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REGULARIZATION OF HIGHER-INDEX DIFFERENTIAL-ALGEBRAIC EQUATIONS WITH RANK-DEFICIENT CONSTRAINTS*

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Abstract. In this paper we present several regularizations for higher-index differential-algebraic equations with rank-deficient or singular constraints. These types of problems arise, for example, in the solution of constrained mechanical systems, when a mechanism's trajectory passes through or near a kinematic singularity. We derive a class of regularizations for these problems which is based on minimization of the norm of the constraints. The new regularizations are analogous to trust-region methods of numerical optimization. We give convergence results for the regularizations and present some numerical experiments which illustrate their effectiveness.

Key words. constrained dynamics, multibody systems, differential-algebraic equations, regularization, kinematic singularity, Baumgarte stabilization

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1. Introduction.

In this paper we consider the numerical solution of higher-index differential-algebraic equations (DAEs) with rank-deficient or singular constraints. The problems that we consider are Hessenberg [10] DAEs of the form

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

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

The system (1.1) is index $m+1$ if GB is nonsingular, where $G = \frac{\partial g}{\partial x}$. These types of systems arise, for example, in the solution of constrained mechanical systems, where a locally rank-deficient constraint matrix can lead to a kinematic singularity [7, 14, 21, 26]. Mechanical systems [19, 30] are described by the Euler–Lagrange equations

$$M(q)q'' = f(q, q', t) + G^T\lambda, \tag{1.2a}$$

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

which are index 3.

High-index systems present difficulties for numerical methods [10]. The index of (1.1) can be reduced by differentiating the constraint one or more times; however, then the solution can "drift" away from the original constraint. Various methods have

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been proposed for stabilizing the constraints [5, 6, 7, 8, 9, 15, 16, 20, 27, 28, 29, 31]. A popular method for (1.1) stabilizes the constraints via Baumgarte's regularization [6]. This method is applicable when GB is nonsingular.

Baumgarte's method replaces the constraints by a linear combination of the constraints and their time derivatives in such a way that the differential equation for the constraints is stable. The constraint (1.1b) is replaced by the equation

$$\sum_{j=0}^{m} \gamma_j \frac{d^j}{dt^j} g(x(t), t) = 0, \tag{1.3}$$

where the γ_j are chosen so that $\gamma_m = 1$ and the roots of the polynomial

$$\sigma(\tau) = \sum_{j=0}^{m} \gamma_j \tau^j$$

are all negative. For instance, one may choose

$$\sigma(\tau) = (\tau + \nu)^m$$

for some $\nu > 0$.

Baumgarte's method has recently been studied in [2], where it was shown how to modify it so that it has better numerical stability properties. The parameters in Baumgarte's method are notoriously difficult to choose. In [2] a choice of $\nu = 1/h$, where h is the stepsize of a numerical method, for index-2 systems was suggested and justified in the case of certain *explicit* methods.

Baumgarte's method can be considered to be a regularization of the differential-algebraic equation. As a regularization it has the property that, unlike many other regularizations, the analytical solution to the Baumgarte stabilization of a DAE is identical to the solution of the original DAE (it does not depend on the parameter in the regularization). However, it cannot by itself handle the case of rank-deficient constraints. Other regularizations have been proposed for high-index DAEs including mechanical systems in [24, 22, 18, 23, 13]; however, none of these regularizations are applicable to the case of rank-deficient constraints.

For problems with singularities, Bayo, Garcia de Jalon, and Serna [8], Bayo and Ledesma [9], and Bayo and Avello [7] propose a method for Euler–Lagrange equations which is based on an augmented Lagrangian formulation. Park and Chiou [26] propose a related method. The augmented Lagrangian method employs a separate iteration to find the Lagrange multipliers at each step. Ascher and Lin [3] have recently developed a variation of this method to handle singular constraints and provide a convergence analysis. A regularization method for Euler–Lagrange systems is proposed in [21, 1] which deals with singularities by first identifying them via Gaussian elimination and then adding their third derivatives to the vanishing and linearly independent constraints.

The methods which we propose here generalize Baumgarte's method to the case where the constraint matrix G is rank deficient or singular. They are easily implemented via standard ODE or DAE solvers and linear equation solvers. They can handle the case of a singular mass matrix for the Euler–Lagrange equations.

Problems with rank-deficient constraints can arise in a variety of contexts. If the constraints are rank deficient but constant rank, the redundant constraints can be identified symbolically or numerically via SVD or QR and, provided they are consistent, removed from the system, along with the corresponding Lagrange multipliers.

It is easy to show in this case that the solution for the state variables x remains unchanged. However, it is not always convenient to remove the redundant constraints. The regularizations which we propose will handle the redundant constraints directly without removing them. If the constraints are singular at an isolated point, a number of situations are possible. If the locally redundant constraints are not consistent, the solution will fail to exist past the singularity. Even if the redundant constraints are consistent, the solution may fail to exist past the singularity; such a situation is sometimes called an impasse point [11]. For many systems, however, the solution for x will be well defined through the singularity. It is those problems that we will address here. It is possible to attempt to remove the redundant constraints and corresponding multipliers locally after identifying them via QR or SVD; however, this can be a lot of work. There is also a problem that at different times, different redundant constraints may be eliminated, leading to problems and inefficiencies in the time integration. Unacceptably inaccurate simulations have been reported [21] using this method, due to errors in not enforcing the constraints near a singular configuration.

In section 2, we show how Baumgarte's method can be derived via optimization, which gives some insight into how to choose the Baumgarte parameters. Then we use the optimization methodology to extend Baumgarte's method to rank-deficient and singular systems, deriving a trust-region [12] method. Finally, we consider another regularization of the Baumgarte method which we call the direct regularization approach. In section 3, we define more precisely for linear DAEs the class of rank-deficient and singular DAEs which the regularizations are designed to handle, and analyze the convergence of the trust-region and direct regularization methods. In section 4, we derive regularizations for rank-deficient and singular DAE systems of index greater than two. The new regularizations are different from Baumgarte's techniques for higher-index systems because they require only first derivatives of the constraints. Numerical results are presented in section 5 which illustrate the effectiveness of the trust-region methods.

2. Regularizations based on the Baumgarte method. In this section we study rank-deficient index 2 systems of the form

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

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

First we modify the Baumgarte minimization for rank-deficient constraints via a trust region. Then we consider a regularization for rank-deficient systems which is based on a perturbation of Baumgarte's method.

Recall that Baumgarte's stabilization for (2.1a) replaces the constraints (2.1b) by

$$\gamma g(x,t) + \frac{d}{dt} g(x,t) = 0, \tag{2.2}$$

where γ is chosen so that $g = 0$ is a stable solution of the differential equation. From (2.2) and (2.1a), we obtain

$$x' = \tilde{f} - \gamma B(GB)^{-1} g, \tag{2.3}$$

where $\tilde{f} = f - B(GB)^{-1}(Gf + g_t)$ and $G = g_x$. In [2], the choice $\gamma = h^{-1}$ is recommended for certain *explicit* discretization methods. The Baumgarte regularization is not defined when GB is singular.

2.1. Baumgarte's method. In this subsection we derive the Baumgarte regularization via optimization. This provides some insight into the selection of the Baumgarte parameters and sets the stage for later generalizations for singular systems of Baumgarte's method.

Consider the solution of the constraint equation (2.1b). We have (x_{n+1}, t_{n+1}), where $x_{n+1} = x_n + hx'_n$ and $t_{n+1} = t_n + h$. By Taylor expansion,

$$\begin{aligned} g(x_{n+1}, t_{n+1}) &= g(x_n + hx'_n, t_n + h) \\ &= g(x_n, t_n) + hg_x(x_n, t_n)x'_n + hg_t(x_n, t_n) + O(h^2). \end{aligned} \tag{2.4}$$

Thus,

$$g(x_n, t_n) + hg_x(x_n, t_n)x'_n + hg_t(x_n, t_n) = 0. \tag{2.5}$$

Substituting (2.1a) into (2.5),

$$g + hG(f - By) + hg_t = 0, \tag{2.6}$$

where $G = g_x$. If $(GB)^{-1}$ exists, then we can solve for y in (2.6):

$$y = (GB)^{-1}(Gf + g_t) + h^{-1}(GB)^{-1}g. \tag{2.7}$$

Substituting (2.7) into (2.1a),

$$\begin{aligned} x' &= \left[f - B(GB)^{-1}(Gf + gt)\right] - h^{-1}B(GB)^{-1}g \\ &= \tilde{f} - \gamma B(GB)^{-1}g, \end{aligned} \tag{2.8}$$

where $\tilde{f} = f - B(GB)^{-1}(Gf + g_t)$, and $\gamma = h^{-1}$.

The stepsize h as defined above, where $\gamma = h^{-1}$, is the *time stepsize which is necessary to locally resolve the constraints* via the Taylor expansion (2.4). This may or may not be related to the time stepsize needed to solve the differential equations to some accuracy criterion. For example, see Example 1 in [5]. This is a problem where the constraints vary rapidly in time, but the differential components are relatively smooth. Experiments in [5] show that the Baumgarte parameter γ needs to be chosen very large for this problem. If γ is chosen so that $\gamma = h^{-1}$, where h is small enough to resolve the constraints, then the Baumgarte method gives a good solution.

2.2. Trust-region approach. For rank-deficient problems, we consider the linearized constraints via a trust region

$$\begin{aligned} &\min_y \frac{1}{2} M_c^T M_c \\ &\text{subject to } \frac{h}{2}^2 y^T y \leq \delta. \end{aligned} \tag{2.9}$$

The Lagrangian function is then given by $L = \frac{1}{2} M_c^T M_c + \epsilon(\frac{h}{2}^2 y^T y - \delta)$.

Letting $M_c = g + hg_t + hGf - h(GB)y$, and setting $\nabla_y L = 0$ to find the minimum, we obtain

$$\begin{aligned} y = &((GB)^T(GB) + \epsilon I)^{-1}(GB)^T(g_t + Gf) \\ &+h^{-1}((GB)^T(GB) + \epsilon I)^{-1}(GB)^T g \end{aligned} \tag{2.10}$$

and, substituting (2.10) into (2.1a),

$$x' = f - By = f - B((GB)^T(GB) + \epsilon I)^{-1}(GB)^T(g_t + Gf) - h^{-1}B((GB)^T(GB) + \epsilon I)^{-1}(GB)^T g, \tag{2.11}$$

where $\frac{h^2}{2}y^T(\epsilon)y(\epsilon) = \delta$. For $\epsilon = 0$, and if $(GB)^{-1}$ exists, the formula reduces to the Baumgarte stabilization (2.3). The trust-region stabilization (2.11) is applicable even when $B \neq G^T$.

2.3. Direct regularization approach. For many systems of physical interest, $B = M^{-1}G^T$, where M^{-1} is symmetric positive definite. Under these circumstances, GB is symmetric positive semidefinite; thus, we can replace GB in (2.7) by $(GB+\epsilon I)$, which is then guaranteed to be nonsingular for $\epsilon > 0$. This yields

$$y = (GB + \epsilon I)^{-1}(Gf + g_t) + h^{-1}(GB + \epsilon I)^{-1}g. \tag{2.12}$$

Substituting into (2.1a), we obtain

$$x' = f - By = f - B(GB + \epsilon I)^{-1}(g_t + Gf) - h^{-1}B(GB + \epsilon I)^{-1}g. \tag{2.13}$$

In subsequent sections, we will investigate the convergence properties of the trust-region regularization (2.11) and the direct regularization (2.13), and show that (2.11) is advantageous because of its greater applicability and robustness, for certain rank-deficient and singular DAE systems.

3. Convergence. In this section we will study the convergence of the trust-region and direct regularization schemes.

DEFINITION 3.1. *Consider the linear DAE*

$$x' = A(t)x + B(t)y + q(t), \tag{3.1a}$$

$$0 = C(t)x + r(t) \tag{3.1b}$$

on $[t_0, t_f]$, *subject to initial conditions in* x *which satisfy the constraints* (3.1b), *where* $x \in \Re^n, y \in \Re^m, C \in \Re^{m\times n}$, *$A$, B, C are time-dependent matrices, and B, C are differentiable. Assume the following hold.*

1. $\mathrm{Rank}(C) = \mathrm{Rank}(B) = r$, $r < m$.
2. *The constraints are consistent,* $r(t) \in \mathit{Im}\ C(t)$.
3. *The reduced problem is index* 2. *Defining* $B^T = U_B\Sigma_B V_B^T$, *we can eliminate the redundant constraints and components of* y *to obtain the reduced problem*

$$x' = Ax + V_B\begin{pmatrix}\bar\Sigma_B\\ 0\end{pmatrix}z_1 + q(t),$$

$$0 = [\bar\Sigma_C, 0]V_C^T x + \bar r_1(t),$$

where

$$\Sigma_C = \begin{pmatrix}\bar\Sigma_C & 0\\ 0 & 0\end{pmatrix}, \quad \Sigma_B = \begin{pmatrix}\bar\Sigma_B & 0\\ 0 & 0\end{pmatrix}.$$

The reduced problem is index 2 *if* $[\bar\Sigma_C, 0]V_C^T V_B\begin{bmatrix}\bar\Sigma_B\\ 0\end{bmatrix}$ *is nonsingular.*

Then (3.1) *will be called a* rank-deficient index-2 DAE.

THEOREM 3.1. *Consider the rank-deficient index* 2 *DAE* (3.1). *For* γ *sufficiently large, the following hold.*

1. *Solutions to the regularization*

$$x' = Ax + By + q(t), \tag{3.2a}$$
$$(CC^T + \epsilon I)y = -(\gamma(Cx + r) + (CAx + Cq + C'x + r')), \tag{3.2b}$$

where $B = C^T$ *and* $N(C^T)$ (*the null space of* C^T) *is constant, converge uniformly as* $\epsilon \to 0$ *in* x *to the solution to* (3.1). *The errors in* x *are* $O(\epsilon)$.

2. *Solutions to the regularization*

$$x' = Ax + By + q(t), \tag{3.3a}$$
$$((CB)^T(CB) + \epsilon I)y = -(CB)^T(\gamma(Cx + r) \tag{3.3b}$$
$$+ CAx + Cq + C'x + r'), \tag{3.3c}$$

where $N(B^T) = N(C)$, *converge uniformly as* $\epsilon \to 0$ *in* x *to the solution to* (3.1). *The errors in* x *are* $O(\epsilon)$.

Proof. Consider first the regularization (3.2) and $B = C^T$. Let $U\Sigma V^T$ be the smooth singular value decomposition of C; i.e.,

$$C = U\Sigma V^T,$$

where

$$\Sigma = \begin{bmatrix} \bar{\Sigma} & 0 \\ 0 & 0 \end{bmatrix},$$

and define $\bar{r}$ by

$$U^T r = \begin{bmatrix} \bar{r} \\ 0 \end{bmatrix}.$$

Partition $U = [U_1, U_2]$. Multiply the constraints in (3.2) by U^T, and let $z = U^T y$, to obtain

$$x' = Ax + V\Sigma z + q(t), \tag{3.4a}$$
$$(\Sigma^2 + \epsilon I)z = -\left(\gamma\left(\Sigma V^T x + \begin{pmatrix} U_1^T r \\ 0 \end{pmatrix}\right) + (\Sigma V^T Ax + \Sigma V^T q + U^T C' x + U^T r')\right). \tag{3.4b}$$

Since $N(C^T)$ is constant, $U_2' \equiv 0$. It follows from $(U^T U)' = 0$ that

$$U^T U' = \begin{bmatrix} U_1^T U_1' & 0 \\ 0 & 0 \end{bmatrix}.$$

Differentiating $U^T r$, we find also that

$$U^T r' = \begin{pmatrix} U_1^T r' \\ 0 \end{pmatrix}.$$

Thus,

$$x' = Ax + V\Sigma z + q(t), \tag{3.5a}$$

$$(\Sigma^2 + \epsilon I)z = -\left[\gamma\left(\Sigma V^T x + \begin{pmatrix} U_1^T r \\ 0 \end{pmatrix}\right) + \Sigma V^T A x + \Sigma V^T q\right.$$

$$\left. +(\Sigma V^T)' x + \begin{bmatrix} (U_1^T U_1')\bar{\Sigma} & 0 \\ 0 & 0 \end{bmatrix} V^T x + \begin{pmatrix} U_1^T r' \\ 0 \end{pmatrix}\right]. \tag{3.5b}$$

Partitioning $z = \binom{z_1}{z_2}$, we see from the bottom block of (3.5) that $z_2 \equiv 0$. Rewriting (3.5) in terms of z_1 only,

$$x' = Ax + V \begin{bmatrix} \bar{\Sigma} \\ 0 \end{bmatrix} z_1 + q(t), \tag{3.6a}$$

$$(\bar{\Sigma}^2 + \epsilon I) z_1 = -d(x), \tag{3.6b}$$

where

$$d(x) = \gamma([\bar{\Sigma}, 0]V^T x + U_1^T r) + [\bar{\Sigma}, 0]V^T A x + [\bar{\Sigma}, 0]V^T q$$
$$+([\bar{\Sigma}, 0]V^T)' x + (U_1^T U_1')[\bar{\Sigma}, 0]V^T x + U_1^T r'.$$

Similar to [4], define

$$v = Rx,$$
$$w = \bar{C}x + \bar{r},$$

where

$$R = [0, I]V^T,$$
$$\bar{C} = [\bar{\Sigma}, 0]V^T,$$
$$\bar{r} = U_1^T r.$$

Then x is given by the inverse transformation

$$x = Sv + Fw - F\bar{r},$$

where S and F are defined by

$$\begin{pmatrix} R \\ \bar{C} \end{pmatrix}^{-1} = (S, F).$$

Changing variables from x to (v, w) in (3.6), we obtain

$$\begin{bmatrix} v' \\ w' \end{bmatrix} = \begin{bmatrix} (R'S + RAS) & (R'F + RAF) \\ O(\epsilon) & -\gamma I + D + O(\gamma\epsilon) \end{bmatrix} \begin{bmatrix} v \\ w \end{bmatrix} + \begin{bmatrix} -R'F\bar{r} - RAF\bar{r} + Rq \\ O(\epsilon) \end{bmatrix}, \tag{3.7}$$

where $D = U_1^{T'} U_1$. The solution to (3.1) satisfies (3.7) with $\epsilon = 0$. It follows from Theorem 10.6 of [17] that for γ sufficiently large, $w = O(\epsilon)$ and the error in v is $O(\epsilon)$. Thus, the error in x is $O(\epsilon)$.

Now consider the second regularization (3.3). Let $C = U_C \Sigma_C V_C^T$ and $B^T = U_B \Sigma_B V_B^T$. Then

$$CB = U_C \Sigma_C V_C^T V_B \Sigma_B^T U_B^T = U_C J U_B^T,$$

where $J = \Sigma_C H \Sigma_B^T$ and $H = V_C^T V_B$. Then (3.3) can be written

$$x' = Ax + V_B \Sigma_B^T z + q(t), \tag{3.8a}$$

$$(J^T J + \epsilon I)z = -J^T U_C^T d, \tag{3.8b}$$

where $z = U_B^T y$ and $d = \gamma(Cx + r) + (CAx + Cq + C'x + r')$. Partitioning $z = \binom{z_1}{z_2}$, where $z_1 \in \Re^r$, from the bottom block of (3.8) we note that $z_2 \equiv 0$. Thus, we can rewrite (3.8) in terms of z_1 only,

$$x' = Ax + V_B \begin{pmatrix} \bar{\Sigma}_B \\ 0 \end{pmatrix} z_1 + q(t), \tag{3.9a}$$

$$(\bar{J}^T \bar{J} + \epsilon I)z_1 = -[\bar{J}^T, 0]U_C^T d, \tag{3.9b}$$

where

$$\bar{J} = \begin{pmatrix} \bar{\Sigma}_C H_{11} \bar{\Sigma}_B & 0 \\ 0 & 0 \end{pmatrix}.$$

Convergence of x and By follows similarly to the first regularization by change of variables to

$$v = Rx = [0, I]V_B^T x,$$
$$w = \bar{C}x = [\bar{\Sigma}_C, 0]V_C^T x$$

to obtain an equation of the form (3.7) from which the results follow. ☐

Now we consider the case where the constraint matrix is singular (i.e., not of constant rank).

DEFINITION 3.2. *Consider the linear DAE* (3.1). *Suppose CB is nonsingular except at an isolated singular point $t^\star$. Assume the following.*

1. *The projector $P = B(CB)^{-1}C$ is differentiable, where*

$$P^{(j)}(t^\star) = \lim_{t \to t^\star} (B(CB)^{-1}C)^{(j)}(t).$$

2. *The inhomogeneity $r(t)$ satisfies $r \in Im\, C(t)$, $t \in [t_0, t_f]$, and $C(t)^+ r(t)$ is differentiable with respect to t.*

Ascher and Lin [3] *have shown that there exists a unique solution to* (3.1) *where x and By are smooth (differentiable). We will call this problem a* kinematically singular index-2 DAE.

Let σ be the smallest singular value of CB, near the singularity. Then the singularity will be called a singularity of multiplicity m *if for t sufficiently close to $t^\star$*

$$|\sigma(t) - \sigma(t^\star)| \leq K|t - t^\star|^m$$

for some constant K.

A linear DAE (3.1) *will be called a* rank-deficient and kinematically singular index-2 DAE *if after eliminating any redundant constraints and Lagrange multipliers as in Definition* 3.1, *the reduced problem is a kinematically singular index*-2 *DAE.*

THEOREM 3.2. *Consider the rank-deficient and kinematically singular index* 2 *DAE* (3.1). *Assume the singularity is of multiplicity m.*

1. *Solutions to the regularization* (3.2) *converge as* $\epsilon \to 0$ *for* γ *sufficiently large to the solution of* (3.1), *for* $B = C^T$. *Errors in* x *due to the regularization are* $O(\epsilon^{1/2})$ *in the region to the left of the interval of length* $O(\epsilon^{1/2m})$ *surrounding the singularity and of order* $O(\epsilon^{1/2\max(m,1)})$ *thereafter.*
2. *The same conclusion holds for the regularization* (3.3) *for* B *such that* $N(B^T) = N(C)$. *Here the errors in* x *are* $O(\epsilon^{1/4})$ *in the region to the left of the interval of length* $O(\epsilon^{1/4m})$ *surrounding the singularity and* $O(\epsilon^{1/4\max(m,1)})$ *thereafter.*

Proof. Without loss of generality, we can remove any global singularity as in Theorem 3.1 and form a reduced system. Hence we will assume that the matrices B and C are of full rank except at the singularity which is assumed to be local.

The regularized solution (3.2) satisfies

$$\begin{aligned} x' = {} & Ax + q(t) \\ & -C^T(CC^T+\epsilon I)^{-1}(C'x + r' + CAx + Cq(t)) \\ & -\gamma C^T(CC^T+\epsilon I)^{-1}(Cx + r(t)). \end{aligned} \tag{3.10}$$

The true solution (3.1) satisfies

$$\begin{aligned} \hat{x}' = {} & A\hat{x} + q(t) \\ & +\hat{x}' - A\hat{x} - q(t) \\ & -\gamma C^T(CC^T+\epsilon I)^{-1}(C\hat{x} + r(t)). \end{aligned} \tag{3.11}$$

Rewriting,

$$\begin{aligned} \hat{x}' = {} & A\hat{x} + q(t) \\ & -C^T(CC^T+\epsilon I)^{-1}C(-\hat{x}' + A\hat{x} + q(t)) \\ & -(I - C^T(CC^T+\epsilon I)^{-1}C)(-\hat{x}' + A\hat{x} + q(t)) \\ & -\gamma C^T(CC^T+\epsilon I)^{-1}(C\hat{x} + r(t)). \end{aligned} \tag{3.12}$$

Substituting $-C\hat{x}' = C'\hat{x} + r'$,

$$\begin{aligned} \hat{x}' = {} & A\hat{x} + q(t) \\ & -C^T(CC^T+\epsilon I)^{-1}(C'\hat{x} + r'(t) + CA\hat{x} + Cq(t)) \\ & -(I - C^T(CC^T+\epsilon I)^{-1}C)(-\hat{x}' + A\hat{x} + q(t)) \\ & -\gamma C^T(CC^T+\epsilon I)^{-1}(C\hat{x} + r(t)). \end{aligned} \tag{3.13}$$

Subtracting (3.13) from (3.10), and letting $e = x - \hat{x}$, we have

$$\begin{aligned} e' = {} & Ae - C^T(CC^T+\epsilon I)^{-1}(C'e + CAe) \\ & -\gamma C^T(CC^T+\epsilon I)^{-1}Ce \\ & -(I - C^T(CC^T+\epsilon I)^{-1}C)(C^T\hat{y}). \end{aligned} \tag{3.14}$$

Rename $e_x = e$. As in [3], there exists a piecewise smooth (differentiable on $[t_0, t^\star]$ and $[t^\star, t_f]$) matrix function $R(t) \in \Re^{(n-m)\times n}$ which has full rank and satisfies $RC^T = 0$. Let $e_v = Re_x$, and $e_w = Pe_x$, where $P = C^T(CC^T)^{-1}C$ and $e_x = e$. Then the inverse transformation is given by

$$e_x = Se_v + e_w,$$

where $S = (I - P)R^T$. Changing variables in (3.14) to (e_v, e_w) yields

$$e_v' = (RAS + R'S)e_v + (RA + R')e_w \tag{3.15a}$$

$$\begin{aligned} e_w' = {} & P'Se_v + P'e_w + PASe_v + PAe_w \\ & -C^T(CC^T + \epsilon I)^{-1}(C'S + CAS)e_v \\ & -C^T(CC^T + \epsilon I)^{-1}(C' + CA)e_w \\ & -\gamma C^T(CC^T + \epsilon I)^{-1}Ce_w \\ & -(P - C^T(CC^T + \epsilon I)^{-1}C)C^T\hat{y}. \end{aligned} \tag{3.15b}$$

Noting that $CS = 0$, hence $C'S = -CS'$,

$$\begin{aligned} e_w' = {} & P'Se_v + P'e_w + PASe_v + PAe_w \\ & -C^T(CC^T + \epsilon I)^{-1}C((S' - AS)e_v + Ae_w) \\ & -C^T(CC^T + \epsilon I)^{-1}C'e_w \\ & -\gamma C^T(CC^T + \epsilon I)^{-1}Ce_w \\ & -(P - C^T(CC^T + \epsilon I)^{-1}C)C^T\hat{y}. \end{aligned} \tag{3.16}$$

Thus, we can write

$$e' = E(t)e + F(t), \tag{3.17}$$

a differential equation for $e = (e_v, e_w)^T$, where the matrix E and function F are defined by (3.15a) and (3.16).

Taking the inner product of both sides of (3.17) with e,

$$\begin{aligned} \frac{1}{2}\frac{d}{dt}\|e\|^2 &= \langle Ee, e\rangle + \langle F, e\rangle \\ &\le \nu(E)\|e\|^2 + \|e\|\|F\|, \end{aligned} \tag{3.18}$$

where $\nu(E)$ is the logarithmic norm (the largest eigenvalue of the symmetric part of E). Let σ be the smallest singular value of CC^T near the singularity $t^\star$. In the subinterval $[t_L^\star, t_R^\star]$, where $|\sigma| \le \epsilon^{1/2}$, we have $\|F\| \le 1$. For large enough γ on this subinterval the eigenvalues of the symmetric part of E are either $O(1)$ or have large negative real part (dominated by the term $\gamma C^T(CC^T + \epsilon I)^{-1}C$). Hence $\nu(E) = O(1)$ on this interval. Let $\bar{e} = \|e\|$. Then from (3.18),

$$\frac{1}{2}\frac{d}{dt}\bar{e}^2 \le O(1)\bar{e}^2 + \bar{e}O(1). \tag{3.19}$$

Thus,

$$\bar{e}' \le O(1)\bar{e} + O(1) \tag{3.20}$$

and it follows that if $\bar{e}$ is $O(\epsilon^{1/2})$ at the beginning of this subinterval, which we will show in a moment, then the size of $\bar{e}$ over $[t_L^\star, t^\star]$ is the maximum of $O(\epsilon^{1/2})$ and the order of the length of the subinterval. At $t^\star$, $R(t)$ may not be continuous. Redefining e via R to the right of the singularity does not change its order of magnitude size. Now by similar arguments, the size of $\bar{e}$ in the subinterval $[t^\star, t_R^\star]$ is the maximum of $O(\epsilon^{1/2})$ and the order of the length of this subinterval.

The length of the subinterval $[t_L^\star, t_R^\star]$ depends on the multiplicity of the singularity. If $t^\star$ is a singularity of multiplicity m, then

$$|\sigma(t) - \sigma(t^\star)| \le K|t - t^\star|^m = O(\epsilon^{1/2}).$$

Thus, $t - t^\star = O(\epsilon^{1/2m})$ and it follows that the errors in x in the subinterval $[t_L^\star, t_R^\star]$ are $O(\epsilon^{1/2\max(m,1)})$.

The rate of convergence thus depends on the multiplicity of the singularity. Convergence is slowest in the subinterval near the root. On the remainder of the interval, where $|\sigma| > \epsilon^{1/2}$, we have the same inequality (3.18), but now $\|F\| = O(\epsilon^{1/2})$. Thus, the accuracy in x in the region to the left of the subinterval of singularity is at least $O(\epsilon^{1/2})$. In the region following the subinterval of singularity, the errors at $t_R^\star$ may already be of order $O(\epsilon^{1/2\max(m,1)})$, hence the order of accuracy following the singularity is $O(\epsilon^{1/2\max(m,1)})$.[1]

For the regularization (3.3), the errors satisfy

$$\begin{aligned} e' = {} & Ae - B((CB)^T(CB) + \epsilon I)^{-1}(CB)^T(C'e + CAe) \\ & -\gamma B((CB)^T(CB) + \epsilon I)^{-1}(CB)^T Ce \\ & -(I - B((CB)^T(CB) + \epsilon I)^{-1}(CB)^T C)(B\hat{y}). \end{aligned} \tag{3.21}$$

We will now examine the last two terms in (3.21) more closely. Let B and C be decomposed $B^T = U_B \Sigma_B V_B^T$, $C = U_C \Sigma_C V_C^T$. Let $J = \Sigma_C H \Sigma_B^T$, where $H = V_C^T V_B$. Then

$$B((CB)^T(CB) + \epsilon I)^{-1}(CB)^T C = V_B \Sigma_B^T (J^T J + \epsilon I)^{-1} J^T \Sigma_C V_C^T. \tag{3.22}$$

Partition $V_C = [V_{C_1}, V_{C_2}], V_B = [V_{B_1}, V_{B_2}]$. Since

$$J = [\bar{\Sigma}_C, 0] \begin{bmatrix} V_{C_1}^T \\ V_{C_2}^T \end{bmatrix} [V_{B_1}, V_{B_2}] \begin{bmatrix} \bar{\Sigma}_B \\ 0 \end{bmatrix}$$

we have

$$J = \bar{\Sigma}_C V_{C_1}^T V_{B_1} \bar{\Sigma}_B.$$

Thus, at all points except the singularity,

$$V_{B_1} \bar{\Sigma}_B = (\bar{\Sigma}_C V_{C_1}^T)^{-1} J. \tag{3.23}$$

Substituting (3.23) into (3.22), we have

$$B((CB)^T(CB) + \epsilon I)^{-1}(CB)^T C = V_{C_1} \bar{\Sigma}_C^{-1} J (J^T J + \epsilon I)^{-1} J^T \bar{\Sigma}_C V_{C_1}^T.$$

Now, since $N(B^T) = N(C)$, we can take $V_{B_1} = V_{C_1}$ [25, Lem. 1]. Then

$$B((CB)^T(CB) + \epsilon I)^{-1}(CB)^T C = V_{C_1} (\bar{\Sigma}_C^2 \bar{\Sigma}_B^2 + \epsilon I)^{-1} \bar{\Sigma}_C^2 \bar{\Sigma}_B^2 V_{C_1}^T$$

and

$$I - B((CB)^T(CB) + \epsilon I)^{-1}(CB)^T C = V_{C_1}(I - (\bar{\Sigma}_C^2 \bar{\Sigma}_B^2 + \epsilon I)^{-1} \bar{\Sigma}_C^2 \bar{\Sigma}_B^2) V_{C_1}^T.$$

Thus, (3.21) has a form analogous to (3.14). The remainder of the proof follows similarly to the first regularization. The error in x due to the regularization is $O(\epsilon^{1/4})$ in the region preceding the subinterval surrounding the singularity and $O(\epsilon^{1/4\max(m,1)})$ elsewhere. □

[1] We suspect from our computational experiences and from the structure of this system that, particularly for $m \le 2$, errors in the interval to the right of the singularity are $O(\epsilon^{1/2})$. However, we have been unable to prove this.

4. Methods for rank-deficient and singular index-3 systems. For higher-index singular systems, one can convert stably [5] to a singular index-2 system and solve via the methods of section 2. It is also possible to solve the index-3 system directly via higher-index versions of Baumgarte's method (1.3), but this requires higher derivatives for the constraint. Here we derive some regularizations for higher-index systems, via the optimization methodology. Unlike the index-2 regularizations, we have not done any convergence analysis on these index-3 regularizations; however, our computational experience with the index-3 trust-region regularization has been positive. These new methods are different from Baumgarte's techniques because they require only first derivatives of the constraint and can be extended as in the index-2 case to rank-deficient and singular systems.

Consider a semiexplicit index-3 differential-algebraic equation of the form

$$x'' = f(x, x', t) - B(x, x', t)y, \tag{4.1a}$$

$$0 = g(x, t). \tag{4.1b}$$

By Taylor expansion

$$x_{n+1} = x(t_n + h) = x_n + hx'_n + \frac{1}{2}h^2 x''_n + O(h^3), \tag{4.2}$$

and

$$0 = g(x_{n+1}, t_{n+1}) \approx g(x_n, t_n) + hg_x \left(x'_n + \frac{1}{2}hx''_n \right) + hg_t.$$

Then by (4.1a), we have

$$g + h(Gx' + g_t) + \frac{1}{2}h^2 Gf - \frac{1}{2}h^2(GB)y = 0, \tag{4.3}$$

where $G = g_x$. If $(GB)^{-1}$ exists, then

$$y = (GB)^{-1}Gf + \frac{2}{h}(GB)^{-1}(Gx' + g_t) + \frac{2}{h^2}(GB)^{-1}g. \tag{4.4}$$

Substituting (4.4) into (4.1), we have

$$x'' = f - B(GB)^{-1}Gf - \frac{2}{h}B(GB)^{-1}(Gx' + g_t) - \frac{2}{h^2}B(GB)^{-1}g. \tag{4.5}$$

4.1. Trust-region approach. If GB is singular, we cannot solve (4.3) for y. We will apply the trust-region approach for solving it.

Consider the trust-region approach for the problem

$$\min_y \frac{1}{2}M_c^T M_c$$
$$\text{subject to} \quad \frac{h^4}{2}y^T y \leq \delta,$$

where $M_c = g + h(Gx' + g_t) + \frac{1}{2}h^2 Gf - \frac{1}{2}h^2(GB)y$. The Lagrangian function $L = \frac{1}{2}M_c^T M_c + \varepsilon(\frac{h^4}{2}y^T y - \delta)$.

Letting $\bigtriangledown_y L = 0$, we have

$$\frac{1}{2}h^2[(GB)^T(GB) + \varepsilon I]y = (GB)^T g + h(GB)^T(Gx' + g_t) + \frac{1}{2}h^2(GB)^T Gf,$$

or

$$
\begin{aligned}
y = {} & [(GB)^T(GB)+\varepsilon I]^{-1}(GB)^T Gf \\
& +\frac{2}{h}[(GB)^T(GB)+\varepsilon I]^{-1}(GB)^T(Gx'+g_t) \\
& +\frac{2}{h^2}[(GB)^T(GB)+\varepsilon I]^{-1}(GB)^T g.
\end{aligned} \tag{4.6}
$$

Substituting y into (4.1), we have

$$
\begin{aligned}
x'' = {} & f - B[(GB)^T(GB)+\varepsilon I]^{-1}(GB)^T Gf \\
& -\frac{2}{h}B[(GB)^T(GB)+\varepsilon I]^{-1}(GB)^T(Gx'+g_t) \\
& -\frac{2}{h^2}B[(GB)^T(GB)+\varepsilon I]^{-1}(GB)^T g.
\end{aligned} \tag{4.7}
$$

For $\varepsilon = 0$, and if $(GB)^{-1}$ exists, the formula (4.7) becomes the formula (4.5).

4.2. Direct regularization approach. We can construct a method which is analogous to the direct regularization approach of section 2.3 by perturbing the matrix GB in (4.5), to obtain

$$
x'' = f - B(GB+\epsilon I)^{-1}Gf - \frac{2}{h}B(GB+\epsilon I)^{-1}(Gx'+g_t) - \frac{2}{h^2}B(GB+\epsilon I)^{-1}g. \tag{4.8}
$$

4.3. Singular mass matrix. The above techniques can be applied directly for solving the Euler–Lagrange equations which describe constrained mechanical systems

$$
M(q)q'' = f(q,q',t) + G^T\lambda, \tag{4.9a}
$$

$$
0 = g(q) \tag{4.9b}
$$

even if the mass matrix M is singular. If M is singular, we consider the original Lagrangian equations for (4.9a)

$$
\min_{q''} \frac{1}{2}||Mq'' - (f+G^T\lambda)||_2^2 \tag{4.10a}
$$

$$
\text{subject to } \ \frac{1}{2}q''^T q'' \le \delta, \tag{4.10b}
$$

$$
0 = g(q). \tag{4.10c}
$$

Then we have

$$
(M^T M + \gamma I)q'' = M^T f + M^T G^T \lambda, \tag{4.11a}
$$

$$
0 = g(q) \tag{4.11b}
$$

for some $\gamma > 0$. Our techniques can then be applied directly to (4.11), even if M is singular in the Lagrangian equations (4.9).

4.4. Higher-index DAE. Consider the DAE of order m

$$
x^{(m)} = f(x,x',\ldots,x^{(m-1)},t) - B(x,x',\ldots,x^{(m-1)},t)y, \tag{4.12a}
$$

$$
0 = g(x,t) \tag{4.12b}
$$

which is index $m+1$ if GB is nonsingular. Applying Taylor series for x_{n+1}, we have

$$x_{n+1} = x(t_n + h) = x_n + hx'_n + \frac{1}{2!}h^2 x''_n + \cdots + \frac{1}{m!}h^m x_n^{(m)} + O(h^{m+1}).$$

Solving the constraint equation by Newton's method,

$$g(x_n, t_n) + g_x\left(hx'_n + \frac{1}{2!}h^2 x''_n + \cdots + \frac{1}{m!}h^m x_n^{(m)}\right) + hg_t = 0$$

or

$$g + h(Gx' + g_t) + \frac{1}{2!}h^2 Gx'' + \cdots + \frac{1}{(m-1)!}h^{m-1}Gx^{(m-1)} + \frac{1}{m!}h^m Gx^{(m)} = 0.$$

Substituting (4.12a),

$$g + h(Gx' + g_t) + \frac{1}{2!}h^2 Gx'' + \cdots + \frac{1}{(m-1)!}h^{m-1}Gx^{(m-1)} + \frac{1}{m!}h^m G(f - By) = 0. \tag{4.13}$$

If GB is nonsingular, then

$$\begin{aligned} y = {} & (GB)^{-1}Gf + \frac{m}{h}(GB)^{-1}Gx^{(m-1)} \\ & + \frac{m(m-1)}{h^2}(GB)^{-1}Gx^{(m-2)} + \cdots + \frac{m!}{2h^{m-2}}(GB)^{-1}Gx'' \\ & + \frac{m!}{h^{m-1}}(GB)^{-1}(Gx' + g_t) + \frac{m!}{h^m}(GB)^{-1}g. \end{aligned} \tag{4.14}$$

We can solve the mth order ODE (4.12a) for $x^{(m)}$:

$$\begin{aligned} x^{(m)} = {} & f - B(GB)^{-1}Gf - \frac{m}{h}B(GB)^{-1}Gx^{(m-1)} \\ & - \frac{m(m-1)}{h^2}B(GB)^{-1}Gx^{(m-2)} - \cdots - \frac{m!}{2h^{m-2}}B(GB)^{-1}Gx'' \\ & - \frac{m!}{h^{(m-1)}}B(GB)^{-1}(Gx' + g_t) - \frac{m!}{h^m}B(GB)^{-1}g. \end{aligned} \tag{4.15}$$

If GB is singular, we apply the trust-region approach for solving (4.13). Consider the problem

$$\min_y \frac{1}{2}M^T M$$
$$\text{subject to} \quad \frac{h^{2m}}{2}y^T y \le \delta,$$

where $M = g + h(Gx' + g_t) + \frac{1}{2}h^2 Gx'' + \cdots + \frac{1}{(m-1)!}h^{m-1}Gx^{(m-1)} + \frac{1}{m!}h^m(Gf - (GB)y)$. We obtain the solution for y:

$$\begin{aligned} y = {} & [(GB)^T(GB) + \varepsilon I]^{-1}(GB)^T \left[Gf + \frac{m!}{h^m}g \right. \\ & \left. + \frac{m!}{h^{m-1}}(Gx' + g_t) + \frac{m!}{2h^{m-2}}Gx'' + \cdots + \frac{m}{h}Gx^{(m-1)}\right]. \end{aligned} \tag{4.16}$$

The solution for x is given by (4.12a).

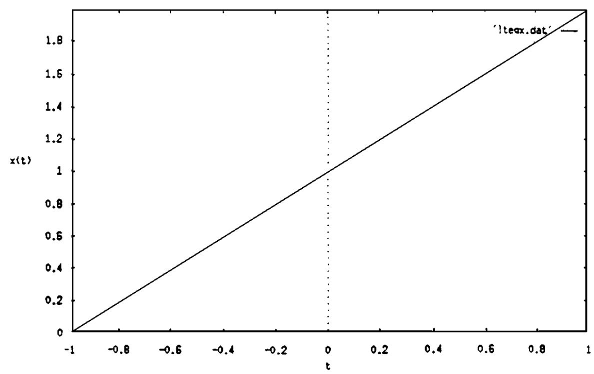

FIG. 5.1. *Example* 5.1*, Baumgarte method,* $\gamma = 10^3$.

5. Numerical experiments. In this section we present the results of some numerical experiments illustrating the effectiveness of the trust-region methods for rank-deficient DAEs.

Example 5.1 (linear test problem). Consider the linear test problem

$$x' = 2 + ty, \tag{5.1a}$$

$$0 = tx - t(t+1). \tag{5.1b}$$

This problem has true solution

$$x = t + 1,$$
$$y = -t^{-1}.$$

Thus, y blows up at the singularity while x remains smooth. We used DASSL [10] to solve the equations given by the Baumgarte method (2.8), the trust-region method (2.11), and the direct regularization method (2.13). For all of our index-2 tests DASSL was modified as recommended in [10]; the root mean square (RMS) norm (DASSL default) was used for all convergence tests with the exception of the error test, which was modified to exclude the index-2 variable. (For the index-3 tests, this norm was modified to exclude the index-2 and index-3 variables). Throughout the testing, the relative error tolerance (RTOL) and absolute error tolerance (ATOL) were fixed at 10^{-5}. All testing was done in double precision.

In Figures 5.1–5.3 we show the results for Example 5.1. For this simple example, the unmodified Baumgarte method (Figure 5.1) works by passing over the singularity (however, we found that for other error tolerances and parameters, this method sometimes fails if the steps get too close to the singularity).

In Figures 5.2 and 5.3, the direct regularization and trust-region approaches are used, with $\gamma = 10^3$ and $\epsilon = 10^{-6}$. We can see the effect of the error due to the regularization, at the singularity. Figure 5.4 shows the trust-region approach with $\gamma = 10^3$ and $\epsilon = 10^{-9}$; we can no longer see the effects of the error due to the regularization.

Example 5.2 (slider-crank mechanism). Next we attempted a more difficult nonlinear singular DAE, arising from the slider-crank mechanism in Figure 5.5 [19].

Here θ_1 and θ_2 act as generalized coordinates and, as shown, all other physical parameters have been given values of unity. After some manipulation, the equations

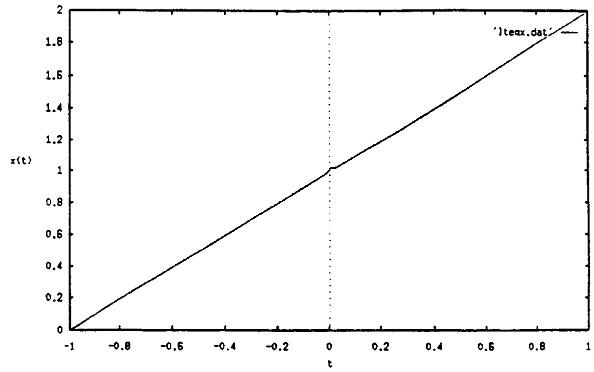

FIG. 5.2. *Example* 5.1, *direct regularization method,* $\gamma = 10^3$, $\epsilon = 10^{-6}$.

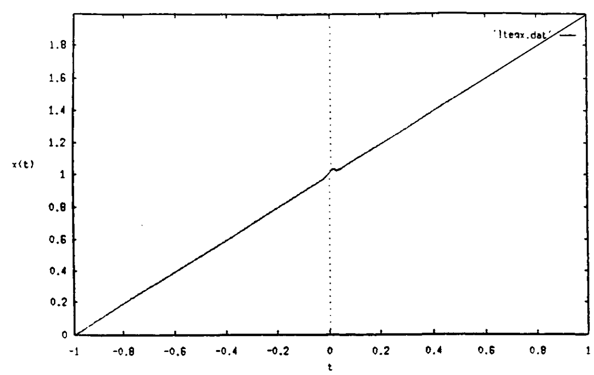

FIG. 5.3. *Example* 5.1, *trust-region method,* $\gamma = 10^3$, $\epsilon = 10^{-6}$.

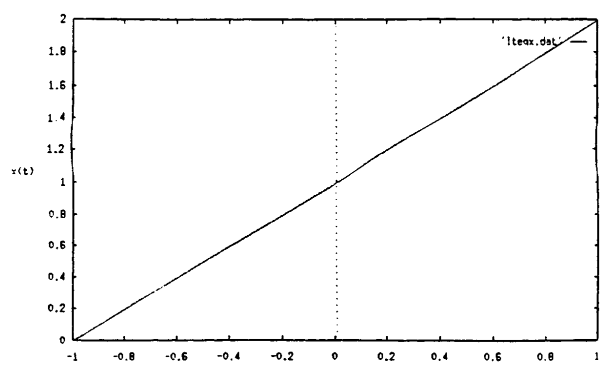

FIG. 5.4. *Example* 5.1, *trust-region method,* $\gamma = 10^3$, $\epsilon = 10^{-9}$.

of motion for the index-3 DAE formulation for this problem take the form

$$\begin{bmatrix} 2.0 & \cos(\theta_d) \\ \cos(\theta_d) & 1.0 \end{bmatrix} \begin{bmatrix} \ddot{\theta_1} \\ \ddot{\theta_2} \end{bmatrix} + \begin{bmatrix} -\sin(\theta_d)(\dot{\theta_2})^2 + 19.6\sin(\theta_1) \\ \sin(\theta_d)(\dot{\theta_1})^2 + 9.8\sin(\theta_2) \end{bmatrix} + \begin{bmatrix} \sin(\theta_1) \\ \sin(\theta_2) \end{bmatrix} \lambda = 0, \tag{5.2}$$

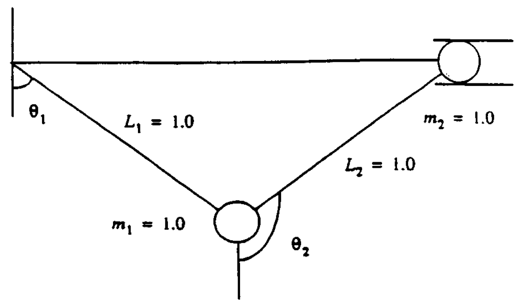

FIG. 5.5. *Example* 5.2*, slider-crank mechanism.*

where $\theta_d = \theta_2 - \theta_1$, with the constraint

$$g_3(\theta, t) = -\cos(\theta_1) - \cos(\theta_2) = 0. \tag{5.3}$$

The equations of motion for the index-2 problem are identical to the above equations, except that the constraint is now differentiated with respect to time

$$g_2(\theta, t) = \sin(\theta_1)\dot{\theta}_1 + \sin(\theta_2)\dot{\theta}_2 = 0. \tag{5.4}$$

The principle reason this problem was chosen as a test case is the presence of a bifurcation singularity (and a lockup-type singularity for $L_1 \neq L_2$) at the point $(\theta_1, \theta_2) = (0, \pi)$, which allows for one of two system configurations. In terms of the index-2 or index-3 DAE formulations, the singularity manifests itself as the rank deficiency of the matrix GB, where $G = \frac{d}{d\theta}(g)$. In fact, for this problem, both the index-2 and the index-3 constraints vanish at $(0, \pi)$, insuring that $\det(GB) = 0$ at the point of singularity.

In Figures 5.6–5.8, we show the results of solving the index-2 equations with the Baumgarte method, the direct regularization method, and the trust-region method, respectively, with $\gamma = 10^3$, $\epsilon = 10^{-6}$. Although the Baumgarte method works for this error tolerance and parameters, our experience is that it is not robust and often fails at the singularities. The direct regularization method fails at the singularity. From Figure 5.8, we can see that the trust-region method is doing a good job. These results are not surprising because the linearization of this problem fails to satisfy $B = C^T$, which is a condition in Theorem 3.2 for convergence of the direct regularization method but is not required for convergence of the trust-region regularization. In Figures 5.9–5.11, we show the results of the three methods for $\gamma = 10^6$, $\epsilon = 10^{-6}$ (here we have used RTOL = ATOL = 10^{-6}). We see that for this choice of parameters, the Baumgarte method and the direct regularization method fail, whereas the trust-region method succeeds. We have also found that the Baumgarte method is very sensitive, near the singularity, to how the equations are formulated. Here we are solving (2.1a) coupled to (2.5), which has been much more robust than solving (2.8) directly.

Finally, we tested the index-3 versions of the methods on the index-3 slider-crank equations. The results are shown in Figures 5.12–5.14. From Figures 5.12 and 5.13, we see that the Baumgarte method and the direct regularization method converge to incorrect solutions. We believe this is due to the loose error control which is (by necessity) used in the index-3 solution. From Figure 5.14, the trust-region method converges. Our experience with the trust-region methods in either the index-2 or index-3 versions is that they are very robust.

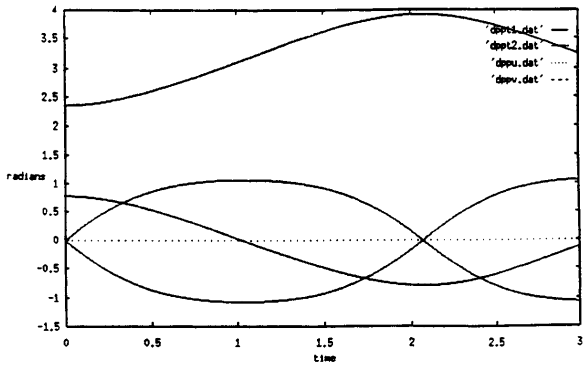

FIG. 5.6. *Example* 5.2*, Baumgarte method,* $\gamma = 10^3$*, index*-2.

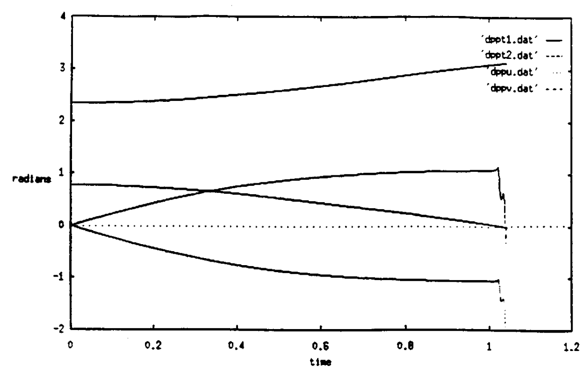

FIG. 5.7. *Example* 5.2*, direct regularization method,* $\gamma = 10^3, \epsilon = 10^{-6}$*, index*-2.

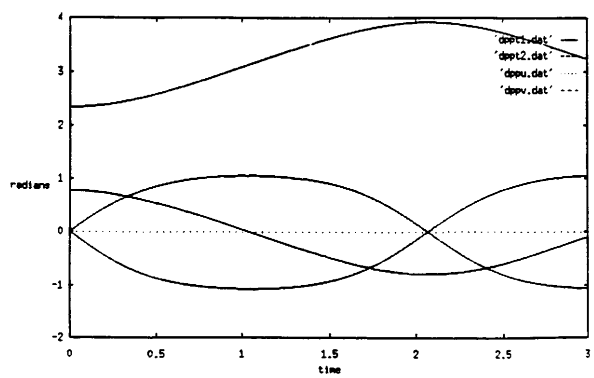

FIG. 5.8. *Example* 5.2*, trust-region method,* $\gamma = 10^3, \epsilon = 10^{-6}$*, index*-2.

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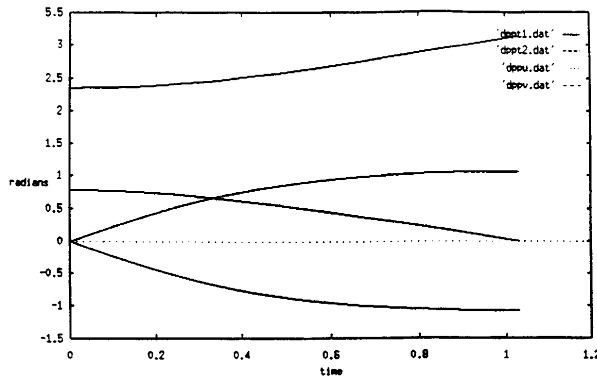

FIG. 5.9. *Example* 5.2, *Baumgarte method,* $\gamma = 10^6$, *index*-2.

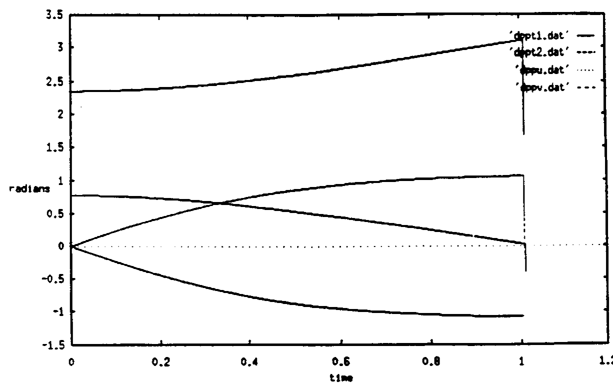

FIG. 5.10. *Example* 5.2, *direct regularization method,* $\gamma = 10^6, \epsilon = 10^{-6}$, *index*-2.

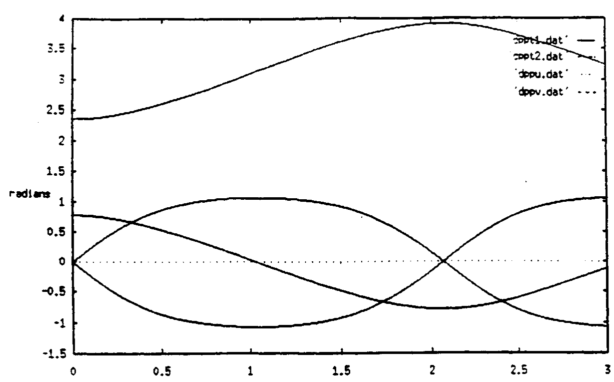

FIG. 5.11. *Example* 5.2, *trust-region method,* $\gamma = 10^6, \epsilon = 10^{-6}$, *index*-2.

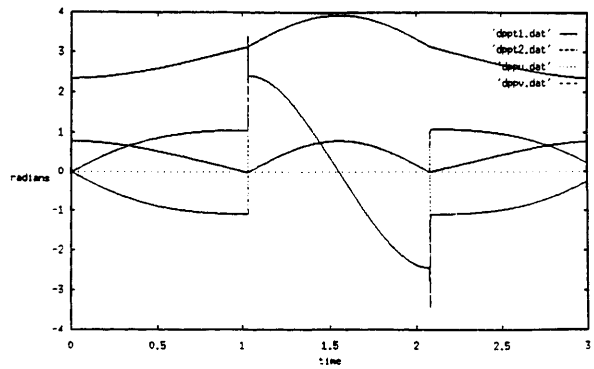

FIG. 5.12. *Example* 5.2, *Baumgarte method,* $\gamma_0 = 2 \times 10^6, \gamma_1 = 2 \times 10^3$, *index*-3.

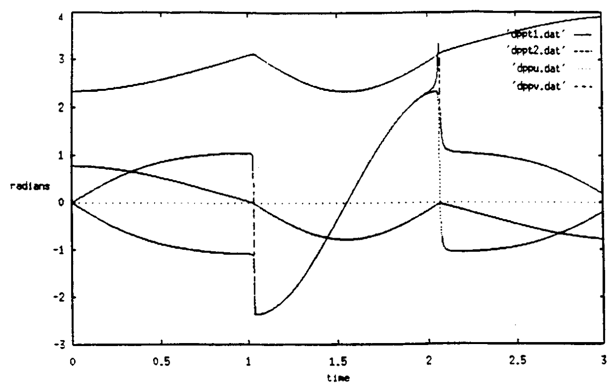

FIG. 5.13. *Example* 5.2, *direct regularization method,* $\gamma_0 = 2 \times 10^6, \gamma = 2 \times 10^3, \epsilon = 10^{-6}$, *index*-3.

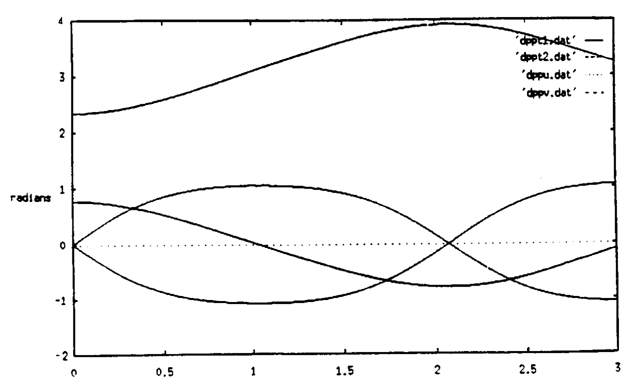

FIG. 5.14. *Example* 5.2, *trust-region method,* $\gamma_0 = 2 \times 10^6, \gamma = 2 \times 10^3, \epsilon = 10^{-6}$, *index*-3.

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