

$$\begin{aligned} PQ_1x(0) = {} & PQ_1P_2A_3^{-1}q(0) + PQ_1Q_2(PP_1Q_2A_3^{-1}q)'(0) \\ & + PQ_1Q_2(PP_1P_2)'(PP_1Q_2A_3^{-1}q(0) + PP_1P_2x(0)) \\ & - PQ_1P_2A_3^{-1}\tilde{B}_1PP_1P_2x(0) \end{aligned} \tag{3.19b}$$

has a unique solution x_ε for sufficiently small $\varepsilon > 0$. Moreover, the asymptotic expansion

$$x_\varepsilon(t) \simeq \sum_{j=0}^{N} (x_j(t) + \overline{x}_j(\tau))\varepsilon^j$$

holds, where $\tau = t/\varepsilon$, $|\overline{x}_j(\tau)| \le Ce^{-\alpha\tau}$, $\alpha > 0$.

Remark. (i) In Theorem 9 we did not obtain unbounded boundary layers. This is due to the fact that we stated the additional initial conditions exactly. Otherwise, unbounded boundary layers would occur. In practice it is very hard to compute these exact initial conditions [LPG].

(ii) For general index 3 problems, (3.14) is of theoretical interest only, because of the complex way the various projectors are involved. When being applied analytical preprocessing is necessary (and possible, e. g. for semiexplicit systems).
(iii) For (2.6), (3.19) has the very simple form

$$0 = B_{32}v(0) + q_3(0), 0 = \frac{d}{dt}(B_{32}v(0) + q_3(0)) \ .$$

4 Steps Towards a Nonlinear Regularization Theory

In the present section we will give an overview of the first steps towards a nonlinear theory of regularization methods. We will do it in the spirit of the consideration of the previous section. Unfortunately, the results are far from being complete. Essentially, we know what to do for semiexplicit systems in Hessenberg form. However, there is some evidence that more general systems can be dealt with, too. It seems to be superfluous to remark that some results about classical Tikhonov regularization have already been derived [EHN90].

In order to be more precise we must introduce some definitions. Again, we will follow [GM86]. Consider the nonlinear boundary value problem

$$F(x'(t), x(t), t) = 0 \tag{4.1}$$

$$G(x(0), x(1)) = 0 \ . \tag{4.2}$$

Here $F : R^m \times R^m \times [0,1] \rightarrow R^m$ and $G : R^m \times R^m \rightarrow R^r$ are continuous and continuously differentiable with respect to their first and second arguments. Later on, when deriving asymptotic representations, more smoothness properties will be necessary. In accordance with the linear theory, (4.1) is called a *normal dae* if $F_y(y,x,t) = \frac{\partial}{\partial y}F(y,x,t)$ is singular for all (y,x,t), the nullspace $\mathcal{N}(t) = \mathcal{N}(F_y(y,x,t))$ is independent of (y,x), and $\mathcal{N}(t)$ is smooth. Putting $P = I - Q$, (4.1) is equivalent to

$$F((Px)' - P'x, x, \cdot) = 0 \ . \tag{4.3}$$

The definition of a solution generalizes to (4.1) and (4.3) in an obvious way.

Definition. The nonlinear dae (4.1) is called *transferable (tractable with index 2, tractable with index 3) at x_0* if the linearized equation

$$A_* x' + B_* x = q \tag{4.4}$$

with

$$A_*(t) = F_y((Px_0)'(t) - P'(t)x_0(t), x_0(t), t)$$
$$B_*(t) = F_x((Px_0)'(t) - P'(t)x_0(t), x_0(t), t)$$

is transferable (tractable with index 2, tractable with index 3).

Let x_0 denote a solution of (4.1), (4.2) and (4.1) be transferable. Hence, the Frechet derivative which is just (4.4) becomes continuously invertible at x_0 provided that the boundary conditions are appropriately stated (Theorem 1). By the Implicit Function Theorem it follows that the nonlinear problem is also well-posed in this case. Intuitively, there is some evidence that the nonlinear problems share the properties of the identically named linear ones. Unfortunately, such an assertion can only be proved under more stringent assumptions. I share the opinion that the connection between nonlinear higher index problems and their linearizations is not fully understood up to now. Nevertheless, for our purposes, the notions introduced above have proved their value.

We consider three cases of semiexplicit dae's which arise in many applications, e. g. dynamical systems subject to balance invariants and constraint mechanical systems:

$$u' = f(u, v, \cdot) \tag{4.5a}$$
$$0 = g(u, v, \cdot) \tag{4.5b}$$

and

$$u' = f(u, v, \cdot) \tag{4.6a}$$
$$0 = g(u, \cdot) \tag{4.6b}$$

and

$$u' = f(u, v, w, \cdot) \tag{4.7a}$$
$$v' = g(u, v, \cdot) \tag{4.7b}$$
$$0 = h(v, \cdot) \tag{4.7c}$$

where all functions involved are sufficiently smooth. We assume g_v in (4.5), $g_u f_v$ in (4.6), and $h_v g_u f_w$ in (4.7) to be nonsingular at least locally around the solutions (u_0, v_0) and (u_0, v_0, w_0), respectively, if the equations are solvable. These systems are special cases of normal dae's with $x = (u, v)$ and $x = (u, v, w)$, respectively. The linearizations of (4.5), (4.6) and (4.7) are just (2.4), (2.5) and (2.6), respectively. Hence, they are transferable, tractable with index 2, and tractable with index 3, respectively, locally at their solutions.

In the introduction we have already seen that (4.5) and (4.6) share all properties of their linear counterparts. This is true for (4.7), too. We try to overcome their ill-posedness by regularization. Applying the pencil regularization (2.13) to (4.1) yields

$$F(x', x + \varepsilon x', \cdot) = 0 \tag{4.8}$$

whereas März' parameterization (2.15) provides

$$F(x', x + \varepsilon P(Px)', \cdot) = 0 \ . \tag{4.9}$$

In the special case of (4.6), (4.8) is equivalent to

$$u' = f(u + \varepsilon u', v + \varepsilon v', \cdot) \tag{4.10a}$$
$$0 = g(u + \varepsilon u', \cdot) \tag{4.10b}$$

whereas (4.9) leads to

$$u' = f(u + \varepsilon u', v, \cdot) \tag{4.11a}$$

$$0 = g(u + \varepsilon u', \cdot). \tag{4.11b}$$

A similar parameterization was investigated by Knorrenschild [Kno88], namely, (4.11b) together with (4.6a). The latter two parameterizations are obviously closely related since (4.11a) is a *regular* perturbation of (4.6a). A simple calculation shows that (4.11) is a singularly perturbed transferable dae, whereas the Jacobian of (4.10) with respect to $x' = (u', v')$ yields $\begin{pmatrix} I - \varepsilon f_u & -\varepsilon f_v \\ -\varepsilon g_u & 0 \end{pmatrix}$, which is nonsingular at least locally around $x_0 = (u_0, v_0)$ showing that (4.10) is an implicit singularly perturbed ordinary differential equation.

What assumptions are necessary in order to guarantee the existence of solutions of the parameterized equations and the convergence of these solutions towards the solution of the original problem? We consider (4.6) subject to the boundary condition

$$G(u(0), u(1)) = 0 \ . \tag{4.12}$$

Here we have taken into account that only boundary conditions for the non-nullspace components of x should be imposed. Let $x_0 = (u_0, v_0)$ be a solution and the index 2 condition be fulfilled at x_0. In order to be precise, let $f : R^n \times R^k \times [0,1] \to R^n$, $g : R^n \times [0,1] \to R^k$, $G : R^n \times R^n \to R^r$. Then, (4.6) is equivalent to

$$u' = f(u, v, \cdot) \tag{4.13a}$$

$$0 = g_u(u, \cdot) f(u, v, \cdot) + g_t(u, \cdot) \tag{4.13b}$$

$$0 = g(u(t_0), t_0) \tag{4.13c}$$

for some fixed $t_0 \in [0,1]$. Having in mind the singularly perturbed equation we choose $t_0 = 0$ since we have learnt from the linear case that boundary layers can only be located at the left-hand boundary. (4.13a), (4.13b) is a transferable dae at x_0 subject to the boundary conditions (4.12), (4.13c). In order to apply the Implicit Function Theorem the linearization of (4.13), (4.12) is required to be continuously invertible. To show this, apply Theorem 1. The linearization of (4.13), (4.12) at x_0 leads to a linear equation (2.1) with

$$A = \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix}, B = \begin{pmatrix} f_u & f_v \\ g_{uu} f + g_u f_u + g_{ut} & g_u f_v \end{pmatrix},$$

$$D_0 = \begin{pmatrix} G_{u(0)} & 0 \\ g_u & 0 \end{pmatrix}, D_1 = \begin{pmatrix} G_{u(1)} & 0 \\ 0 & 0 \end{pmatrix},$$

where all functions are evaluated at $x_0 = (u_0, v_0)$. For the boundary conditions,

$$\begin{pmatrix} D_0 & D_1 \\ Q(0) & 0 \end{pmatrix} = \begin{pmatrix} G_{u(0)} & 0 & G_{u(1)} & 0 \\ g_u & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & I & 0 & 0 \end{pmatrix}.$$

This matrix has full rank $m = n + k$ if and only if

$$\text{rank} \begin{pmatrix} G_{u(0)} & G_{u(1)} \\ g_u & 0 \end{pmatrix} = n \ .$$

Now, the homogeneous boundary value problem

$$\begin{aligned} z' + (PA_1^{-1}B_0 - P')z = 0 \\ D_0 z(0) + D_1 z(1) + 0, Qz(0) = 0 \end{aligned}$$

is equivalent to

$$u' = \{f_v(g_u f_v)^{-1}[g_{uu}f + g_u f_u + g_{ut}] - f_u\}u \tag{4.14a}$$
$$0 = g_u u(0) \tag{4.14b}$$
$$0 = G_{u(0)}u(0) + g_{u(1)}u(1) \tag{4.14c}$$

where $z = (u, 0)$. On the other hand, the linearization of (4.6), (4.12) is

$$\begin{aligned} u' &= f_u u + f_v v \\ 0 &= g_u u \\ 0 &= G_{u(0)}u(0) + G_{u(1)}u(1) \ . \end{aligned}$$

Differentiating the second equation once we see that this system is equivalent to

$$u' = f_u u + f_v v \tag{4.15a}$$
$$0 = g_{uu}fu + g_{ut}u + g_u(f_u u + f_v v) \tag{4.15b}$$
$$0 = g_u u(0) \tag{4.15c}$$
$$0 = G_{u(0)}u(0) + G_{u(1)}u(1) \ . \tag{4.15d}$$

Substituting $v = -(g_u f_v)^{-1}[g_{uu}f + g_u f_u + g_{ut}]\,u$ in (4.14a) shows that (4.14) and (4.15) are equivalent.[6] Summing up, the boundary value problem (4.6), (4.12) is isolatedly solvable if Assumption (NP2, 0, i, ii) below is fulfilled.

Assumption (NP2). (0) $f : R^n \times R^k \times [0,1] \to R^n$, $g : R^n \times [0,1] \to R^k$, $G : R^n \times R^n \to R^r$.
(i) (4.6), (4.12) has a solution (u_0, v_0) and $g_u(u_0(t), t)f_v(u_0(t), v_0(t), t)$ is nonsingular for every $t \in [0,1]$.
(ii) $r = n - k$, the matrix

$$\begin{pmatrix} G_{u(0)}(u_0(0), u_0(1)) & G_{u(1)}(u_0(0), u_0(1)) \\ g_u(u_0(0), 0) & 0 \end{pmatrix}$$

has full rank n, and the homogeneous linearized boundary value problem

$$\begin{aligned} u' &= f_u(u_0, v_0, \cdot)u + f_v(u_0, v_0, \cdot)v \\ 0 &= g_u(u_0, \cdot)u \\ 0 &= G_{u(0)}(u_0(0), u_0(1))u(0) + G_{u(1)}(u_0(0), u_0(1))u(1) \end{aligned}$$

[6] For short: Linearization and index reduction commute for semiexplicit systems.

has the trivial solution only.
(iii) The nonlinear equation

$$g_u(u_0(0),0)f(u_0(0),\beta,0)=0 \tag{4.16}$$

has a solution $\beta_0 \in R^k$ sufficiently close to $v_0(0)$.

Remark. (i) Because of (NP2, i), (4.6) is tractable with index 2 locally around (u_0,v_0). Moreover, $k \leq n$ such that $r \geq 0$ in (NP2, ii). $r=0$ means simply that no boundary conditions are allowed.
(ii) Since (u_0,v_0) is a solution of (4.6), we obtain, by differentiating (4.6b), $g_u(u_0(0),0)f(u_0(0),v_0(0),0)+g_t(u_0(0),0)=0$, i. e. (NP2, iii) is fulfilled if g is an autonomous constraint.

Equation (4.12) gives only $r<n$ boundary conditions. In order to obtain a full set of boundary conditions, namely n, one should add

$$0=g(u(0),0)\ . \tag{4.17}$$

Compare Theorem 7 and the remark following it.

The importance of (4.17) lies in the fact that no unbounded boundary layers are allowed. Besides its practical significance this fact allows to handle the nullspace component v and the non-nullspace component u together without decoupling. In contrast to the linear case, such a decoupling is impossible for nonlinear systems.

For transferable dae's, $v_\varepsilon(0)$ is given by $u_\varepsilon(0)$ and the algebraic relations. (NP2, iii) guarantees that (i) $v_\varepsilon(0)$ is uniquely deteremined for sufficiently small $\varepsilon>0$, (ii) $v_\varepsilon(0)$ has an asymptotic expansion in powers of ε with the solution β_0 of (4.16) giving its first term, and (iii) β_0 belongs to the domain of attraction of the attraction point $v_0(0)$ of the auxiliary equation

$$\begin{aligned}\tilde{v}' = &-[g_u(u_0(0),0)f_v(u_0(0),v_0(0),0)]^{-1}\times\\ &\{g_u(u_0(0),0)f_v(u_0(0),\tilde{v},0)+g_t(u_0(0),0)\}\end{aligned}$$

which is the equivalent of hypothesis (vi) of Theorem 6.

As one expects from the linear case, after some tedious calculations one obtains that the relevant matrix $W(t)$ is the negative identity. Theorem 6 yields now immediately

Theorem 10 [Han90b]. *Let (NP2) hold. Then, for sufficiently small $\varepsilon>0$, the boundary value problem (4.11), (4.12), (4.17) has exactly one solution $(u_\varepsilon,v_\varepsilon)$ in a neighbourhood of (u_0,v_0). These solutions have asymptotic expansions*

$$u_\varepsilon(t)\simeq u_0(t)+\sum_{j=1}^{N}(u_j(t)+\overline{u}_j(\tau))\varepsilon^j \tag{4.18a}$$

$$v_\varepsilon(t)\simeq \sum_{j=0}^{N}(v_j(t)+\overline{v}_j(\tau))\varepsilon^j \tag{4.18b}$$

where $\tau=t/\varepsilon$, $|\overline{u}_j(\tau)|,|\overline{v}_j(\tau)|\leq Ce^{-\alpha t}$, $\alpha>0$.

Remark. Obviously, the same result is true for Knorrenschild's parameterization (4.6a), (4.11b) subject to the boundary conditions (4.12), (4.17).

Corollary 11. *Let (NP2) hold. Then, for sufficiently small $\varepsilon > 0$, the pencil regularization (4.10) subject to the boundary conditions (4.12), (4.17) and some* fixed *initial condition $v_\varepsilon(0) = v^0$ has exactly one solution $(u_\varepsilon, v_\varepsilon)$ in a neighbourhood of (u_0, v_0). These solutions possess asymptotic expansions (4.18).*

Proof. Replace $v + \varepsilon v'$ by r in (4.10). This yields März' parameterization (4.11) for u, r. Applying Theorem 10 with $v_0 = r_0$ provides (4.18a) and (4.18b) for r_ε. Now, v_ε is determined by the initial value problem

$$\varepsilon v' + v = r_\varepsilon, v(0) = v^0 \ .$$

Repeating the proof of the corollary of Theorem 7 shows that (4.18b) holds for v_ε, too. □

Remark. Our philosophy of stating the necessary additional boundary conditions has two aims: Firstly, the inherent structure of a dae with an index greater than 0 determines the nullspace component completely once u is given, and secondly, we try to use easily available information from the given system. In [Kno88] another method for initial value problems is proposed. Instead of $G(u(0)) = 0$, $g(u(0), 0) = 0$ the initial condition

$$u(0) + \varepsilon f(u(0), v_0(0), 0) = u_0(0)$$

is used. The advantage of this choice is that even in v_ε there are no boundary layers, i. e. $\overline{v}_0 = 0$. But usually $u_0(0)$ and $v_0(0)$ are not known, and the numerical computation of these values is a severe problem for higher index equations (see the paper of Hansen in this volume).

We shortly describe the results in the index 3 case. The general idea follows the lines of the proofs for (4.11). Unfortunately, the technical expense is enormous.

Consider the nonlinear semiexplicit dae which is tractable with index 3

$$u' = f(u, v, w, \cdot) \tag{4.19a}$$
$$v' = g(u, v, \cdot) \tag{4.19b}$$
$$0 = h(v) \tag{4.19c}$$

subject to the boundary condition

$$G(u(0), v(0), u(1), v(1)) = 0 \ . \tag{4.20}$$

Instead of using (4.9) directly we propose a simplified version

$$u' = f(u, v, w, \cdot) \tag{4.21a}$$
$$v' = g(u + \varepsilon u', v, \cdot) \tag{4.21b}$$
$$0 = h(v + \varepsilon v') \tag{4.21c}$$

which is a regular perturbation of (4.9). We introduce

Assumption (NP3). (0) $f : R^n \times R^k \times R^l \times [0,1] \to R^n$, $g : R^n \times R^k \times [0,1] \to R^k$, $h : R^k \to R^l$, $G : R^n \times R^k \times R^n \times R^k \to R^r$.
(i) w appears only linearly in f, i. e. $f_{ww}(u, v, w, \cdot) \equiv 0$.
(ii) The problem (4.19), (4.20) has a solution (u_0, v_0, w_0) and

$$h_v(v_0(t))g_u(u_0(t), v_0(t), t)f_w(u_0(t), v_0(t), w_0(t), t)$$

is nonsingular for every $t \in [0, 1]$.
(iii) $r = n - k + 2l$, the matrix

$$\begin{pmatrix} G_{u(0)}(\phi_1) & G_{v(0)}(\phi_1) & G_{u(1)}(\phi_1) & G_{v(1)}(\phi_1) \\ 0 & h_v(v_0(0)) & 0 & 0 \\ h_v(v_0(0))g_u(\phi_2) & h_v(v_0(0))g_v(\phi_2) & 0 & 0 \end{pmatrix},$$

where $\phi_1 = (u_0(0), v_0(0), u_0(1), v_0(1))$ and $\phi_2 = (u_0(0), v_0(0), 0)$, has full rank $n + k$, and the homogeneous linearized boundary value problem

$$\begin{aligned} u' &= f_u(u_0, v_0, w_0, \cdot)u + f_v(u_0, v_0, w_0, \cdot)v + f_w(u_0, v_0, w_0, \cdot)w \\ v' &= g_u(u_0, v_0, \cdot)u + g_v(u_0, v_0, \cdot)v \\ 0 &= h_v(v_0)v \\ 0 &= G_{u(0)}(\phi_1)u(0) + G_{v(0)}(\phi_1)v(0) + G(u(1)(\phi_1)u(1) + G_{v(1)}(\phi_1)v(1) \end{aligned}$$

has the trivial solution only.
(iv) The equation

$$\begin{aligned} &h_v(v_0(0))g_u(u_0(0), v_0(0), 0)f(u_0(0), v_0(0), \beta_0, 0) = \\ &-\frac{1}{2}h_{vv}(v_0(0))g^2(u_0(0), v_0(0), 0) \end{aligned}$$

has a solution $\beta_0 \in R^l$ sufficiently close to $w_0(0)$.

Remark. (i) Because of (NP3, ii), (4.19) is tractable with index 3 locally around (u_0, v_0, w_0). Moreover, $n, k \geq l$ such that $r \geq 0$ in (NP3, iii). $r = 0$ means simply that no boundary conditions are allowed at all.
(ii) (NP3, iii) causes (4.19), (4.20) to be uniquely solvable in a neighbourhood of (u_0, v_0, w_0).
(iii) In (4.19c) we assumed the algebraic constraint to be autonomous. This is a severe restriction. Since (4.21) is a transferable dae, $w_\varepsilon(0)$ is completely determined by $u_\varepsilon(0)$ and $v_\varepsilon(0)$. In agreement with the index 2 case, an asymptotic expansion of $w_\varepsilon(0)$ has to be established. This expansion does *not* exist for general nonautonomous constraints. However, (4.19c) can be slightly relaxed, namely, $h_t(v_0(0), 0) = 0$ for nonautonomous h.
(iv) In general, $\beta_0 \neq w_0(0)$ since $w_0(0)$ is the solution of

$$\begin{aligned} &h_v(v_0(0))g_0(u_0(0), v_0(0), 0)f(u_0(0), v_0(0), w_0(0), 0) = \\ &- h_{vv}(v_0(0))g^2(u_0(0), v_0(0), 0) - h_v(v_0(0))g_t(u_0(0), v_0(0), 0) \\ &- h_v(v_0(0))g_v(u_0(0), v_0(0), 0)g(u_0(0), v_0(0), 0) \end{aligned}$$

(v) (NP3, i) is necessary for the asymptotic expansion in powers of ε to hold. By a straightforward computation one obtains an auxiliary problem which is a singular singularly perturbed problem. Using (NP3, i) this problem can be further reduced. It is not known whether expansions in noninteger powers of ε exist if (NP3, i) is not fulfilled. However, in many applications w represents some kind of a Lagrange multiplier such that (NP3, i) is no serious restriction.

For the solution of (4.19), $h(v_0(0)) = 0$ and $h_v(v_0(0))g(u_0(0), v_0(0), 0) = 0$. In order to obtain additional boundary conditions, besides (4.20), we use (cf. Theorem 9)

$$0 = h(v(0)) \tag{4.22a}$$

$$0 = h_v(v(0))g(u(0), v(0), 0) \ . \tag{4.22b}$$

Theorem 12 [Han90b]. *Let (NP3) hold. Then, for sufficiently small $\varepsilon > 0$,*
(i) (4.21) is a transferable dae;
(ii) (4.21), (4.20), (4.22) has exactly one solution $(u_\varepsilon, v_\varepsilon, w_\varepsilon)$ in a neighbourhood of (u_0, v_0, w_0);
(iii) the asymptotic expansions

$$u_\varepsilon(t) \simeq u_0(t) + \sum_{j=1}^{N}(u_j(t) + \overline{u}_j(\tau))\varepsilon^j$$

$$v_\varepsilon(t) \simeq v_0(t) + \sum_{j=1}^{N}(v_j(t) + \overline{v}_j(\tau))\varepsilon^j$$

$$w_\varepsilon(t) \simeq \sum_{j=0}^{N}(w_j(t) + \overline{w}_j(\tau))\varepsilon^j$$

hold, where $\tau = t/\varepsilon$, $|\overline{u}_j(\tau)|, |\overline{v}_j(\tau)|, |\overline{w}_j(\tau)| \le Ce^{-\alpha t}$, $\alpha > 0$.

Remark. Analogous results are valid if (4.8) or (4.9) are used for (4.19).

5 Numerical Solution and Examples

Last but not least there remains the problem of numerically solving the regularized equations. At present a number of methods and codes for solving boundary value problems for transferable dae's are known (see this volume). 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 we are interested in the solution for $\varepsilon \to 0$ only, 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 [Sto72, Ste73]. Assuming that some quantity q (say, with values in a Banach space) is a smooth function of a parameter ε, some values $q(\varepsilon_0),\dots,q(\varepsilon_n)$ are computed. An estimation of $q(0)$ is obtained via an interpolation function (usually a polynomial or a rational function) interpolating the known values. A justification of such a process can be given using asymptotic expansions. We quote a related result.

Theorem 13 ([Ste73], Theorem 1.4.2, Corollary 1.4.4). *Let $q:(0,\overline{\varepsilon})\to X$, for some Banach space X, have an asymptotic expansion*

$$q(\varepsilon)=q_0+\sum_{j=l}^{l+k}q_j\varepsilon^j+O(\varepsilon^{l+k+1})\ .$$

Denote, for $\rho=0,\dots,k$, $T_0^\rho=q(\varepsilon_\rho)$, $0<\varepsilon_k<\varepsilon_{k-1}<\cdots<\varepsilon_0$. Let p_r^i be the polynomial in ε with $(p_r^i)'(0)=\cdots=(p_r^i)^{(l-1)}(0)=0$ and $p_r^i(\varepsilon_\rho)=T_0^\rho$ $(\rho=i,\dots,i+r)$. Now define $T_r^i=p_r^i(0)$. Then

$$T_r^i=q_0+(\varepsilon_{i+r}^l\prod_{\rho=i}^{i+l-1}\varepsilon_\rho)K_{lr}(\varepsilon_i,\dots,\varepsilon_{i+r})q_{l+r}+R_{ir}$$

where K_{lr} are homogeneous functions of the 0^{th} order of their arguments. In particular, $K_{1r}\equiv(-1)^r$. If, moreover, $\varepsilon_\rho=\beta\varepsilon_{\rho-1}$ for some fixed $0<\beta<1$, then

$$T_r^0=q_0+O(\varepsilon^{l+r})\ .$$

The assertion of the theorem shows that the order of convergence will be better after extrapolation. The computation of the T_r^i can be carried out by Neville's algorithm [Sto72] or, for $p>1$, by a similar one [BS64].

Corollary 14. *Let $x_\varepsilon\in C[0,1]$ have an asymptotic expansion*

$$x_\varepsilon(t)\simeq\sum_{j=0}^{N}(x_j(t)+\overline{x}_j(\tau))\varepsilon^j$$

with $\tau=t/\varepsilon$, and $|\overline{x}(\tau)|\le Ce^{-\alpha\tau}$, $\alpha>0$. Assume $\varepsilon_\rho=\beta\varepsilon_{\rho-1}$, $\rho=1,\dots,N$ for some $0<\beta<1$. Then, for the extrapolated values, it holds

$$T_r^0(t)=\begin{cases}x_0(0)+\overline{x}_0(0)+O(\varepsilon^{r+1}), & \text{if } t=0\\ x_0(0)+O(\varepsilon^{r+1}), & \text{if } t\in(0,1]\end{cases}\ .$$

Moreover, for every $0<a<1$,

$$\sup_{t\in[a,1]}|T_r^0(t)-x_0(t)|\le C(a)\varepsilon^{r+1}.$$

The proof is obvious.

As a simple example we 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 order to obtain a system in standard form, introduce $p = \dot{x}$, $q = \dot{y}$ such that (5.1) becomes

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

This system has the form (4.19) with $u = (p, q)$, $v = (x, y)$, $w = \lambda$, and $h_v g_u f_w = -2x^2 - 2y^2 \equiv -2$ in a solution of (5.2). Hence, (5.2) is tractable with index 3. In order to obtain an index 2 system we follow a proposal of [GGL85]: Introduce an artificial Lagrange multiplier μ that vanishes identically in a solution:

$$\begin{aligned} \dot{x} &= p - x\mu \\ \dot{y} &= q - y\mu \\ \dot{p} &= -x\lambda \\ \dot{q} &= -g - y\lambda \\ x^2 + y^2 &= 1 \\ 2xp + 2yq &= 0 \ . \end{aligned} \tag{5.3}$$

Equation (5.3) has the form (4.6) with $u = (x, y, p, q)$, $v = (\lambda, \mu)$, and

$$g_u f_v = -\begin{pmatrix} 0 & 2x^2 + 2y^2 \\ 2x^2 + 2y^2 & 2xp + 2yq \end{pmatrix} = \begin{pmatrix} 0 & -2 \\ -2 & 0 \end{pmatrix}$$

in a solution. Hence, (5.3) is tractable with index 2. We will compute the period of the pendulum if its initial state is the horizontal position $x = 1$, $y = 0$ with no impulse, i. e. $\dot{x} = 0$, $\dot{y} = 0$. Introducing T to be one fourth of the period we obtain the following boundary value problem

$$\begin{aligned} \dot{x} &= T(p - x\mu) \\ \dot{y} &= T(q - y\mu) \\ \dot{p} &= -Tx\lambda \\ \dot{q} &= -T(g + y\lambda) \\ \dot{T} &= 0 \\ x^2 + y^2 &= 1 \\ 2xp + 2yq &= 0 \\ y(0) &= 0 \\ q(0) &= 0 \\ x(1) &= 0 \ . \end{aligned} \tag{5.4}$$

Equation (5.4) is again an index 2 problem of the form (4.6). In the following computations we have chosen $g = 13.750371636041$, which leads to $T = \frac{1}{2}$.

As a standard boundary value solver we used a simplification of Degenhardt's algorithm (a fourth order collocation code with automatic grid selection and error control) for semiexplicit systems (see this volume). Since the computations were done in double precision on an AT-386 running MS-DOS, the main restriction was the small memory of about 500k. Nevertheless, we were able to solve the parameterized problem (4.6a), (4.11b) for parameters $\varepsilon = 10^{-1} \cdots 10^{-8}$ and tolerances of $10^{-5} \cdots 10^{-6}$. For $\varepsilon > 10^{-1}$, Newton's method did not converge when solving the discretized equation, and, for $\varepsilon < 10^{-8}$, the code reported that the system was not transferable. We always used $\beta = \frac{1}{2}$.

The exact solution of (5.1) cannot be analytically expressed. Only the period can be obtained via incomplete elliptic integrals. Instead, we used a solution computed by means of the program RADAU5 [HW88] with a high precision (10^{-8}) in an initial value formulation 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 "boundary layer region" and $[0.2, 1]$ as the "smooth region".

Table 1 contains typical results.[7] The theoretical values $T_i^{\rho+1}/T_i^{\rho}$ should approach 2.0, 4.0, 8.0, 16.0. For the pendulum, the third columns show that even $u_1 = 0$ and $v_1 = 0$, and no boundary layers are present. Unfortunately, I was not able to prove this behaviour strictly. Taking into account this observation we tried a new extrapolation experiment (Table 2). Now, the results were as expected from the theory and the used tolerance. In the non-nullspace components they were even better.

We also tried to solve the same problem in the index 3 formulation. However, for our initial guess, Newton's method converged only for $\varepsilon = 5 \times 10^{-3} \cdots 10^{-4}$. We were not able to obtain approximations for tolerances below 10^{-3} due to memory limitations. So Table 3 is of limited value only. In this table, one can see that $w = \lambda$ has a boundary layer as predicted by the theory.

6 Conclusions

We investigated two approaches to the regularization problem for higher index differential-algebraic equations which are closely related. One approach aimed at transferable dae's, the other one at implicit ordinary differential equations. From an analytic point of view, the first one seems to be more elegant and more flexible than the second one. If both parameterizations are applicable, the pencil regularization leads to singular singularly perturbed equations which can be handled by a wide variety of known methods. On the other hand, this singular perturbation is more severe than März' parameterization (and its derivatives), which lead to singularly perturbed dae's. In the index 2 case, for a constant nullspace, standard solvers work well for the latter problem. If this nullspace is time-dependent, it is shown that the backward differentiation formulae do

[7] In the tables we denote $\alpha_i = T_i^{\rho+1}/T_i^{\rho}$. The notation $a.b(c)$ means $a.b \times 10^c$.

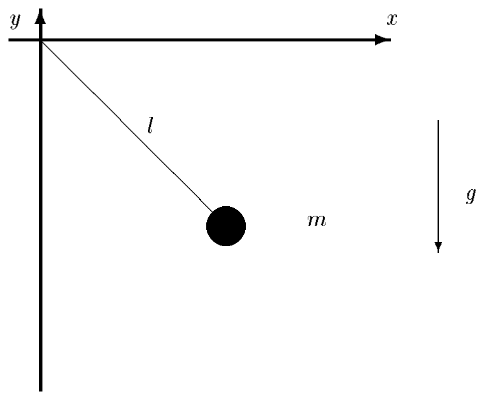

Fig. 1. The mathematical pendulum

not work [KM89] in contrast to what could be expected from the ode case. Recall that the pencil regularization does not apply for a non-constant nullspace. For index 3 systems, the situation is even worse. With the exeption of constant coefficient systems and systems, that are transferable to constant coefficient systems by simple methods [Cam83], the pencil regularization is not applicable. This behaviour reminds of similar properties of backward differentiation formulae [Mar90a]. For semiexplicit index 3 systems in Hessenberg form, the results of [BE88] are also discouraging. Runge-Kutta methods seem to work a little bit better [HLR89] for initial value problems. Applying our regularization method to index 3 systems, we expect difficulties for small ε, too. This is indicated by the bad behaviour of our collocation solver[8], which works very efficient and reliable for well-conditioned problems [Deg88], for the index 3 problem. To overcome these troubles, extrapolation procedures seem to be favourable as indicated above. In order to construct an efficient code many important questions must be answered. For instance, how to discretize, how to estimate the error, how accurate to solve the discrete equations, how far to extrapolate and so on. While the experience from boundary value problems for ode's suggests to use symmetric collocation methods, we think that, on account of the boundary layer at the left-hand side, Radau methods would behave better than symmetric formulae. All these questions are under investigation now. Results will be published elsewhere.

[8] This code bases on symmetric Lobatto formulae.

Table 1. $\varepsilon_0 = 10^{-2}$, tolerance 10^{-5}

u - boundary layer region

ε	T_0^ρ	α_0	T_1^ρ	α_1	T_2^ρ	α_2	T_3^ρ	α_3	T_4^ρ
1.00(-2)	2.64(-4)								
5.00(-3)	6.86(-5)	3.8	1.27(-4)						
2.50(-3)	1.75(-5)	3.9	3.37(-5)	3.8	2.98(-6)				
1.25(-3)	4.40(-6)	4.0	8.66(-6)	3.9	3.72(-7)	8.0	3.28(-8)		
6.25(-4)	1.11(-6)	4.0	2.19(-6)	3.9	4.62(-8)	8.0	9.30(-10)	35.2	2.26(-9)

u - smooth region

ε	T_0^ρ	α_0	T_1^ρ	α_1	T_2^ρ	α_2	T_3^ρ	α_3	T_4^ρ
1.00(-2)	7.56(-4)								
5.00(-3)	1.91(-4)	3.9	3.74(-4)						
2.50(-3)	4.80(-5)	4.0	9.50(-5)	3.9	7.57(-6)				
1.25(-3)	1.20(-5)	4.0	2.40(-5)	3.9	8.14(-7)	9.3	2.52(-7)		
6.25(-4)	3.01(-6)	4.0	6.02(-6)	4.0	9.64(-8)	8.4	9.56(-9)	26.3	7.09(-9)

v - boundary layer region

ε	T_0^ρ	α_0	T_1^ρ	α_1	T_2^ρ	α_2	T_3^ρ	α_3	T_4^ρ
1.00(-2)	4.46(-3)								
5.00(-3)	1.11(-3)	4.0	2.23(-3)						
2.50(-3)	2.79(-4)	4.0	5.58(-4)	4.0	1.43(-5)				
1.25(-3)	6.99(-5)	4.0	1.39(-4)	4.0	7.53(-6)	1.9	1.04(-5)		
6.25(-4)	1.83(-5)	3.8	3.54(-5)	3.9	8.43(-6)	0.9	8.59(-6)	1.2	8.46(-6)

v - smooth region

ε	T_0^ρ	α_0	T_1^ρ	α_1	T_2^ρ	α_2	T_3^ρ	α_3	T_4^ρ
1.00(-2)	1.93(-2)								
5.00(-3)	4.78(-3)	4.0	9.70(-3)						
2.50(-3)	1.19(-3)	4.0	2.40(-3)	4.0	3.05(-4)				
1.25(-3)	3.06(-4)	3.9	5.92(-4)	4.0	1.62(-4)	1.9	2.28(-4)		
6.25(-4)	1.49(-4)	2.0	1.37(-4)	4.3	1.83(-4)	0.9	1.86(-4)	1.2	1.83(-4)

Table 2. $\varepsilon_0 = 10^{-2}$, tolerance 10^{-5}

u - boundary layer region								
ε	T_0^ρ	α_0	T_1^ρ	α_1	T_2^ρ	α_2	T_3^ρ	α_3	T_4^ρ
1.00(-2)	2.64(-4)								
5.00(-3)	6.86(-5)	3.8	3.97(-6)						
2.50(-3)	1.75(-5)	3.9	4.95(-7)	8.0	2.20(-8)				
1.25(-3)	4.40(-6)	4.0	6.18(-8)	8.0	5.48(-9)	4.0	7.29(-9)		
6.25(-4)	1.11(-6)	4.0	8.29(-9)	7.4	2.88(-9)	1.9	2.71(-9)	2.7	2.57(-9)

u - smooth region									
ε	T_0^ρ	α_0	T_1^ρ	α_1	T_2^ρ	α_2	T_3^ρ	α_3	T_4^ρ
1.00(-2)	7.56(-4)								
5.00(-3)	1.91(-4)	3.9	9.84(-6)						
2.50(-3)	4.80(-5)	4.0	1.14(-6)	8.6	1.60(-7)				
1.25(-3)	1.20(-5)	4.0	1.69(-7)	6.7	4.62(-8)	3.5	5.99(-8)		
6.25(-4)	3.01(-6)	4.0	4.23(-8)	4.0	2.78(-8)	1.7	2.66(-8)	2.2	2.55(-8)

v - boundary layer region									
ε	T_0^ρ	α_0	T_1^ρ	α_1	T_2^ρ	α_2	T_3^ρ	α_3	T_4^ρ
1.00(-2)	4.46(-3)								
5.00(-3)	1.11(-3)	4.0	1.14(-5)						
2.50(-3)	2.79(-4)	4.0	1.49(-6)	7.6	3.31(-6)				
1.25(-3)	6.99(-5)	4.0	2.94(-6)	0.5	3.57(-6)	0.9	4.03(-6)		
6.25(-4)	1.83(-5)	3.8	5.68(-6)	0.5	6.07(-6)	0.6	6.24(-6)	0.6	6.31(-6)

v - smooth region									
ε	T_0^ρ	α_0	T_1^ρ	α_1	T_2^ρ	α_2	T_3^ρ	α_3	T_4^ρ
1.00(-2)	1.93(-2)								
5.00(-3)	4.78(-3)	4.0	2.39(-4)						
2.50(-3)	1.19(-3)	4.0	4.13(-5)	5.8	7.73(-5)				
1.25(-3)	3.06(-4)	3.9	6.42(-5)	0.6	7.81(-5)	1.0	8.82(-5)		
6.25(-4)	1.49(-4)	2.0	1.24(-4)	0.5	1.32(-4)	0.6	1.36(-4)	0.6	1.37(-4)

Table 3. $\varepsilon_0 = 5 \times 10^{-3}$, tolerance 10^{-3}

(u,v) - boundary layer region			
ε	T_0^ρ	$T_0^{\rho+1}/T_0^\rho$	T_1^ρ
5.00(-3)	1.81(-3)		
2.50(-3)	9.00(-4)	2.0	6.50(-5)

(u,v) - smooth region			
ε	T_0^ρ	$T_0^{\rho+1}/T_0^\rho$	T_1^ρ
5.00(-3)	1.10(-1)		
2.50(-3)	5.59(-2)	2.0	1.54(-3)

w - boundary layer region			
ε	T_0^ρ	$T_0^{\rho+1}/T_0^\rho$	T_1^ρ
5.00(-3)	1.04(-3)		
2.50(-3)	8.79(-4)	1.2	2.80(-3)

w - smooth region			
ε	T_0^ρ	$T_0^{\rho+1}/T_0^\rho$	T_1^ρ
5.00(-3)	9.05(-1)		
2.50(-3)	4.62(-1)	1.9	1.90(-2)

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