Sequential Regularization Methods for Nonlinear Higher Index DAEs

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Abstract

Sequential regularization methods relate to a combination of stabilization methods and the usual penalty method for differential equations with algebraic equality constraints. The present paper extends an earlier work [4] to nonlinear problems and to DAEs with index higher than 2. Rather than having one "winning" method, this is a class of methods from which a number of variants are singled out as being particularly effective methods in certain circumstances.

We propose sequential regularization methods for index-2 and index-3 DAEs, both with and without constraint singularities. In the case of no constraint singularity we prove convergence results. Numerical experiments confirm our theoretical predictions and demonstrate the viability of the proposed methods. The examples include constrained multibody systems.

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1 Introduction

It is well-known that differential-algebraic equations (DAEs) can be difficult to solve when they have a higher index, i.e. index greater than one (cf. [9]). Higher index DAEs are ill-posed in a certain sense, especially when the index is greater than two [6], and a straightforward discretization generally does not work well. An alternative treatment is the use of index reduction methods, whose essence is the repeated differentiation of the constraint equations until a low-index problem (an index-1 DAE or ODE) is obtained. But repeated index reduction by direct differentiation leads to instability of the resulting ODE, and this causes drift-off — the numerical error in the original constraint grows. Hence, stabilized index reduction methods were proposed to overcome the difficulty. A popular stabilization technique was introduced first in the computation of constrained multibody systems by Baumgarte [7]. Various improvements and additional techniques have been proposed and analyzed since, see e.g. [2, 3] and references therein. Another approach is the so-called regularization of DAEs where a small perturbation term (measured by a small positive parameter ϵ) is added to the original DAE (see, e.g., [11, 15, 14, 13, 19]). The regularized problem usually is a singular perturbation problem and the DAE becomes the reduced problem of this singular perturbation problem. Then a stiff solver is typically needed to solve the regularized problem. In a recent paper [4], a new method called *sequential regularization method* (SRM) was proposed for linear index-2 DAEs with initial or boundary conditions. It relates to a combination of Baumgarte's stabilization with the usual penalty method and to a method proposed in [22] in an optimization context. In [4], we have indicated that this method is particularly useful for DAEs with constraint singularities and that, unlike usual regularization, the regularization parameter (say, ϵ) does not have to be chosen very small. Therefore the regularized problem is less stiff and/or more stable. For a given ϵ a linear convergence analysis yields a much faster convergence rate for the SRM than for the method proposed in [19]. Furthermore, when there are no constraint singularities the regularized problem can be made essentially non-stiff for any ϵ, or it can be simplified in other ways. Because of these facts we believe that our SRM is an important improvement over the usual regularization methods.

In this paper, we generalize the SRM to nonlinear higher index DAEs, and then apply it to constrained multibody systems with or without singularities. As in [6, 2], we consider a nonlinear model DAE of order ν

$$x^{(\nu)} = f(x, x', \ldots, x^{(\nu-1)}, t) - B(x,t)y, \tag{1.1a}$$

$$0 = g(x,t). \tag{1.1b}$$

It has index $\nu + 1$ if GB is nonsingular for all t, $0 \leq t \leq t_f$, where $G = g_x$. We are interested in the cases $\nu = 1$ or 2. The Euler-Lagrange equations for mechanical systems with holonomic constraints are in this form with $\nu = 2$. The discussion also involves systems with constraint singularities, i.e. the case where GB is singular at some isolated t. A singularity in the constraints (or in the algebraic solution components) of a DAE may cause various phenomena to occur, including impasse points and bifurcations [21, 20]. In this paper, however, we consider a class of singular problems arising from multibody mechanical systems [1, 8, 12] (see the slider-crank example in §5) and assume that the solution sought is smooth and unique in the passage through isolated singularity points.

The paper is organized as follows: In §2 we consider index-2 problems without constraint singularities. SRM variants involving $\frac{dg}{dt}$ are analyzed in §2.1 (Theorem 2.1). They lead to nonstiff problems; the variant (2.12) with $E = I$ there is particularly attractive. Iterations not involving $\frac{dg}{dt}$ are considered in §2.2 (Theorem 2.2). Here the choice $E = I$ in (2.15), where possible, is recommended.

Index-2 nonlinear problems with constraint singularities are considered in §3. The SRM (3.2) is proposed for such problems. This variant works well in practice, but our proofs extend only to the linear case.

In §4 we analyze and discuss various methods for index-3 problems. A number of SRM variants are possible, combining regularization with Baumgarte's or an invariant's stabilization. Their relative utility depends on the application, and they each offer significant advantages in suitable circumstances. Of particular interest, in case of no constraint singularity, are the methods (4.12) and (4.14)–(4.16). The choice $E = I$ leads to particularly simple iterations. A corresponding convergence result is given in Theorem 4.1. In case of a possible constraint singularity the SRM (4.23) is recommended.

These methods are reformulated in §5 for the special case of multibody systems with holonomic constraints. The "winning" methods are (5.3)-(5.4) with $E = I$ for the nonsingular case and (5.5)-(5.6) for the case where the constraint Jacobian may have isolated rank deficiencies. In §6 we report the results of numerical experiments confirming our theoretical predictions and demonstrating the effect of the proposed methods.

2 Nonlinear, nonsingular index-2 problems

We consider the following nonlinear index-2 model problem ($\nu = 1$ in (1.1))

$$x' = f(x,t) - B(x,t)y \tag{2.1a}$$
$$0 = g(x,t) \tag{2.1b}$$

where f, B and g are sufficiently smooth functions of $(x,t) \in \mathbf{R}^{n_x} \times [0, t_f]$, and $y \in \mathbf{R}^{n_y}$. We consider this DAE subject to $n_x - n_y$ boundary conditions

$$b(x(0), x(t_f)) = \beta \, . \tag{2.2}$$

These boundary conditions are assumed to be such that they yield a unique[1] and bounded solution for the ODE (2.1a) on the manifold given by (2.1b). Concretely, if

[1]locally unique, or isolated solution in a sufficiently large neighborhood would suffice.

we were to replace (2.1b) by its differentiated form

$$0 = Gx' + g_t \quad (= \frac{dg}{dt}) \tag{2.3a}$$

$$g(x(0), 0) = 0 \tag{2.3b}$$

and use (2.3a) in (2.1a) to eliminate y and obtain n_x ODEs for x, then the boundary value problem for x with (2.2) and (2.3b) specified has a unique solution. In the initial value case (i.e. b is independent of $x(t_f)$), this means that (2.2) and (2.3b) can be solved uniquely for $x(0)$.

In this section we consider the case where GB is nonsingular. Generalizing the idea in [4], we have the following SRM formulation for the nonlinear index-2 differential-algebraic problem (2.1): for $s = 1, 2, \ldots,$

$$x_s' = f(x_s, t) - B(x_s, t)y_s, \tag{2.4}$$

where

$$y_s = y_{s-1} + \frac{1}{\epsilon}E(x_s, t)(\alpha_1 \frac{d}{dt}g(x_s, t) + \alpha_2 g(x_s, t)), \tag{2.5}$$

subject to the boundary conditions (2.2) and (2.3b). Note that $y_0(t)$ is a given initial iterate which we assume is sufficiently smooth and bounded and that $\epsilon > 0$ is the regularization parameter. The regularization matrix E is nonsingular and has a uniformly bounded condition number; possible choices are $E = I$, $E = (GB)^{-1}$ and others (e.g. $E = (GB)^T$, cf. [4, 19]). We note that if we take $y_0 \equiv y$ then $x_1 \equiv x$, where x and y are the solution of (2.1). If we take $y_0 \equiv 0$, then one SRM iteration is the usual penalty method (cf. [17, 18, 13]). As customary for the penalty method, we assume:

$H1$ *The problem (2.4), (2.5),(2.2),(2.3b) has a unique solution and the solution is bounded if y_{s-1} is bounded.*

Assumption $H1$ is generally true for initial value problems. For general boundary value problems, we expect that $H1$ would hold for most practical cases since (2.4) (with (2.5) plugged in) may be seen as a perturbed problem of (2.1) according to the proof of *Theorem 2.1* (see below), where the perturbation and its first derivative are both small if ϵ is small.

To analyze the SRM, we assume the following perturbation inequality: For $0 \le t \le t_f$,

$$\|\hat{x}(t) - x(t)\| \le M \max_{0 \le \tau \le t_f} (|\delta(\tau)| + |\delta'(\tau)|), \tag{2.6a}$$

$$\|\hat{y}(t) - y(t)\| \le M \max_{0 \le \tau \le t_f} (|\delta(\tau)| + |\delta'(\tau)|), \tag{2.6b}$$

where $\|\cdot\|$ is some l_p norm (say, maximum norm), and $\hat{x}$ and $\hat{y}$ satisfy the following perturbed version of (2.1):

$$\hat{x}' = f(\hat{x}, t) - B(\hat{x}, t)\hat{y}, \tag{2.7a}$$

$$0 = g(\hat{x}, t) + \delta(t) \tag{2.7b}$$

with the same boundary conditions as (2.2). For initial value problems, (2.6) has been proved in [10], pp. 478-481. It is actually the definition of the perturbation index introduced in [10]. Furthermore, (2.6) also holds for boundary value problems if we impose some boundedness conditions on the corresponding Green's function (cf. [5]).

The case $\alpha_1 \neq 0$ in (2.5) is sufficiently different from the case $\alpha_1 = 0$ to warrant a separate treatment.

2.1 The case $\alpha_1 = 1$

Now we estimate the error of the sequential regularization method (2.4)-(2.5). We prove a theorem which says that the error after s SRM iterations is $O(\epsilon^s)$ (i.e., each iteration improves the error by $O(\epsilon)$) everywhere in t.

Theorem 2.1 *Let all functions in the DAE (2.1) be sufficiently smooth and the above assumptions hold. Then, for the solution of iteration (2.4),(2.5) with $\alpha_1 \neq 0$, we have the following error estimates:*

$$\begin{aligned} x_s(t) - x_e(t) &= O(\epsilon^s), \\ y_s(t) - y_e(t) &= O(\epsilon^s), \end{aligned}$$

for $0 \le t \le t_f$ and $s \ge 1$.

Proof: Let $v_s = g(x_s, t)$. Then, from (2.4),

$$v_s' = G(x_s,t)x_s' + g_t(x_s,t) = G(x_s,t)f(x_s,t) - G(x_s,t)B(x_s,t)y_s + g_t(x_s,t).$$

Using (2.5), we thus have

$$\begin{aligned} (\epsilon(GBE)^{-1} + I)v_s' + \alpha_2 v_s &= \epsilon(GBE)^{-1}(Gf + g_t) - \epsilon E^{-1} y_{s-1}, && \text{(2.8a)} \\ v_s(0) &= 0. && \text{(2.8b)} \end{aligned}$$

Therefore it is not difficult to get

$$v_s = g(x_s,t) = O(\epsilon), \; v_s' = g(x_s,t)' = O(\epsilon), \tag{2.9}$$

if y_{s-1} is bounded (which implies that x_s is bounded).

For $s = 1$, we have

$$\begin{aligned} x_1' &= f(x_1,t) - B(x_1,t)y_1 \\ &\quad g(x_1,t) = O(\epsilon), \; g(x_1,t)' = O(\epsilon) \end{aligned}$$

since y_0 is chosen to be bounded. From assumption (2.6), we immediately get

$$x_1 - x_e = O(\epsilon), \; y_1 - y_e = O(\epsilon). \tag{2.10}$$

Then it is easy to see that y_1 is bounded. So for $s = 2$, we obtain

$$\begin{aligned} x_2' &= f(x_2, t) - B(x_2, t) y_2 \\ & \quad g(x_2, t) = O(\epsilon),\ g'(x_2, t) = O(\epsilon) \end{aligned}$$

By using assumption (2.6) again, this yields

$$x_2 - x_e = O(\epsilon).$$

Hence it can be verified, by substituting (2.3a),(2.1a) for the exact solution, that the right hand side of (2.8a) becomes $O(\epsilon^2)$. So, from (2.8), we can get

$$g(x_2, t) = O(\epsilon^2),\ g'(x_2, t) = O(\epsilon^2).$$

Applying assumption (2.6), it follows that

$$x_2 - x_e = O(\epsilon^2),\ y_2 - y_e = O(\epsilon^2). \tag{2.11}$$

This also gives the boundedness of y_2.

We can repeat this procedure, and, by induction, conclude the results of the theorem. □

From (2.8) it is clear that *there is no stiffness here*, so we can choose $\epsilon > 0$ very small, so small in fact that one SRM iteration would suffice for a desired accuracy, and discretize the regularized ODE possibly using a nonstiff method like explicit Runge-Kutta. This gives a modified penalty method

$$[I + \epsilon^{-1} BEG] x' = f - By_0 - \epsilon^{-1} BE(g_t + \alpha_2 g) \tag{2.12}$$

where B, E, g etc, all depend on x, with the subscript $s = 1$ suppressed.

For the choice $E = (GB)^{-1}$, let $P = BEG = B(GB)^{-1}G$ be the associated projection matrix. Multiplying (2.12) by $\frac{1}{1+\epsilon^{-1}} P$ and by $I - P$, respectively, and then adding together, we have

$$x' = f - \frac{1}{1 + \epsilon^{-1}} By_0 - \frac{\epsilon^{-1}}{1 + \epsilon^{-1}} B(GB)^{-1}[Gf + g_t + \alpha_2 g]$$

So the obtained iteration is similar to Baumgarte's stabilization

$$x' = f - B(GB)^{-1}[Gf + g_t + \alpha_2 g] \tag{2.13}$$

In fact, the single SRM iteration tends to (2.13) in this case when $\epsilon \to 0$. Indeed, the parameter α_2 is the usual Baumgarte parameter, and choosing $\alpha_2 > 0$ obviously makes equation (2.8a) asymptotically stable for the drift v_s. For both of these methods we can apply post-stabilization instead, i.e. take $\alpha_2 = 0$ but stabilize after each discretization step [2, 3].

For reasons of computational expense, it may be better to choose $E = I$ in (2.12). The obtained iteration is simple, although a possibly large matrix (with a special structure) must be "inverted".

Example 2.1 *The choice of $E = I$ was utilized in [16] for the time-dependent, incompressible Navier-Stokes equations governing fluid flow. The advantage gained is that no treatment of pressure boundary conditions is needed, unlike methods based on Baumgarte-type stabilizations which lead to the pressure-Poisson equation.* $\Box$

2.2 The case $\alpha_1 = 0$

For this case the drift equation (2.8) is clearly stiff for $0 < \epsilon \ll 1$. If we assume

$$y_0(0) = y_e(0),\, y_0'(0) = y_e'(0), \ldots, y_0^{(m)}(0) = y_e^{(m)}(0), \tag{2.14}$$

where $m = -1$ if $y_0(0) \neq y_e(0)$, then we can prove the same result as of *Theorem 2.1* for $s \leq m+1$ by a similar procedure. We omit the proof (see also *Theorem 3.1* of [4]), but state the theorem:

Theorem 2.2 *Let the assumptions of Theorem 2.1 plus (2.14) hold. In addition, suppose that the matrix function $E(x,t)$ has been chosen so that GBE is positive definite. Then, for the solution of iteration (2.4),(2.5) with $\alpha_1 = 0$, we have the following error estimates:*

$$\begin{aligned} x_s(t) - x_e(t) &= O(\epsilon^s), \\ y_s(t) - y_e(t) &= O(\epsilon^s), \end{aligned}$$

for $1 \leq s \leq m+1$ and $0 \leq t \leq t_f$. The convergence result holds for all s (i.e. also for $s > m+1$) away from an initial layer of size $O(\epsilon)$ in t.

Note that we may choose y_0 satisfying (2.14) for some $m \geq 0$ by expressing y in terms of x at $t = 0$ for initial value problems, but this starting procedure generally does not work for boundary value problems.

Taking $\alpha_2 = 1$ without loss of generality, we obtain the iteration

$$x_s' = f - By_{s-1} - \epsilon^{-1}BEg(x_s, t) \tag{2.15}$$

This is a singular, singularly perturbed problem (so ϵ should not be taken extremely small compared to machine precision even if a stiff solver is being used). If GB is positive definite then we may choose $E = I$, and this yields a very simple iteration in (2.15) which avoids the inversion necessary in stabilization methods like Baumgarte's. However, if an explicit discretization method of order p is contemplated then approximately p SRM iterations like (2.15) are needed, because one must choose $\epsilon = O(h)$, where h is the step size.

3 Nonlinear, singular index-2 problems

Next we consider the nonlinear index-2 problem (2.1) with an isolated singular point $t^\star$, i.e. GB is singular at $t^\star$. For simplicity, we assume that B and g are independent of t. Denote $P(x) = B(GB)^{-1}G$. Motivated by constrained multibody systems (see §4), we assume $P(x)$ to be differentiable in t, but $\frac{\partial P}{\partial x}(x)$ may be unbounded. For this reason, we consider only the case $\alpha_1 = 0$ in this section (cf. [4]). In the drift equation (2.8) we then have essentially the singularly perturbed operator $\epsilon v' + GBEv$ to consider. The choices of $E = I$ or $E = (GB)^T$ yield a turning point problem, which complicates the analysis, even in the linear case [4], and degrades the numerical performance as well in our experience. Therefore, we choose $E = (GB)^{-1}$. In the sequel we will be careful to evaluate the effect of E only when its singularity limit is well-defined, as e.g. in $P(x)$.

A direct generalization of [4] would give the SRM formulation (2.4) where instead of updating y (because y may be unbounded at t^*) we update By by

$$B(x_s)y_s = B(x_{s-1})y_{s-1} - \frac{1}{\epsilon}B(x_s)(G(x_s)B(x_s))^{-1}g(x_s). \qquad (3.1)$$

However, (3.1) needs to be modified, since we may have $RangeB(x_s) \neq RangeB(x_{s-1})$. So we use the projection $P(x_s)$ to move from $RangeB(x_{s-1})$ to $RangeB(x_s)$. Then we consider the following SRM formulation for singular problems:

$$x'_s = f(x_s, t) - B(x_s)y_s, \qquad (3.2a)$$

$$B(x_s)y_s = P(x_s)B(x_{s-1})y_{s-1} + \frac{1}{\epsilon}B(x_s)(G(x_s)B(x_s))^{-1}g(x_s), \qquad (3.2b)$$

where x_s satisfies the boundary condition (2.2).

If the assumptions given at the beginning of this section and in *Theorem 2.2* remain valid, then the result of *Theorem 2.2* (which generalizes the results of *Theorem 2.1*) still holds. Unfortunately, for the singular problem, assumption (2.6) may not be true in general. To see this, consider one iteration, i.e. $s = 1$. The accuracy for the approximation of x depends on the extent that the bound (2.6a) holds. Numerical experiments show that we can get a pretty good approximation of x near the singularity. But the situation for By is worse, and the bound (2.6b) often does not hold. Indeed, assume for the moment that we have a good, smooth approximation of x, say $x_s = \hat{x}$, i.e. (2.7) holds with $\delta, \delta' = O(\epsilon)$, and $B(\hat{x})\hat{y}$ is defined by (3.2b) for some $B(x_{s-1})y_{s-1}$. From (2.7) we have

$$B(\hat{x})\hat{y} = P(\hat{x})f(\hat{x}, t) + \eta, \qquad (3.3)$$

where $\eta = B(\hat{x})(G(\hat{x})B(\hat{x}))^{-1}\delta'$. It is not difficult to find that the exact $B(x)y$ from (2.1) satisfies

$$B(x)y = P(x)f(x, t). \qquad (3.4)$$

Yet, even if η is small, $B(\hat{x})\hat{y}$ may not be a good approximation of By because $\frac{\partial P}{\partial x}$ may be unbounded at the singular point so that $P(\hat{x})$ is not a good approximation of $P(x)$.

Example 3.1 *In (2.1) let* $x = (x_1, x_2)$*,* $g(x) = -\cos x_1 - \cos x_2$*, and* $G = B^T = (\sin x_1 \quad \sin x_2)$*. Then* $P(x) = (\sin^2 x_1 + \sin^2 x_2)^{-1} \begin{pmatrix} \sin^2 x_1 & \sin x_1 \sin x_2 \\ \sin x_1 \sin x_2 & \sin^2 x_2 \end{pmatrix}$*. Clearly, at a singularity point* $x = (0, \pi)$ *the value of* P *depends on the direction from which it is approached. Thus,* $\frac{\partial P}{\partial x}$ *is unbounded, even though* P *is a differentiable function of* t*.*

Letting further $f = (\sin x_2 - \sin x_1)^{-1} (\sin x_1 \quad 2\sin x_2 - \sin x_1)^T$*, and given the initial conditions* $x_1(0) = -\pi/2$*,* $x_2(0) = \pi/2$*, the exact solution is*

$$x(t) = (\, t - \pi/2 \quad t + \pi/2\,)^T, \; y = (\sin x_2 - \sin x_1)^{-1}$$

So, as t *crosses* $t^* = \pi/2$*,* $y(t)$ *blows up but* $By = (\sin x_2 - \sin x_1)^{-1} (\sin x_1 \quad \sin x_2)^T$ *remains bounded. However, it is easy to perturb* $x(t)$ *slightly and smoothly in such a way that the perturbed* By *blows up at* $t = t^*$*, still satisfying (2.7) with a small* δ*.* □

Note that for the linear model problem (see [4]), $P \equiv P(t)$ is independent of x. Hence we do not have the above difficulty in the linear case. For the nonlinear problem, the accuracy near the singular point is reduced and no longer behaves like $O(\epsilon^s)$ for more than one iteration. However, we do expect $O(\epsilon^s)$ accuracy away from the singular point, assuming that no bifurcation or impasse point is encountered by the approximate solution, because once we pass the singular point, *Theorem 2.2* with $m = -1$ can be applied again.

4 The SRM for nonlinear higher-index problems

We next generalize the SRM to the more general problem (1.1). Particularly, we consider the index-3 problem ($\nu = 2$). The Euler-Lagrange equations for multibody systems with holonomic constraints yield a practical instance of the problem. The SRM formulations presented in this section are easy to generalize for more general problems (1.1). The index-3 problem reads:

$$\begin{aligned} x'' &= f(x, x', t) - B(x, t)y, && (4.1a) \\ 0 &= g(x, t), && (4.1b) \end{aligned}$$

with given $2(n_x - n_y)$ boundary conditions,

$$b(x(0), x(t_f), x'(0), x'(t_f)) = 0. \tag{4.2}$$

The meaning of G, B and the stabilization matrix E below remain the same as in the index-2 problems considered in previous sections.

4.1 The case of nonsingular GB

We first use an idea from [4], viz. a combination of Baumgarte's stabilization with a modified penalty method, to derive the SRM for the nonlinear index-3 problem (4.1). Then we apply a better stabilization [2] to generate a new SRM which is expected to have better constraint stability. Finally, we seek variants which avoid evaluation of complicated terms in the second derivative of the constraints. Here "stabilization" means stabilized index reduction.

At first consider, instead of (4.1b), the Baumgarte stabilization

$$\alpha_1 \frac{d^2}{dt^2} g(x,t) + \alpha_2 \frac{d}{dt} g(x,t) + \alpha_3 g(x,t) = 0, \tag{4.3a}$$

$$g(x(0),0) = 0, \ \frac{d}{dt} g(x(0),0) = 0, \tag{4.3b}$$

where $\alpha_j, j = 1,2,3$ are chosen so that the roots of the polynomial

$$\sigma(\tau) = \sum_{j=1}^{3} \alpha_j \tau^{3-j}$$

are all negative. Following the same procedure as in [4] or in §2, we can write down an SRM for (4.1): for $s = 1, 2, \ldots$ and y_0 given,

$$x_s'' = f(x_s, x_s', t) - B(x_s, t) y_s, \tag{4.4}$$

where x_s satisfies boundary conditions (2.2) and (4.3b) and y_s is given by

$$y_s = y_{s-1} + \frac{1}{\epsilon} E(x_s, t)(\alpha_1 \frac{d^2}{dt^2} g(x_s, t) + \alpha_2 \frac{d}{dt} g(x_s, t) + \alpha_3 g(x_s, t)). \tag{4.5}$$

It is not difficult to repeat the approach of §2 for the present case. Under assumptions similar to the index-2 case, i.e. (2.6) with a change to include $\delta''(\tau)$ at the right hand side (cf. [10]) and *H1* with the addition that the derivative of the solution is also bounded, we readily obtain extensions of Theorems 2.1 and 2.2 for the cases $\alpha_1 \neq 0$ and $\alpha_1 = 0$ (with $\alpha_2 \neq 0$), respectively. We do not allow for $\alpha_1 = \alpha_2 = 0$ since in this case equations (4.4),(4.5) have different asymptotic properties. Note that the SRM (4.4),(4.5) with $\alpha_1 = 0$ avoids computing g_{xx}; however, the obtained iteration now calls for solving problems which become stiff when ϵ gets small, and to avoid g_{xx} one should use a non-stiff discretization method.

Another way to generalize the SRM to higher index problems is based on invariant stabilization. Its advantages over Baumgarte's stabilization have been discussed in [2, 3]. We first describe this stabilization. By two direct differentiations of the constraints (4.1b), we can eliminate y and get an ODE

$$x'' = \tilde{f}(x, x', t), \tag{4.6}$$

for which the original constraint (4.1b) together with its first derivative give an invariant. The idea of the method is to reformulate the higher index DAE (4.1) as a first order ODE (cf. (4.6)):

$$z' = \hat{f}(z,t) \tag{4.7}$$

with an invariant

$$0 = h(z,t), \tag{4.8}$$

where

$$z = \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = \begin{pmatrix} x \\ x' \end{pmatrix}, \; \hat{f}(z,t) = \begin{pmatrix} z_2 \\ \tilde{f}(z,t) \end{pmatrix}, \; h(z(t),t) = \begin{pmatrix} g(x(t),t) \\ \frac{d}{dt} g(x(t),t) \end{pmatrix} \tag{4.9}$$

and to consider the stabilization families

$$z' = \hat{f}(z,t) - \gamma F(z,t) h(z,t), \tag{4.10}$$

where $F = D\tilde{E}$ for some appropriate matrix functions D and $\tilde{E}$ such that $\tilde{E}$ and HD are nonsingular, and $H = h_z$. The ODE (4.10) coincides with Baumgarte's stabilization for the index-2 problem (2.1) with $D = B$ and $\tilde{E} = E = (HD)^{-1}$. One choice for D here is $D = H^T$, but others will be mentioned below. Note that (4.10) has the same solution as the original problem (4.1) for any parameter value γ. Although the method has better constraint stabilization, both the evaluation of $\tilde{f}$ and that of H involve g_{xx} which may be complicated to calculate in practice. Next, we derive SRM iterations based on this stabilization.

One SRM variant is obtained by writing (4.7) as

$$z' = \hat{f}(z,t) - D\zeta \tag{4.11}$$

which, together with (4.8) gives an index-2 DAE, and apply the methods of §2 directly. An obvious choice for ζ_0 is the exact $\zeta_0 = \zeta \equiv 0$. Choosing $\alpha_1 = 0$, $D = \begin{pmatrix} G^T & 0 \\ 0 & G^T \end{pmatrix}$ say, and $E = I$, we obtain the simple, though potentially stiff, iteration

$$z_s' = \hat{f}(z_s) - D\zeta_s \tag{4.12a}$$

$$\zeta_s = \zeta_{s-1} + \frac{1}{\epsilon} h(z_s) \tag{4.12b}$$

Next, we present an SRM method based on invariant stabilization which avoids the computation of $\tilde{f}$. In fact, we can avoid g_{xx} altogether using the new stabilization. If we do not eliminate y by differentiations, then $\hat{f}(z,t)$ in the stabilization (4.10) becomes

$$\hat{f}(z,t) = \begin{pmatrix} z_2 \\ f(z,t) - B(z_1,t)y \end{pmatrix}. \tag{4.13}$$

Since y is not known in advance, we use an iterative SRM procedure to calculate y as in [8, 4]. The solutions of the iterative procedure no longer satisfy (4.1) precisely.

Hence the iterative procedure has to be a regularization procedure and the parameter in (4.10) is changed to $\gamma = \frac{1}{\epsilon}$ to emphasize that it must be chosen sufficiently large. These lead to the following SRM formulation (for simplicity of notation, we only consider the special case where B and g are independent of t):

$$z_s' = \begin{pmatrix} z_{1s} \\ z_{2s} \end{pmatrix}' = \begin{pmatrix} z_{2s} \\ f(z_s, t) - B(z_{1s})y_{s-1} \end{pmatrix} - \frac{1}{\epsilon}F(z_s)h(z_s), \tag{4.14}$$

where z_s satisfies boundary conditions (4.2), (4.3b) and $h = (g(z_1), G(z_1)z_2)^T$. Thus the Jacobian of h is

$$H = \begin{pmatrix} G(z_1) & 0 \\ L(z) & G(z_1) \end{pmatrix}, \quad \text{where} \quad L = z_2^T g_{xx}(z_1).$$

We choose D and $\tilde{E}$ so that

$$F = BE \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} = \begin{pmatrix} BE & 0 \\ 0 & BE \end{pmatrix} \tag{4.15}$$

where, as in §2.2, E is chosen such that GBE is symmetric positive definite. Updating y by

$$y_s = y_{s-1} + \frac{1}{\epsilon}E(z_{1s})G(z_{1s})z_{2s} \tag{4.16}$$

yields that the second part of the original index-3 system holds exactly, i.e.

$$z_{2s}' = f(z_s, t) - B(z_{1s})y_s.$$

Next we analyze the convergence of (4.14)–(4.16). Again we assume that the solutions of (4.14), (4.2), (4.3b) exist uniquely and are bounded if y_{s-1} is bounded (see assumption *H1*). Assumption (2.6) changes a bit: We first rewrite the system (4.1) as

$$\begin{aligned} z_1' &= z_2, && (4.17a) \\ z_2' &= f(z,t) - B(z_1)y, && (4.17b) \\ 0 &= g(z_1). && (4.17c) \end{aligned}$$

Then we assume the following perturbation bound,

$$\begin{aligned} \|\hat{z}(t) - z(t)\| &\le M \max_{0 \le \tau \le t_f} (|\delta(\tau)| + |\delta'(\tau)| + |\delta''(\tau)| + |\theta(\tau)| + |\theta'(\tau)|), && (4.18a) \\ \|\hat{y}(t) - y(t)\| &\le M \max_{0 \le \tau \le t_f} (|\delta(\tau)| + |\delta'(\tau)| + |\delta''(\tau)| + |\theta(\tau)| + |\theta'(\tau)|), && (4.18b) \end{aligned}$$

where $\hat{z}$ and $\hat{y}$ satisfy a perturbed problem of (4.17),

$$\begin{aligned} \hat{z}_1' &= \hat{z}_2 + \theta(t), && (4.19a) \\ \hat{z}_2' &= f(\hat{z},t) - B(\hat{z}_1)\hat{y}, && (4.19b) \\ 0 &= g(\hat{z}_1) + \delta(t), && (4.19c) \end{aligned}$$

with the same boundary conditions (4.2). Again, for the initial value problems, (4.18) can be easily proved by following the technique presented in [10], and this can be extended for boundary value problems as well.

Similarly to the proof of *Theorem 2.1*, let $w_s = h(z_s) = \begin{pmatrix} v_s \\ v_s' \end{pmatrix}$, where $v_s = g(z_{1s})$. From (4.14), we get

$$\begin{aligned} \epsilon v_s' &= -GBE(z_s)v_s + \epsilon G(z_{1s})z_{2s} && (4.20a) \\ \epsilon v_s'' &= -GBE(z_s)v_s' - LBE(z_s)v_s + \epsilon[Lz_{2s} + Gf(z_s) - GB(z_s)y_{s-1}] && (4.20b) \end{aligned}$$

with the initial conditions $w_s(0) = 0$. Applying (4.20a) and then (4.20b) for $s = 1$, we obtain $h_1, h_1' = O(\epsilon)$ if y_0 satisfies (2.14) for $m \geq 0$. Therefore (4.14), (4.16) becomes

$$\begin{aligned} z_{11}' &= z_{21} + \theta, && (4.21a) \\ z_{21}' &= f(z_1, t) - B(z_{11})y_1, && (4.21b) \\ g(z_{11}) &= \delta, && (4.21c) \end{aligned}$$

where $\delta, \delta', \delta'' = O(\epsilon)$ and $\theta = -\frac{1}{\epsilon}BEv_1$. To use (4.18), we have to estimate θ. But from (4.20a) we obtain $v_1 = O(\epsilon^2)$ since $G(z_{11})z_{21} = \delta' = O(\epsilon)$. So $\theta = O(\epsilon)$. Furthermore, from the initial conditions of w_s, $v_1'(0) = 0$, and differentiating (4.20a) once, we get $v_1' = O(\epsilon^2)$ similarly. From this it follows that $\theta' = O(\epsilon)$. Applying (4.18) to (4.21) we immediately have

$$z_1 = z_e + O(\epsilon), \ y_1 = y_e + O(\epsilon),$$

where $\{z_e, y_e\}$ is the exact solution of the index-3 problem. Then following the proof procedure of *Theorem 2.1*, we obtain:

Theorem 4.1 *Let all functions in the DAE (4.1) be sufficiently smooth and the above assumptions (particularly (4.18)) hold. Assume in addition that y_0 satisfies (2.14). Then, for the solution of iteration (4.14)–(4.16), the following error estimates hold:*

$$\begin{aligned} z_s(t) - z_e(t) &= O(\epsilon^s), && (4.22a) \\ y_s(t) - y_e(t) &= O(\epsilon^s) && (4.22b) \end{aligned}$$

for $1 \leq s \leq m+1$.

Remark 4.1 We note that, unlike *Proposition 2.2* of [2], we do not assume

$$\|H(z)\hat{f}(z)\|_2 \leq \gamma_0 \|h(z)\|_2$$

to discuss the stability and accuracy of the constraints. Also, from (4.20), we see the difference of the constraint stability or accuracy between SRM formulations based on Baumgarte's stabilization and the new stabilization. For the former, we only have

$$v_1' = G(z_{11})z_{11}' = G(z_{11})z_{21}$$

So if we obtain $G(z_{11})z_{21} = O(\epsilon)$ then $v_1 = O(t\epsilon)$. This can be much worse than what we get from (4.20a). □

Remark 4.2 For $s > m$ we expect initial layer terms in the estimates (4.22) (cf. *Theorem 2.2* and *Theorem 3.1* of [4]). □

4.2 The case for constraint singularities

For the singular case we allow that GB may be singular at some isolated point t^* as described in the introduction §1. The situation here is similar to that for index-2 problems. An examination of the drift equations (4.20) suggests that here, too, the choice $E = (GB)^{-1}$ is preferable to $E = I$ or $E = (GB)^T$. The iteration for y_s is modified as well. Still assuming for simplicity that g and B do not depend explicitly on t, this gives in place of (4.14)–(4.16) the iteration

$$\begin{aligned} z'_{1s} &= z_{2s} - \frac{1}{\epsilon}B(GB)^{-1}g(z_s) &\quad (4.23\text{a})\\ z'_{2s} &= f(z_s, t) - \hat{y}_s &\quad (4.23\text{b})\\ \hat{y}_s &= P(z_s)\hat{y}_{s-1} + \frac{1}{\epsilon}P(z_s)z_{2s} &\quad (4.23\text{c}) \end{aligned}$$

Also, as indicated in §3 for index-2 problems, we cannot expect $O(\epsilon^s)$ approximation near the singular point any more. But we do expect that (4.22) holds away from the singular point, because the singularity is in the constraint and the drift manifold is asymptotically stable (following our stabilization). A numerical example in §6 will show that we do get improved results by using SRM iterations for the singular problem.

5 The SRM for constrained multibody systems

Constrained multibody systems provide an important family of applications of the form (4.1) and (2.1). We consider the system

$$\begin{aligned} q' &= v &\quad (5.1\text{a})\\ M(q)v' &= f(q, v) - G(q)^T\lambda &\quad (5.1\text{b})\\ 0 &= g(q) &\quad (5.1\text{c}) \end{aligned}$$

where q and v are the vectors of generalized coordinates and velocities, respectively; M is the mass matrix which is symmetric positive definite; $f(q, v)$ is the vector of external forces (other than constraint forces); $g(q)$ is the vector of (holonomic) constraints; λ is the vector of Lagrange multipliers; and $G(q) = \frac{d}{dq}g$. For notational simplicity, we have suppressed any explicit dependence of M, f or g on the time t. We first consider the problem without singularities.

Corresponding to (4.1) in §4, we have $B = M^{-1}G^T$, so $GB = GM^{-1}G^T$. Other quantities like h and H retain their meaning from the previous section. In some applications it is particularly important to avoid terms involving g_{xx}, since its computation is somewhat complicated and may also easily result in mistakes and rugged terms. So [3] suggests post-stabilization using the stabilization matrix

$$F = M^{-1}G^T(GM^{-1}G^T)^{-1}\begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} \tag{5.2}$$

twice, instead of involving H, at the end of each time step or as needed. They find that this F performs very well in many applications. However, while this stabilization avoids the g_{xx} term in F, g_{xx} is still involved in obtaining $\tilde{f}$, although only through matrix-vector multiplications (see (4.6)). The SRM formulation (4.14)–(4.16) enables us to avoid the computation of $\tilde{f}$ in the absence of constraint singularities. For the multibody system (5.1) we write the iteration as follows:

For $s = 1, 2, \ldots$, find $\{q_s, v_s\}$ by

$$q_s' = v_s - \frac{1}{\epsilon}BE(q_s)g(q_s) \tag{5.3a}$$

$$v_s' = M^{-1}f(q_s, v_s) - B(q_s)\lambda_{s-1} - \frac{1}{\epsilon}BEG(q_s)v_s \tag{5.3b}$$

Then update λ by

$$\lambda_s = \lambda_{s-1} + \frac{1}{\epsilon}EG(q_s)v_s. \tag{5.4}$$

It is easy to see that in this SRM formulation the g_{xx} term is avoided completely. Moreover, since $GM^{-1}G^T$ is positive definite, we can choose $E = I$ in (5.3),(5.4), obtaining a method for which *Theorem 4.1* applies which avoids computing $(GM^{-1}G^T)^{-1}$. Although it requires an iterative procedure, a small number of iterations (p if an explicit discretization method of order p is used) typically provide sufficient accuracy. Numerical experiments will show the $O(\epsilon^s)$ error estimate.

Next we consider the singular problem, i.e. the matrix $GM^{-1}G^T$ is singular at some isolated point t^*, $0 < t^* < t_f$. A typical example of singular multibody systems is the two-link slider-crank problem (see Figure 5.1) consisting of two linked bars of equal length, with one end of one bar fixed at the origin, allowing only rotational motion in the plane, and the other end of the other bar sliding along the x-axis. Various formulations of the equations of motion for this problem appear, e.g., in [12, 8, 4, 19]. In our calculations we have used the formulation of [4], to make sure that the problem is not accidentally too easy. It consists of 6 ODEs and 5 constraints, with the last row of the Jacobian matrix G vanishing when the mechanism moves left through the point where both bars are upright ($\phi_1 = \frac{\pi}{2}$, $\phi_2 = \frac{3\pi}{2}$, where x_i, y_i, ϕ_i are the coordinates of the centre of mass of the ith bar). The last row of G vanishes at this one point and a singularity is obtained. We note that the solution is smooth in the passage through the singularity with a nonzero velocity.

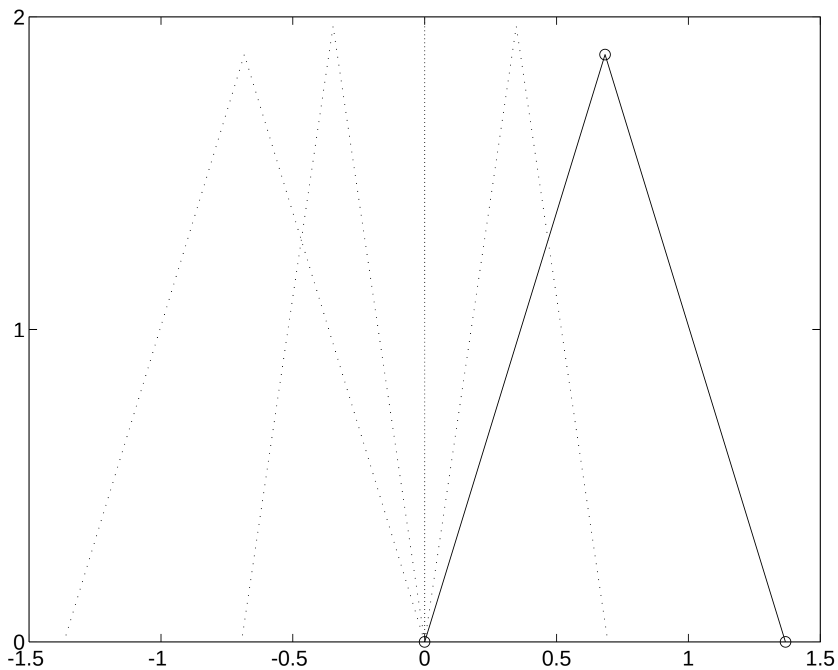

Figure 5.1: planar slider-crank: initial state in solid line, subsequent states in dotted lines

When we attempt to integrate this system using a stabilization method like [2] which ignores the singularity, the results are unpredictable, depending on how close to the singular time point the integration process gets when attempting to cross it. In fact, radically different results may be obtained upon changing the value of an error tolerance. (Similar observations are made in [19].) In some instances a general purpose ODE code would simply be unable to "penetrate the singularity", and yield a solution which, after hovering around the upright (singular) position for a while, turns back towards the initial position (solid line in Figure 5.1). Such a motion pattern may well look deceptively plausible.

Methods which do not impose the constraints on the position level (e.g. methods consisting of differentiating the constraints once and solving the obtained index-2 problem numerically, or of projecting only on the velocity-level constraint manifold) perform particularly poorly here (cf. numerical results in [19]). This is easy to explain: The position-level constraint corresponds to ensuring that the two bars have equal length. If this is not strictly imposed in the process of numerical solution, inevitable numerical errors due to discretization may yield a model where the lengths are not close enough to being equal, and this leads to the lock-up phenomena described e.g. in [12], which have a vastly different solution profile.

We now wish to generalize the SRM to the problem (5.1) with singularities since we have seen its success for the linear index-2 case in [4]. From the two-link slider crank problem, we find that, although $GM^{-1}G^T$ is singular at t^*, $P(q) \equiv$

$M^{-1}G^T(GM^{-1}G^T)^{-1}G$ and $M^{-1}G^T(GM^{-1}G^T)^{-1}g$ are smooth as functions of t for the exact solution or functions q satisfying the constraints, while $M^{-1}G^T(GM^{-1}G^T)^{-1}$, $M^{-1}G^T(GM^{-1}G^T)^{-1}G_q$ and the derivative $\frac{dP(q)}{dq}$ are not. Also, as indicated in [4], λ is no longer smooth, while $B\lambda$ is since we assume the solution q to be sufficiently smooth. We only include terms which are most possibly smooth in the SRM formulation.

Applying (4.23), we obtain the method

$$\begin{aligned} q_s' &= v_s - \frac{1}{\epsilon}M^{-1}G^T(GM^{-1}G^T)^{-1}g(q_s), && (5.5a) \\ v_s' &= M^{-1}f(q_s, v_s, t) - \hat{\lambda}_s, && (5.5b) \end{aligned}$$

$$\hat{\lambda}_s = P(q_s)\hat{\lambda}_{s-1} + \frac{1}{\epsilon}P(q_s)v_s \tag{5.6}$$

As we indicated in §3, we do not expect $O(\epsilon^s)$ accuracy near the singular point. However, we do expect that the SRM iteration would improve the accuracy and that we still get $O(\epsilon^s)$ accuracy away from the singular point. Numerical experiments in §6 will show such improvements.

6 Numerical experiments

We now present a few examples to demonstrate our claims in the previous sections. Throughout this section we use a constant step size h and select the simple initial iterate $y_0 \equiv 0$. To make life difficult we choose h when we can so that there is an i such that $t_i = t^*$, namely, there is a mesh point hitting the singularity point t^*, for singular test problems. At a given time t, we use $'ex'$ to denote the maximum over all components of the error in x_s. Similarly, $'drift'$ denotes the maximum residual in the algebraic equations.

Example 6.1 *Consider the DAE (2.1),(2.2) with*

$$\begin{aligned} f &= \begin{pmatrix} 1-e^t \\ \cos t + e^t \sin t \end{pmatrix}, \; B = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \\ g &= \frac{1}{2}(x_1^2 + x_2^2 - e^{-2t} - \sin^2 t). \end{aligned}$$

subject to $x_1(0) = 1,\ x_2(0) = 0.$

The exact solution is $x_e = (\,e^{-t},\ \ \sin t\,)$, $y_e = e^t$. *This is a problem without singularities.*

Using an explicit second order Runge-Kutta method with $h = 0.001$ *we test various choices of* E *and* α_1 *(always taking* $\alpha_2 = 1$ *in our computations) of the SRM formulation in §2. We list the computational results in Table 6.1. Observe that, for* $\alpha_1 \neq 0$, *the SRM works well for various choices of* E. *Its error is as good as Boumgarte's* *method whose parameter is taken corresponding to α_2 of the SRM. For $\alpha_1 = 0$, we see that the error improves at a rate of about $O(\epsilon)$ for various choices of E, including the simplest $E = I$. (Observe the errors at $t = 1$; the error situation near $t = .1$ is different because of the existence of an initial layer.) Such an error improvement continues until the accuracy of the second order explicit Runge-Kutta method, i.e. $O(h^2)$, is reached.* $\Box$

The next two examples are for problems with singularities. In the index-2 case of the Baumgarte stabilization the worst term is $B(GB)^{-1}g_t$ for the type of the singularities we discuss in this paper. So, to show what happens when the Baumgarte method does not work well, we choose nonautonomous problems (i.e. $g_t \neq 0$) as index-2 singular examples.

Example 6.2 *Consider the nonlinear DAE (2.1) with*

$$\begin{aligned} f &= \begin{pmatrix} 1 + (t - \frac{1}{2})e^t \\ 2t + (t^2 - \frac{1}{4})e^t \end{pmatrix}, \; B = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \\ g &= \frac{1}{2}(x_1^2 + x_2^2 - (t - \frac{1}{2})^2 - (t^2 - \frac{1}{4})^2) \end{aligned}$$

subject to the initial condition $x_1(0) = -\frac{1}{2}$, $x_2(0) = -\frac{1}{4}$.

The exact solution is $x_e = (\, t - \frac{1}{2}, \quad t^2 - \frac{1}{4}\,)$, $y_e = e^t$. A singularity is located at $t^* = \frac{1}{2}$. Using this example we test the SRM formulations of §3. We list the computational results in Table 6.2, where we take $h = \epsilon = 0.001$ for the case of $\alpha_1 = 0$, and $h = 0.001$, $\epsilon = 10^{-10}$ for the case of $\alpha_1 \neq 0$, and use the explicit second order Runge-Kutta scheme to easily see the iteration improvement (Ij stands for results of the jth iteration).

From Table 6.2, we see error deterioration for the Baumgarte method and the SRM with $\alpha_1 \neq 0$. The SRM with $\alpha_1 = 0$ performs better in the singular case. $\Box$

Next we try an example in which y is unbounded at the singularity.

Example 6.3 *Consider the nonlinear DAE (2.1) with*

$$\begin{aligned} f &= \begin{pmatrix} -x_1 + x_2 - \sin(t) - (1 + 2t) \\ 0 \end{pmatrix}, \; B = \begin{pmatrix} 0 \\ x_1 \end{pmatrix} \\ g &= x_1^2 + x_1(x_2 - \sin(t) - 1 + 2t), \end{aligned}$$

subject to the initial condition $x_1(0) = 1$, $x_2(0) = 0$.

The exact solution is $x_e = (\, 1 - 2t, \quad \sin t\,)$, $y_e = -\cos t/(1 - 2t)$. Taking the same parameters and using the same method as before, we get the results listed in Table 6.3. Clearly, the SRM with $\alpha_1 = 0$ performs well for this situation as well, while Baumgarte's method blows up upon hitting the singularity. $\Box$

Our next example tests the formulation (4.14)–(4.16) or (5.3)–(5.4) for index-3 problems.

Example 6.4 *This example is made up from Example 2 in [3], which describes a two-link planar robotic system. We use the notation of (5.1). Let* $q = (\theta_1, \theta_2)^T$ *and*

$$M = \begin{pmatrix} m_1 l_1^2/3 + m_2(l_1^2 + l_2^2/3 + l_1 l_2 c_2) & m_2(l_2^2/3 + l_1 l_2 c_2/2) \\ m_2(l_2^2/3 + l_1 l_2 c_2/2) & m_2 l_2^2/3 \end{pmatrix},$$

where $l_1 = l_2 = 1$, $m_1 = m_2 = 3$ *and* $c_2 = \cos\theta_2$. *The constraint equation is*

$$g(q) = l_1 \sin\theta_1 + l_2 \sin(\theta_1 + \theta_2) = 0.$$

We choose the force term

$$f = \begin{pmatrix} (l_1 \cos\theta_1 + l_2 \cos(\theta_1 + \theta_2)) \cos t - 3 \sin t \\ l_2 \cos(\theta_1 + \theta_2) \cos t + (1 - \frac{3}{2} c_2) \sin t \end{pmatrix}$$

which yields the exact solution $\theta_1 = \sin t$, $\theta_2 = -2\sin t$ *and* $\lambda = \cos t$. *Because* M *is symmetric positive definite and* $B = M^{-1}G^T$ *we can take* $E = I$ *in the SRM formula (5.3)–(5.4). Again we use the second- order explicit Runge-Kutta scheme, and set* $h = 0.001$, $\epsilon = 0.005$. *The results are listed in Table 6.4, where eq and ev stand for maximum errors in* q *and* $v = q'$, *resp., and* $pdrift$ *and* $vdrift$ *stand for drifts at position level and velocity level, resp. We see that the accuracy is improved significantly by the first two iterations. The third iteration is unnecessary here, because the error is already dominated by the Runge-Kutta discretization error. Qualitatively similar results are obtained for* $E = (GB)^T$ *and* $E = (GB)^{-1}$. *More interestingly, though, for* $E = I$ *we neither form nor invert* $GM^{-1}G^T$, *so a particularly inexpensive iteration is obtained.*

□

Next we solve for the dynamics of the slider-crank mechanism described in §5. To recall, this is a nonlinear index-3 DAE with isolated, "smooth" singularities.

Example 6.5 *We take* $h = \epsilon = 0.0001$ *and use the explicit second order Runge-Kutta method again. Singularities are located at* $(\phi_1, \phi_2) = (\frac{\pi}{2}, \frac{3\pi}{2})$ *(i.e., they occur each time the periodic solution crosses this point). Corresponding to the case shown in [19], we choose* $\phi_1(0) = \frac{7\pi}{4}$ *and* $\phi_1'(0) = 0$ *and compute*

$$\theta_1 = \phi_1 - \frac{3\pi}{2}, \; \theta_2 = \phi_2 + \frac{\pi}{2},$$

θ_1' *and* θ_2'. *Using the formulation (5.6), (5.5), we calculate until* $t = 70$ *without any difficulty (see Figure 6.1).*

We also list the drift improvement as a function of the SRM iteration in Table 6.5.

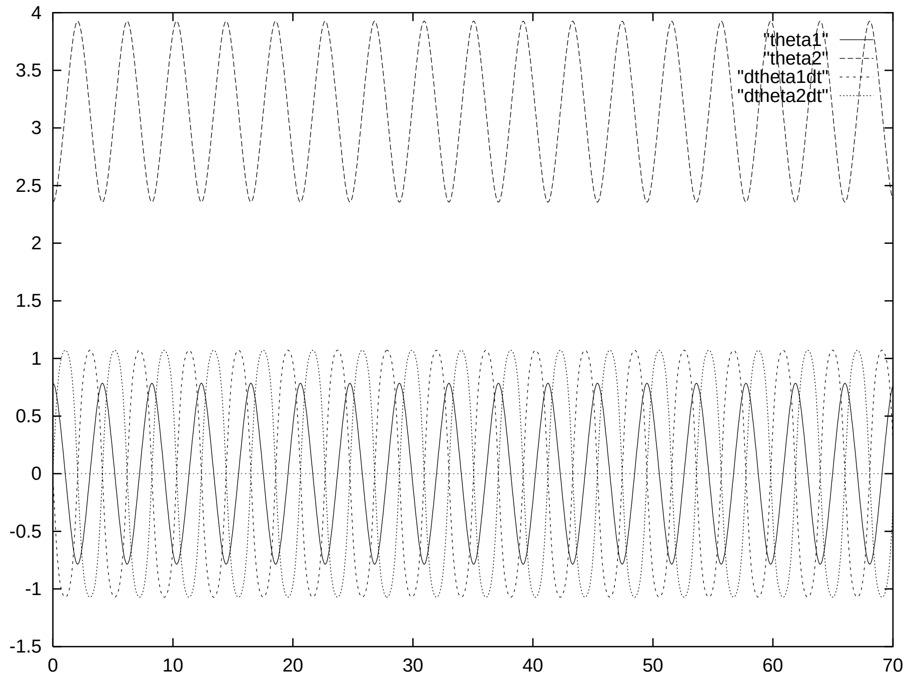

Figure 6.1: Solution for slider-crank problem with singularities

If we use the SRM formulations considered in §§4 and 5 for problems with no singularities, or one of the usual stabilization methods with strict tolerances, the results become wildly different from the correct solution after several periods.

Next we calculate the acceleration of the slider end in the horizontal direction under the initial data $\phi_1(0) = \frac{\pi}{4}$ and $\phi_1'(0) = 2\sqrt{2}$. The same problem was discussed in [8]. The result shown in [8] is not perfect since the maximum and minimum values in each period appear to differ. Our result looks better (see Figure 6.2). □

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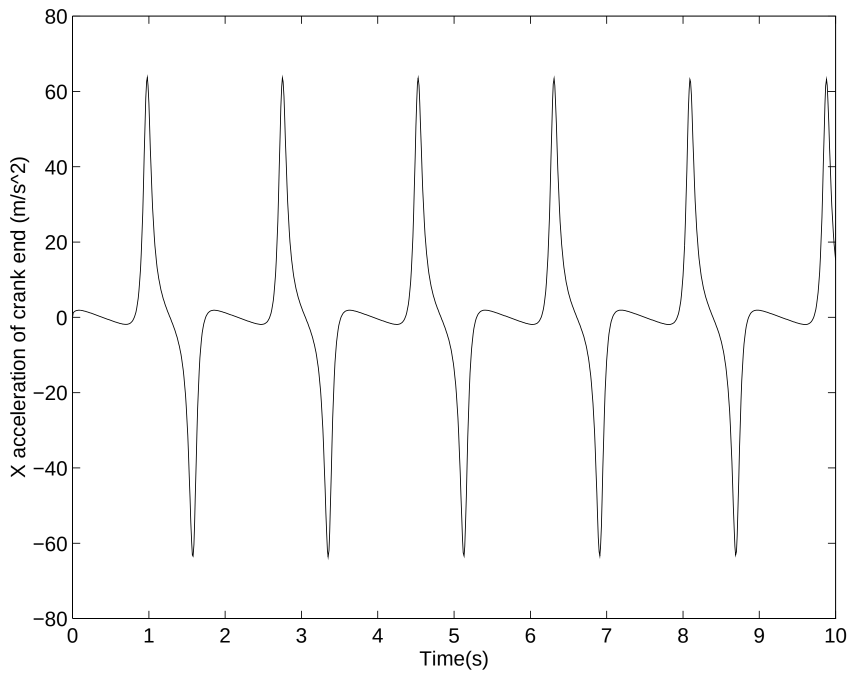

Figure 6.2: Acceleration of slider end

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methods	ϵ	*iteration*	*error at* $\rightarrow$	*t=.1*	*t=.5*	*t=1.0*
$\alpha_1 = 1$	1e-8	1	ex	.11e-7	.94e-7	.19e-6
$E = I$			drift	.79e-8	.56e-7	.14e-6
$\alpha_1 = 1$	1e-8	1	ex	.11e-7	.92e-7	.18e-6
$E = (GB)^T$			drift	.78e-8	.53e-7	.14e-6
$\alpha_1 = 1$	1e-8	1	ex	.11e-7	.95e-7	.19e-6
$E = (GB)^{-1}$			drift	.80e-8	.58e-7	.15e-6
Baumgarte			ex	.45e-6	.16e-6	.35e-6
			drift	.40e-6	.70e-7	.29e-6
$\alpha_1 = 0$	5e-3	1	ex	.60e-2	.11e-1	.11e-1
$E = I$			drift	.54e-2	.80e-2	.13e-1
		2	ex	.11e-3	.26e-3	.22e-3
			drift	.96e-4	.20e-3	.27e-3
		3	ex	.32e-5	.65e-5	.46e-5
			drift	.29e-5	.47e-5	.54e-5
		4	ex	.26e-6	.23e-6	.28e-6
			drift	.13e-6	.51e-7	.12e-6
$\alpha_1 = 0$	5e-3	1	ex	.70e-2	.12e-1	.13e-1
$E = (GB)^T$			drift	.64e-2	.13e-1	.15e-1
		2	ex	.22e-3	.65e-3	.31e-3
			drift	.20e-3	.49e-3	.29e-3
		3	ex	.11e-4	.16e-4	.69e-5
			drift	.10e-4	.10e-4	.52e-5
		4	ex	.85e-6	.91e-7	.29e-6
			drift	.75e-6	.77e-6	.14e-6
$\alpha_1 = 0$	5e-3	1	ex	.51e-2	.66e-2	.10e-1
$E = (GB)^{-1}$			drift	.46e-2	.49e-2	.12e-1
		2	ex	.35e-4	.11e-3	.21e-3
			drift	.30e-4	.79e-4	.24e-3
		3	ex	.86e-6	.23e-5	.47e-5
			drift	.77e-6	.17e-5	.53e-5
		4	ex	.26e-6	.18e-6	.26e-6
			drift	.26e-7	.31e-7	.13e-6

Table 6.1: Errors for Example 6.1 using the explicit second order Runge-Kutta scheme

methods	error at →	t=.1	t = .3	t = .5	t= .7	t= 1.0
$\alpha_1 = 1$	ex	.39e-6	.13e-5	.12e-3	.14e-3	.76e-4
	drift	.24e-6	.16e-6	.10e-7	.39e-6	.75e-6
$\alpha_1 = 0$ (I1)	ex	.46e-3	.32e-3	.43e-4	.49e-3	.20e-2
	drift	.24e-3	.89e-4	.18e-8	.20e-3	.22e-2
$\alpha_1 = 0$ (I2)	ex	.81e-6	.11e-5	.41e-5	.29e-5	.68e-5
	drift	.24e-6	.30e-6	.15e-10	.13e-5	.76e-5
$\alpha_1 = 0$ (I3)	ex	.23e-6	.26e-6	.34e-6	.29e-6	.29e-6
	drift	.90e-9	.11e-8	.78e-13	.35e-8	.18e-7
$\alpha_1 = 0$ (I4)	ex	.23e-6	.26e-6	.36e-6	.27e-6	.29e-6
	drift	.47e-11	.33e-11	.10e-12	.29e-11	.28e-10
Baumgarte	ex	.43e-6	.45e-6	.34e-3	.39e-3	.21e-3
	drift	.24e-6	.16e-6	.61e-7	.24e-6	.75e-6

Table 6.2: Example 6.2 – bounded y and singularity at $t^* = .5$

methods	error at →	t=.1	t = .3	t = .5	t= .7	t= 1.0
SRM ($\alpha_1 = 0$)	ex	.40e-6	.25e-6	.14e-6	.46e-7	.60e-7
(I3)	drift	.25e-8	.76e-9	.16e-15	.28e-9	.40e-9
Baumgarte	ex	.49e-7	.15e-6	.93e+1	NaN	NaN
	drift	.39e-7	.59e-7	.52e+13	NaN	NaN

Table 6.3: Example 6.3 – unbounded y and singularity at $t^* = .5$

methods	ϵ	iteration	error at →	t=.1	t=.5	t=1.0
$E = I$	5e-3	1	eq	.41e-4	.66e-3	.26e-2
			ev	.75e-2	.74e-2	.69e-2
			pdrift	.22e-4	.28e-4	.22e-4
			vdrift	.49e-2	.41e-2	.27e-2
		2	eq	.13e-6	.66e-6	.36e-6
			ev	.19e-5	.81e-6	.20e-4
			pdrift	.42e-9	.13e-7	.17e-6
			vdrift	.91e-7	.21e-5	.21e-4
		3	eq	.10e-6	.58e-6	.12e-5
			ev	.86e-6	.10e-5	.16e-5
			pdrift	.96e-11	.60e-9	.48e-8
			vdrift	.10e-8	.99e-7	.59e-6

Table 6.4: Errors for Example 6.4 using SRM (5.3)-(5.4)

iteration number	*position drift at t=30*	*velocity drift at t = 30*
1	*.669e-8*	*.671e-4*
2	*.730e-11*	*.731e-7*

Table 6.5: Drifts of the SRM for the slider-crank problem