On the Accurate Solution of
Differential-Algebraic Optimization Problems

by

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Abstract

Differential - algebraic optimization problems arise often in chemical engineerting processes. Current numerical methods for differential - algebraic optimization problems rely on some form of approximation in order to pose die problem as a nonlinear program. Here we explore an appropriate discretization and formulation of this optimization problem by considering stability and error properties of implicit Runge * Kutta (IRK) methods for differential • algebraic equation (DAE) systems. From these properties we are able to enforce appropriate error constraints and method orders in a collocation based nonlinear programming (NLP) formulation.

After demonstrating the IRK properties on a small DAE system, we show from variational conditions that optimal control problems can have the same difficulties as higher index DAE systems. This is illustrated for a number of small chemical engineering optimization examples that exhibit higher index characteristics. For these cases the NLP formulation in this paper yields efficient and accurate solutions.

I. Introduction

The determination of optimal control profiles is of major importance for process applications. Examples within chemical engineering include problems in reactor design, process startup, batch process operation, etc. However, solution of optimization problems with differential and algebraic equation modehstiD remains a diflBcniltproblem. At present, optimization problems with [illegible] algebraic equations can be solved in a straightforward way as nonlinear programs. On die other hand, unconstrained problems with differential equation models can be handled through die calculus of variations. However, models that combine both of these features are currently optimized by imposing some level of approximation to the problem. The purpose of this paper is to develop and discuss a nonlinear programming formulation that leads to the accurate solution (within an e tolerance) of the general differential-algebraic optimal control problem.

Current methods for handling these problems either apply an approximation to the control variable profile or to both the state and control profiles. A straightforward approach adopted by Sargent and Sullivan (1977) is to parameterize the control profile (e.g. piecewise constant) over variable-length finite elements and to solve the differential equations with this parameterization. A nonlinear programming algorithm is then applied to the control parameters in an outer calculation loop. Similar strategies have been proposed by Ray (1981) and Morshedi (1986). This "feasible path" approach requires the repeated and expensive solution of the differential-algebraic eqautions. Also, state variable inequality constraints cannot be handled in a straightforward way. Finally, the quality of the solution is strongly dependent on die parameterization of the control profile.

Early studies with the second approach, parameterization of both the state and control profiles, were reported by Neuman and Sen (1972), Tsang et al (1974) and Lynn et al (1971). Here state and control profiles and die differential equations were parameterized using some method of weighted residuals (eg. orthogonal collocation). This leads to a large nonlinear program (NLP) with algebraic equality constraints. However, since NLP algorithms were less developed at that time, this approach was either inefficient when compared to feasible path methods, or was restricted to specialized (e.g. linear) problems.

With advances in NLP methods through the development of Successive Quadratic Programming (SQP) and MINOS, these NLP's could be solved more efficiently and could handle nonlinear state and control profile constraints in a straightforward manner. Biegler

(1984) demonstrated this approach on a small batch reactor problem. Renfro et al (1987) solved much larger problems with orthogonal collocation on finite elements and piecewise constant approximations to the control profile. In order to obtain accurate finite element solutions, however, Cuthrell and Biegler (1986,1989) imposed additional constraints in the NLP formulation in Older to enforce accurate state profiles. They classified the role of finite elements in terms of knot locations (over which die error was equidistributed, hence minimiTfri) and breakpoints that allowed for control profile discontinuities. This led to a formulation that enforced the accurate solution of the differential equations and allowed for a general description of the control profile. In this paper we explore the theoretical development of these finite element constraints and present a formulation that leads to arbitrarily accurate state variable and control variable profiles. Here finite elements serve as decision variables in the optimization problem and are simultaneously required to satisfy approximation error constraints and to locate control profile discontinuities.

This formulation will be considered from the perspective of a discretized Differential-Algebraic Equation (DAE) system. Recent approximation error and stability results by Petzold and coworkers will be tailored to optimal control problems and incorporated into the NLP. The next section will review the equivalence between the variatibnal conditions for general optimal control problems and die Kuhn-Tucker conditions for the corresponding NLP formulation. Section 3 then discusses recent stability and approximation error results for Runge-Kutta methods (including collocation methods) ipplied to DAE systems. In particular we will discuss the appropriate selection of collocation methods for higher index (i.e., more difficult) DAE systems. The following section then discusses how these higher index DAE systems arise in optimal control problems with path constraints and singular arcs. Section 5 presents the solution of a number of higher index optimal control examples with our approach. Here it is shown that arbitrarily accurate solutions can be found with our NLP formulation. Finally, section 6 summarizes die paper and discusses approaches to dealing with large-scale optimal control problems.

2. Analysis of the Opdmalhy CotKlitwns for Optimal Control ProWems

In this section we briefly review the equivalence between the calculus of variations and the math programming approach. Special cases for optimal control problems such as singular arcs and path constraints will be discussed after this section. Consider the following general problem:

Min ¥(z(b)) + J *(z(t),ii(t)) dt

u(t).x(t)

SL 2(0 « F(z(t), u(t))
g(u(t),:e(t)) ^ 0
g_f(z(b)) £ 0
z(a) = z_0
$z(t)^L$ £ z(t) ^ $z(t)^U$
$u(t)^L$ ^ u(t) £ $u(t)^U$

where:

- Y(z(b)) * component of objective function due to final conditions

I <J>(z(t)$_f$u(t))dt = component of objective function due to integral of state and control vectors

g « inequality design constraint vectors
z(t) « state profile vector
u(t) « control profiles
gj « final conditions inequality constraints
ZA K frwtifti condition for ttfttf vector

$z(t)^L$$_f$ $z(t)^U$ « sate profile bounds

$u(t)^L$, $u(t)^U$ * control profile bounds

The variational conditions for Ais problem are:

(a) du du du = 0

$$\text{(b)} \quad \frac{\partial \Phi}{\partial z} + \frac{\partial F}{\partial z} \Lambda + \frac{\partial g}{\partial z} M + \dot{\Lambda}(t) = 0$$

$$\text{(c)} \quad g\,(\,u(t),\, z(t)\,) \leq 0$$

$$\text{(d)} \quad M(t)\; g\,(z\,(t)\,) = 0\,, \quad M(t) \geq 0$$

$$\text{(e)} \quad \dot{z}\,(t) = F\,(\,z(t)\,,\, u(t)\,)\,, \quad z(a) = z_0$$

$$\text{(f)} \quad \dot{\lambda}\,(\,b) = -[\frac{\partial \Psi}{\partial z} + \frac{\partial g_f}{\partial z} M_f]_{t_f = b}$$

where $M(t)$ and $\Lambda(t)$ are adjoint functions for the constraint $g\,(\,u(t),\, z(t)\,) \leq 0$,and the ODE model respectively. Note that these conditions form a DAE system. Here the algebraic relation (a) is used to determine the optimal control profile. Also, when constraints (d) are active, these additional algebraic conditions can cause an additional degree of difficulty in the solution of the DAE system. This difficulty is classified by the index of the system and is considered later. Finally, if (a) is not explicitly a function of u, then singular arcs can be encountered for the DAE system.

Kreindler (1982) showed that the above equations are stronger necessary conditions than those presented in Bryson and Ho (1975). Cuthrell and Biegler (1987) showed the similarity between the solution solved with a nonlinear programming formulation and the corresponding variational conditions of the optimal control problem. The Kuhn - Tucker conditions for the DAE's discretized with finite element collocation are considered next.

Here we include the integration lengths, $\Delta\alpha_i$, as decision variables in order to find the breakpoints for control profile discontinuities. Later, in section 4 we also impose constraints for the approximation error. The nonlinear program to be solved by applying collocation on finite elements now has the following form:

$$\underset{z_{ij},\, u_{ij},\, \Delta\alpha_i}{\text{Min}} \quad \Psi\,(z_f) + \sum_{i=1}^{NE} \sum_{j=1}^{K} w_{ij} \Phi(\, z_{ij},\, u_{ij},\, \Delta\alpha_i)$$

$$\text{s.t.} \quad r\,(t_{ij}) = \dot{z}_{k+1}(t_{ij}) - F\,(\, z_{ij},\, u_{ij},\, \Delta\alpha_i, t_{ij}) = 0$$

$$g\,(\, z_{ij},\, u_{ij},\, \Delta\alpha_i\,) \leq 0$$

$$g_f\,(\, z_f) \leq 0$$

$$z_{10} - z_0 = 0$$

$$z_{i0} - z_{k+1}^{i-1}(\alpha_i) = 0 \qquad i = 2,\ldots,NE$$

$$z_f - z_{k+1}^{NE}(\alpha_{NE+1}) = 0$$

$$z_{ij}^L \le z_{ij} \le z_{ij}^U$$

$$u_{ij}^L \le u_{ij} \le u_{ij}^U$$

$$\Delta\alpha^L \le \Delta\alpha_i \le \Delta\alpha^U$$

$$\sum_{i=1}^{NE} \Delta\alpha_i = \alpha_{Total}$$

where i is the element, and j is the collocation point. Also, $\Delta\alpha_i$ are finite element lengths $i = 1,\ldots, NE$, z_f is the value of the state at the final time, and the constraint g_f is evaluated at the final time.
Note that z_{ij}, u_{ij} are collocation coefficients for the state and control profiles.

As shown in Cuthrell and Biegler (1989), the optimality conditions for the NLP can be simplified to the following equations:

$$\text{(a)} \qquad \frac{\partial \Phi(t_{ij})}{\partial z_{ij}} + \left(\frac{\partial F(t_{ij})}{\partial z_{ij}}\right)\lambda_{ij} + \dot{\lambda}_{k+1}(t_{ij}) + \left(\frac{\partial g}{\partial z_{ij}}\right)\mu_{ij} = 0$$

$$\lambda_{k+1}^{i-1}(\alpha_i) = \lambda_{k+1}^{i}(\alpha_i) \qquad i = 2,\ldots,NE$$

These equations (a) are the discrete analog of the adjoint equations. Then the discrete analog of the variational conditions for the control variables are given in (b):

$$\text{(b)} \qquad \frac{\partial \Phi(t_{ij})}{\partial u_{ij}} + \left(\frac{\partial F(t_{ij})}{\partial u_{ij}}\right)\lambda_{ij} + \left(\frac{\partial g}{\partial u_{ij}}\right)\mu_{ij} = 0$$

The final and initial conditions on the adjoint variables are:

$$\text{(c)} \qquad \frac{\partial \Psi}{\partial z_f} + \frac{\partial g_f}{\partial z_f}\mu_f - \lambda_{k+1}(\alpha_{NE+1}) = 0$$

$$\text{(d)} \qquad \lambda_{k+1}(\alpha_1) = 0 \qquad \text{if } z_0 \text{ not specified}$$

The feasibility conditions for the ODE and the problem constraints are:

$$(e) \quad \dot{z}_{k+1}(t_{ij}) - F(z_{ij}, u_{ij}, t_{ij}) = 0 \quad , z_{10} = z_0$$

$$z^{i-1}_{k+}i\,(\alpha P \quad - \quad *L_{+}i(a) \qquad i = 2..........NE$$

$$(0 \quad g(z_{ij}, u_{ij}) \wedge \quad 0$$

$$(g) \quad gfUf) \quad * \quad 0$$

$$(h) \quad ki_r \bullet Mij \quad \geq \quad 0$$

$$(i) \quad \wedge (g U \wedge)) = O \quad \mu_f (g_f(z_f)) - 0$$

For optimal control problems, numerical difficulties are encountered for problems that have control profiles with state path constraints enforced and/or singular arc segments. These characteristics can be classified by considering properties of DAE systems. In the next section we define the index of a DAE system and relate this to optimal control problems.

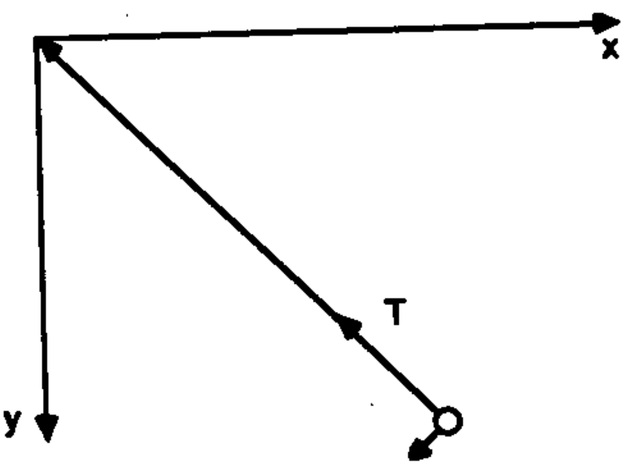
3. Definition of Index **and** Impact on Solution of DAE's

Implicit in the solution of the nonlinear programming formulation for the optimal control problem is an accurate approximation to the solution of the differential equations. Here we assume that the finite elements are kept sufficiently small so that the local error is controlled within the element. However, it has recently been pointed out (Petzold (1982)) that numerical problems can occur with discretized differential equations solved in conjuction with the algebraic equations. Methods can fail due to incorrect error control strategies or instabilities resulting firom the error propagation during the integration. These numerical problems are characteristic of classes of DAE's and can be classified by the index of the system.

Consider the semUxplicit form described by Petzold and LBtstedt (1986) and Brenan(1983):

$$\cancel{\begin{aligned} \dot{u} &= f(u,v,t) \\ 0 &= g(u,v,t) \end{aligned}} \qquad \begin{aligned} \dot{x} &= f(x,y,t) \\ 0 &= g(x,y,t) \end{aligned} \quad (1)$$

Now the difficulty of solution can be characterized by die index of the system, which is simply the number of times Ac algebraic equations of the system must be differentiated in order to obtain a standard form ODE system. As an example, consider the mechanical system of a simple pendulum pictured in Figure 1.



Fielire 1. Pendulum System

For the case of a unit mass on a unit length of string, the following system of equations describe the model:

• u . W
x *
m V (b)
y
u « -Tx (c)
• g-iy (d)
V « 2 2
1 - (0
x(0) x - • »o y
y(0) * yo

(2)

This is an index three system because (e) must be differentiated (and ODE's substituted) three times to yield a first order ODE in T. The first differentiation yields:

$$0 \ll xu + yv \qquad (f) \qquad \text{Index 2}$$

Differentiating (f) gives:

$$0 \ll -T + yg + u^2 + v^2 \qquad (g) \qquad \text{Index 1}$$

And differentiating *pffo. Ifaris to *i*

$$t \ll 3vg-2Tux-2Tvy \qquad (h) \qquad \text{Index 0}$$

Using the index 0 formulation $_t$ one can solve this problem with any standard ODE solver once consistent initial conditions have been specified (Pantelides (1988)). The solution of this problem in the higher index forms has been studied for linear multistcp methods such as the BDF (backward - differentiation formulas) first proposed by Gear (1971) and currently used in codes such as DASSL (1982) and LSODE (1980). Convergence proofs have been established for fixed step-size BDF methods for index 2 and index 3 problems by Petzold and Lötstedt(1986) and Brenan and Engquist (1985). Theory for variable step-size BDF for index 2 systems was established by Gear et al (1985).

Runge-Kutta methods for DAE's have been studied by Petzold (1986), März(1981), Brenan and Petzold (1987), and Burrage and Petzold (1988). Petzold showed that the Runge-Kutta methods can suffer order reduction for index erne problems. Brenan and Petzold (1987) studied the order, stability, and convergence of implicit Runge-Kutta (IRK) methods applied to differential-algebraic systems. Burrage and Petzold (1988) established die convergence and stability properties of index 1 systems solved by IRK methods. For example, two point orthogonal collocation falls into the class of IRK methods which are stable and have good error control for index 1 systems.

The higher index problem is of concern, however, because it is often desirable to solve the DAE system directly rather than die differentiated form. Moreover, for optimal control problems, the solution may be governed by different sets of constraints over different parts of the trajectory and the reformulation is difficult to implement Also the differentiation may introduce additional constants of integration which may not remain invariant under integration. As an example, consider the index 1 problem

$$0 - y - \frac{t^2}{2} \qquad (3)$$

which can be differentiated to obtain:

$$\dot{y} - * \qquad (4)$$

Even with the correct initial condition y(0) « 0, integration errors due to truncation and roundoff errors could cause the numerical solution of (4) to differ from that of (3). We would also prefer to use the formulation of the DAE's in the higher index form because this-is the natural statement of the physical models.

Finally, the nonlinear programming formulation of the optimal control problem requires a self-starting method. Consequently, the properties associated with Runge-Kutta methods are especially useful to us. In particular, the method we have chosen to discretize the differential equations is orthogonal collocation on finite elements. The method must possess strong stability properties and control the local integration error because the stability of the method and the local error determine the global error. Since collocation is an implicit Runge-Kutta method, we can directly apply their stability and error properties for index one and higher systems (Petzold(1986), Brenan and Petzold(1987), Burrage and Petzold (1988)). The next section will briefly review these properties. This is necessary in order to determine what order method (i.e., number of collocation points) is needed to obtain a stable and accurate solution for different classes of optimal control problems.

3-1 Review oT Runge-Kutta Analysis:

The standard Runge-Kutta analysis starts with the consideration of an initial value problem:

$$\dot{y} « f(t.y), \quad y(to)«y(O) \qquad (5)$$

The s-stage Runge-Kutia method applied to (5) yields

$$Y_i = y_n + h\sum_{j=1}^{s} a_{ij} f(t_n + c_j h, Y_j), \quad i = 1, \ldots, s$$

$$y_{n+1} = y_n + h\sum_{j=1}^{s} b_j f(t_n + c_j h, Y_j) \tag{6}$$

where

$b^T = (b_1, \ldots, b_s)$,

$A = (a_{ij})_{i,j=1,\ldots,s}$ the Butcher block coefficients

$c^T = (c_1, \ldots, c_s) = A e_M$

$c^{j^T} = (c_1^j, c_2^j, \ldots, c_s^j)$

$e_M = (1, \ldots, 1)^T$, unit vector

h = step length of integration

For example, the 2-stage Gauss - Legendre method (2 point orthogonal collocation) is represented by the following Butcher block notation:

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array} = \begin{array}{c|cc} \frac{3-\sqrt{3}}{6} & \frac{1}{4} & \frac{3-\sqrt{3}}{6} - \frac{1}{4} \\ \frac{3+\sqrt{3}}{6} & \frac{3+\sqrt{3}}{6} - \frac{1}{4} & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

Now the local error has been shown by Petzold (1986) to be $O(h^{k_a+1})$ for index one systems if **and** only if

$$b^T A^{-1} c^j = 1, \quad j = 1, \ldots, k_a \tag{7}$$

For the above two point orthogonal collocation method it is easily shown that the Butcher block coefficients satisfy the error relationship (7) for $k_a = 2$. For higher index systems, we need to consider the stage order or algebraic order of the method. Here the stage order k_I is the largest integer w that satisfies the following tests:

$$C(w): \quad \sum_{j=1}^{s} a_{ij}\, c_j^{k-1} = c_i^{k}/k \;, \quad i = 1,\dots s \qquad k = 1,\dots w \tag{8}$$

$$B(w): \quad \sum_{j=1}^{s} b_j\, c_j^{k-1} = 1/k \;, \quad k = 1,\dots w \tag{9}$$

If $C(k_I)$ and $B(k_I)$ hold for the Runge-Kutta method with s stages then it has a stage order k_I and the local error is $O(h^{k_I})$. For collocation the stage order is the number of internal points and C(w) and B(w) are self-generating (Burrage and Petzold (1988)).

Therefore, collocation methods have stage order k_I and the stability and error relationships developed by Brenan and Petzold (1987) can be used to predict the integration error and stability behavior of the system. First let us consider the error relationship for the local error. The general relationship is:

$$d_{n,v} = O(h^{(k_{a,v}-v+2)}) + O(h^{(k_{a,v}-v+3)}) + \dots + O(h^{(k_{a,I}+1)})$$

where $\quad v \;=$ the index of the system

and $\quad k_{a,v} =$ the largest integer k that satisfies the following tests.

$$b^T A^{-i} e_M = b^T A^{-v} c^{v-i}/(v-i)! \qquad i = 1,2,\dots\dots v-1$$
$$b^T A^{-v} c^i = i(i-1)\dots\dots(i-v+1) \qquad i = v, v+1,\dots k$$

Specifically, for index 2 systems, the algebraic order k satisfies:

$$b^T A^{-1} e_M = b^T A^{-2} c^1$$
$$b^T A^{-2} c^i = i \qquad i = 2,3,\dots k$$

And for index 3 systems

$$b^T A^{-1} V^2 e_M = b W$$
$$b^T A^{-1} V e_M = b^T A^{-3} V c J_2$$
$$b V V = i(i-1) \qquad i = 3,4,\ldots k$$

Then the local error for index one and index zero systems is simply the last term for $d_{n,v}$ and the higher index systems terms are added as required Thus, by noting that the stage order for collocation methods is the number of internal points, one can find die local order of the errors for the following methods:

Index 1. Two-point collocation - O (h**1 *! V O (h0))
Index 2. Three-point collocation - O C h 0 ^ - O(h(3>)
Index 3. Four-point collocation - O (h(k○ "! ^ - O (h°)

These results are valid for A-stable and L-stable collocation systems in that these systems satisfy the tests outlined above. Note that there is an order reduction in the local error for the higher index systems. Let us now consider the stability of the methods. Brenan and Petzold (1987) developed the general stability relation for the error propagation from step to step:

$$e_{n,v} = (1 - b^T A^{-1} e_M)\, e_{n-1,v} - (b^T A^{-1} \delta_{n,v} - \delta_{n,v}^{M+1}) - \sum_{i=1}^{v-1} \frac{(-1)^i}{h^i} b^T A^{-i-1} (\delta_{n,v-i} + e_M e_{n-1,v-i})$$

where $\delta_{n,v}$ = perturbations due to roundoff error and machine precision:

They defined a stability constant r, as

$$r = 1 - b^T A^{-1} e_M$$

and $|r| < 1.0$ for strict stability.

For two point orthogonal collocation, the value of $|r| = 1.0$ because $b^T A^{-1} e_M = 0$. Note that this does not satisfy the sufficient strict stability condition of

$|r| <$ LO. However* further work by Bimage and Pttzold (1988) showed this method to be stable for index 1 systems and proved the convergence properties for linear constant coefficient systems of index 1. Also, index 1 systems have been shown to be stable and to not suffer any order reduction for semi-explicit systems (Roche (1987), Deuflhaid et al. (1985), and Griepentrog and Man (1986)).

Note that for the local enor analysis, three point collocaticm was found to satisfy the index 2 order tests and four point was found to satisfy ihe index 3 tests. Also, two point collocation failed the index 2 tests . Note that orthogonal and non-orthogonal collocation will satisfy the local enor tests because die butcher block coefficients axe self generating for collocation. However, the difference between die methods (orthogonal and non-orthogonal) becomes apparent when computing the stability coefficient. The orthogonal roots will yield $b^T A^{-1} e_M \approx 0$ for two and four points and $b^T A^{-1} e_M = 2$ for three point collocation. This will cause the methods to be A-stable ($|r| \approx 1.0$), but not L-stable. However, L-stable methods can be achieved by using the Legendre roots in the A-stable method and, in addition, applying a collocation point at the end of the element. This leads to $b^T A^{-1} e_M \approx 1$ and $|r| \approx 0$- (Recall that a method is A-stable if it stably integrates the test equation $\dot{y} = \lambda y$ where λ is a complex number with negative real part The method is L-stable if Ac method is A -stable and fim$_{Re0A)}$^_« p ^{1} ^] * 0.)

With the stability results and local error estimates, one can estimate the global error for an implicit Runge-Kutta method as shown by Brenan and Petzold(1987). The order is of $O(h^{k_{c,v}})$ for all solvable linear constant coefficient systems of index $\leq v$. The constant coefficient order $k_{c,v}$ is given by

$$k_{c,v} = \min_{1 \leq i \leq v} (k_d, k_{a,i} - v + 2)$$

where

k_d tofteoderofilrciirthalte the purely differential part of the system

$k_{a,i}$ is the algebraic order.

For optimal control problems, the solution trajectories could be composed of mixed index portions due to the existence of path constraints and singular arc sections. When a higher index section exists in conjuction with lower index sections, then the errors will be different and an error control strategy will have to be able to control the different order of errors for the different indices.

From theoretical properties developed by Brenan and Petzold (1987), systems of equations of higher index can now be considered by choosing die appropriate method and by coo trolling the integration «™r. Tte minimum wny iinwiw»«* for these methods are listed below:

1. Index 1 problems - two point collocation
2. Index 2 problems - three point collocation
3. Index 3 problems - four point collocation

Note that for higher index systems, care will have to be exercised to prevent the error propagation from the index variable. These inaccuracies will, with enough integration steps, cause the solution to become unstable. Here either an L-stable method could be used for the solution and/or a separate error control strategy for the index variable could be used to control the error if die number of elements in the higher index portion is small.

32 Numerical Experiment:

The stability and error properties of Brenan and Petzold (1987) are verified in this subsection using the pendulum problem. Here the " true " solution was generated by using the index zero formulation and solved with LSODE. The system of differential equations was integrated forward in time, using a constant integration step size of 0.005 from a set of consistent initial conditions;

$$x_0 = 1.0_f\ yo«O.O,yo*O\text{-}OtV_O«O.O_f\ u_o«O.O,T_o«O.O.$$

Further, two point collocation was used for the index 1 system, achieving a solution that matched the index zero solution, but it failed for the index 3 formulation as predicted by Brenan and Petzold (1987). On die other hand, four point (non-orthogonal, L - stable) collocation was found to solve the index 3 formulation. However, when orthogonal roots (A-stable method) were used, the emir propagation caused the solution to become unstable as the integration proceeded forward. The non-orthogonal roots remained stable because the L-stable method effectively damps out the *error* propagation for each finite dement These results CTable 1) follow the stability properties shown by Brenan andPetzold (1987).

Table 1 Pendulum Results

Index	x	y	u	v	T
after 100 elements					
0	0.391044	0.920376	-3.91109	1.661727	27.086565
1	0.391048	0.920369	-3.91104	1.661734	27.086487 +
3	0.391048	0.920369	-3.91104	1.661736	27.086496 *
3	0.391048	0.920369	-3.91106	1.661705	31.684719 •*
after 2000 elements					
0	0.275085	0.961419	-4.175598	1.194742	28.294455
3	0.275087	0.961419	-4.175598	1.194749	28.294575 *
3	-0.137607	0.951803	40924.18	-283047	1.068el2 **

Key + two-pointA-stable (orthogonal)

* four point L-stable (nonorthogonal)

+* four point A-stable (orthogonal)

The A-stable cases are obtained by using orthogonal collocation, and the L-stable cases are obtained by also collocating at the endpoint Note that die error propagates in the algebraic (or control) variable and as the enor grows with time it causes die differential variables to become unstable (as shown by the A-stable case when the integration required a significant number of elements for the total integration period-For fids j«>blem the error propagation did not cause solution problems untQ after the 20* dement). The above results were obtained by careful selection of a fixed integration step size (h«0-005).

Inthe next section *wt* will investigate tie similarity between path constraints and singular arc conditions for optimal control problems and die index problem for solving DAE systems. We will consider path constraints and singular arcs from a variational standpoint and show how these conditions can arise in a math programming formulation.

4. DAE DifBcultio in Optimal Control

Bryson and Ho (1975) developed the case for an equality path constraint as a p^{1h} order state variable constraint when the equation is a function of states only (the control is implicit in the equation). Consider the state variable constraint:

$$S(x_f t) -0 \tag{10}$$

For this condition to hold for a section of the path, t© £ t £ tj_t its time derivative along that section of the path must vanish:

$$as= \frac{25.}{* \cdot at} + \frac{25.}{8x} f(x.u.t) \; s. \; o \qquad (»)$$

Now the order (p) of (11) is defined as the number of times that (11) has to be differentiated in order to recover the dependence of the control, u. For a DAE system, the corresponding constraints will occur when a path constraint, $g(z,u)$ £ 0, becomes active, e.g., when a state reaches one of its bounds. As discussed earlier, the index of the problem is p+1, which is the number of differentiations required to obtain a differential equation for the control variable. To control the integration error and maintain the stability of the solution, we need to anticipate that higher index constraints may become active and thus use the appropriate level of discretization for the collocation constraints. As mentioned in the previous section, die appropriate number of collocation points per element as well as the use of an A-stable (orthogonal collocation) or an L-stable (additional collocation point at the end of the element) form can be applied once the index of die algebraic constraints has been analyzed.

A less obvious instance of higher index algebraic constraints occurs when singular arcs are present Normally, this can occur with variational problems which are linear in the control variable. To see die influence of singular axes, consider the following simple optimal control problem (Bryson and Ho (1975)) with a single control profile:

$$\begin{aligned} &\text{Min} \quad \Phi(x_{tf}) \\ &\text{s.t} \quad \dot{x} « f(x) + g(x)u \\ &\qquad\quad to \text{ £ } t \text{ £ } t, \end{aligned} \tag{12}$$

Here, die Hamiltonian is linear in u and assumed to be non-linear in x :

$$H « X^T [f(x)+g(x)u] \tag{13}$$

Necessary conditions include

$$\frac{dH}{du} « X^T g(x) « O \tag{14}$$

$$\dot{X}^T « -[X^T (f_s + g_x u)] \tag{15}$$

$$X^T(t_f) « -(O_x) \tag{16}$$

Note that equation (14) does not detennine the control u (x, X) but it may be possible to find u(t) over a finite time period so that (14) is satisfied. If this happens, then

$$\frac{d}{dt}\frac{\partial H}{\partial u} = \lambda^T \dot{g} + \dot{\lambda}^T g$$

$$= ? \quad 3x \tag{17}$$

$$= 0$$

Substituting (12) and (IS) into (17) yields

$$\frac{d}{du} ft.X^T \frac{\partial g}{dx} fg.ix^T [\frac{\partial f}{dx} + \frac{\partial g}{\partial x} u] g$$

$$-X^T q(x) « 0 \tag{18}$$

where $q(x) = \frac{\partial g}{\partial x} f - \frac{\partial f}{\partial x} g$

Note mat the terms in n cancel each other so we are forced to take the second derivative of $\frac{\partial H}{du}$ in order to recover u:

$$\frac{d^2}{dt^2}\left(\frac{\partial H}{\partial u}\right) = \lambda^T \dot{q} + \dot{\lambda}^T q = \lambda^T \frac{\partial q}{\partial x}(f+gu) - \lambda^T \left(\frac{\partial f}{\partial x} + \frac{\partial g}{\partial x} u\right) q$$

$$= \lambda^T \left(\frac{\partial q}{\partial x} f - \frac{\partial f}{\partial x} q\right) + \lambda^T \left(\frac{\partial q}{\partial x} g - \frac{\partial g}{\partial x} q\right) u \qquad (19)$$

Then

$$u = \frac{-\lambda^T \left(\frac{\partial q}{\partial x} f - \frac{\partial f}{\partial x} q\right)}{\lambda^T \left(\frac{\partial q}{\partial x} g - \frac{\partial g}{\partial x} q\right)} \qquad \text{if} \quad \lambda^T \left(\frac{\partial q}{\partial x} g - \frac{\partial g}{\partial x} q\right) \neq 0 \qquad (20)$$

Therefore, singular arcs that occur for the above type of problems would be at least index 3 because at least three differentiations of $\frac{\partial H}{\partial u}$ are required to obtain an expression for $\dot{u}$. From a DAE standpoint, we can examine equation (a) for the first order variation in the control. Note that when the Hamiltonian is linear and singular arcs exist, the quantity $\left(\frac{\partial F(t)}{\partial u}\right)\lambda$ is equal to zero. On the other hand, if this quantity is not equal to zero, the control will be on one of the bounds. Here, the index of the system is one because we have an active inequality constraint in u. Finally, even though we have potential for the singular arc to exist, it does not mean that the singular arc will be on the optimal trajectory since second order conditions (Legendre - Clebsch) must be satisfied (Lewis (1980)).

In closing this section, a natural question to ask is:

Why isn't the problem reformulated as a lower index form where the stability concerns and error propogation concerns are not an issue ?

The answer is that the constraints would have to be differentiated explicitly to obtain the form of the equations with the control appearing in the equations. It is not desirable to use the differentiated form because, over the solution trajectory, different constraints may be active and we do not know , a priori, where the higher index constraints will be active. Also, the issue of numerical errors from using the differentiated form would have to be considered. We would therefore like our method to be robust so that reformulation of the problem will not be required during the solution of the optimal control problem.

5. Dement Placement to Control Approximation Error

In the previous section, die NLP and variational formulations were shown to be equivalent as long as the elements were sufficiently small to allow for an accurate discretization. To ensure this, we include the element lengths as decision variables in the NLP formulation and E*M additional inequality constraints to keep the flpp.m*.hTmtinn error small. Note that discontinuous control profiles are allowed at die end of each element Thus, any element may determine an optimal breakpoint location as long as it is small enough to satisfy the error constraints.

To derive the error approximation constraints, we consider the discussion in Russell and Christiansen (1978) of various strategies for adaptive mesh selection to solve two-point boundary value problems. Here, a residual based criterion was developed for collocation methods which is effective for finding die element locations or breakpoints (switching times). The criterion is useful for index one or index zero problems where all the errors are of the same magnitude. (There is no order reduction due to a higher index variable being present) The criterion is based on evaluating a residual at a non-collocation point for an error estimate:

$$
\begin{aligned}
|e(t)|| &\approx C\, r(t_{nc})\, h + O(h^{\wedge 1}) \\
&\approx O(hS
\end{aligned}
$$

where h « step length (Le., element length)

$r(t_{nc})$ « residual evaluated at a non-collocation point

We compute ihe residual at a non- collocation points within the element (we used the endpoint) by extrapolating die states and controls to that point. To illustrate the procedure, owii?vte.!r die two-point collocation case shown in Figure 2.

»ij «ij "ij "ij "ij »ij

z_{i0} z_{1i} Z_{2i} z_{i0} z_{1i} $Z_{2»}$ · z_{i0} z_{1i} Z_{2i} z_{iE}

1__*______*___!___*______*____1___*_______*____1

|<------ $\Delta\alpha_i$ ----->|

0 1

Figure 2. Two - point collocation

For each differential equation equality constraint,

$$\dot{z}j = F(Zi, Adj, u) \tag{21}$$

we construct the residual at another point by extrapolating the states found from the solution of the collocation equations in the element. Here the extrapolated derivative is given by:

$$Aa_{i2i} = \underset{j«o}{£}—\underset{dt}{±}(T=1)\ z? \tag{22}$$

and the right hand side terms can be calculated by using the states and controls extrapolated to the point of interest

$$z_{i0} = \sum_{j=0}^{k} \theta_j(t=1)\ z_{i-1j} \tag{23}$$

$$u_{i0} = \sum_{j=1}^{k} \gamma_j(\tau=1)\ u_{i-1j}$$

where

8j ,Yj = Lagrange polynomial basis functions evaluated at x = 1.

x s normalized length along dement i-1.

The residual for each differential equation is then evaluated as follows:

$$\Delta\alpha_i r_i = \sum_{j=0}^{k} z_i \dot{\theta} - \Delta\alpha_i F(z_{i0}, u_{i0}) \tag{24}$$

Next we choose an error norm to control the overall error within the element for all the differential equations. We found the sum of the squares to be effective:

$$\pi_{overall} = \frac{1}{2} \sum_{w}^{M} (r_i^2 \Delta\alpha_i) \leq \varepsilon \tag{25}$$

We can cither enforce this inequality constraint in the optimization formulation directly , or monitor the residuals in an outer loop and take corrective action as required to ensure an accurate solution. Note that this enforcement is only effective for index one problems. However, for higher index problems, the order of the error is reduced. This reduction in the order of the approximation error particularly affects the accuracy of the higher index variables, i.e., those variables for which no differential equations appear. Here, a different error control strategy is required for the control of the integration error of the higher index variables. For optimal control problems, this variable is usually the control variable. Here we use an error control strategy based on derivative information which can also be found in Russell and Christiansen (1978). The highest nonzero derivative of the approximate solution, v(x), bounds the approximation error by the following relation:

$$\| e(x) \| \leq C(h_i^{k-1}) \left\| v_i^{k-1} \right\|$$

For example, with four point collocation, we required the third derivative of the control profile to be less than a tolerance. This can be enforced as an algebraic constraint on the control profile.

6. Example Problems

In this section, examples art presented which demonstrate that mathematical programming using SQP (with finite elements using orthogonal collocation for the discretization) can obtain accurate numerical solutions for higher index optimal control problems. The key to obtaining results for die higher index systems is to control the integration error as discussed in die previous section, thus ensuring that die state profiles are accurate for the next clement For the higher index systems* the integration error was controlled through enforcement of residuals at a noncollocation point Additionally, for singular arc segments, the integration error control requires enforcement of a constraint relating directly to the control variable. We require that the control profile be of an order such that its k^{tb} derivative would be less than a tolerance. The enforcement of these constraints, along with the proper order of the collocation method for the index of the problem, was used to obtain satisfactory control profiles. For index one problems, it was not necessary to directly enforce the residual constraints, provided that the elements were monitored and kept sufficiently small.

6.1 Index One Problems-Batch Reactor Problems

The first example is the batch reactor example found in Ray(1981) and discussed by Biegler (1984) and Renfro (1987). This problem is of interest because the control profile becomes saturated and moving elements are required to find the exact profile. The optimal control problem is

$$
\begin{aligned}
\text{Max} \quad & y_2 O.0) \\
\text{s.t.} \quad & \dot{} \; - \qquad - \; \frac{u}{2}) y_1 \\
& \dot{y}_2 = (u) y_1 \\
& y_1(0) = 1, \; y_2(0) = 0 \\
& 0 \;£\; u \;£\; 5
\end{aligned}
$$

This problem is index 1 because one differentiation is required to obtain an expression for $\dot{u}$ from the optimality conditions .The stability results presented earlier indicate that two-point collocation should achieve die solution within a good accuracy. Since the problem is linear in the states , we solve for die states within each element for a set of control variables. Figure 3 shows the control profile (using two - point collocation) and Table 2 summarizes the control profile.

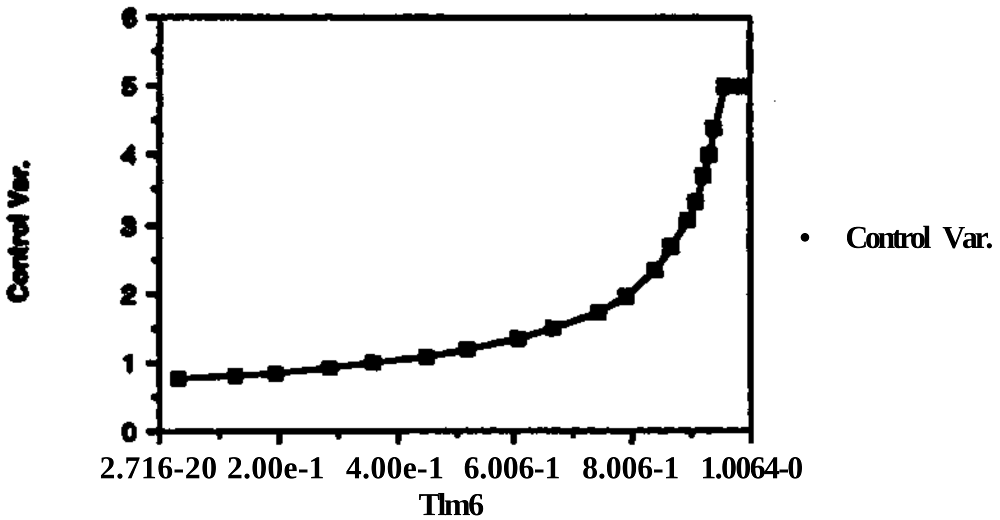


Figure 3. Optimal Temperature Profile
Example No. 1

Table 2 Example # 1 Results

Element	Aa;	Control variables inclement u_1	u_2	Residual
1	.15932	.76175	.80922	2.7987C-7
2	.16496	.85010	.92967	1.2399e-6
3	.16338	.98663	1.8042	1.5999e-6
4	.15218	1.1839	13547	5.3628e-6
5	.13024	1.4785	1.7303	7.7268e-6
6	.08931	1.9519	2.3354	&5961e-6
7	.04655	2.6572	3.0419	7.6322e-7
8	.02193	33327	3.7057	5.7064c-8
9	.01776	4.0033	4.4000	3.8208e-8
10	.05432	5.0	5.0	13414C-5

The solution required S3 iterations to reach a Kuhn-Tuckcr tolerance of 10^{-6} with the objective function being a yield of 0.57353. The CVI (control vector iteration) result was 037349 and the CVP (control vector parameterization) result was 036910 for the case of a starting profile of u « 1.0 (Biegler (1984)). The elements were allowed to vary slightly and the residual errors were simply monitored. Tea elements were required to obtain a control profile with the saturation portion bciny exhibited*

The second example is also found in Ray (1981) and is an index one problem with nonlinear states and controls. Renfro (1986) solved this problem by using piecewise constant controls and by scaling the problem to avoid numerical difficulties. We did not need to apply this restriction to the solution of the problem. The problem is a batch reactor with temperature as the control variable. The objective function is the maximization of one of the products after a fixed reaction time. This example considers die following reaction:

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

The problem is nonlinear in the rate equations for the concentration of A. By letting the following represent the concentration of A and B ($c_1 = [A]$, $c_2 = [B]$), the optimal control problem becomes:

$$\text{Max} \quad c_2(1.0)$$

$$\text{s.t.} \quad \frac{dc_1}{dt} = -k_1(T)c_1^2$$

$$\frac{dc_2}{dt} = k_1(T)c_1^2 - k_2(T)c_2$$

$$k_i(T) = A_{i0} \exp^{[-E_i/RT]} \qquad i = 1,2$$

$$c_1(0) = 1.0, \quad c_2(0) = 0$$

$$298 \le T \le 398$$

Figure 4 shows the solution obtained using two-point collocation. Table 3 summarizes the results.

Table 3 Example #2 Results

Element	$\Delta\alpha_i$	Control variables in element u_1	u_2	Residual
1	.0281	391.9	375.4	1.14e-4
2	.0318	366.6	357.0	7.08e-6
3	.0856	352.9	347.4	4.05e-5
4	.0792	344.2	340.2	3.29e-6
5	.1997	338.2	335.4	3.78e-5
6	.3094	333.6	331.4	3.48e-5
7	.256	329.9	328.0	1.68e-6
8	.009	326.9	325.0	4.48e-13

This solution required 88 iterations to achieve a Kuhn - Tucker tolerance of 10^{-7} with an objective function of 0.610767. Renfro obtained his solution in 14 iterations (objective function of 0.610) but did not find the steep portion of the profile. To show that the objective function is fairly flat, our method also found a solution (objective function of 0.606) in 11 iterations with a Kuhn - Tucker convergence of 10^{-6}. Figure 4 compares this solution with the steeper profile.

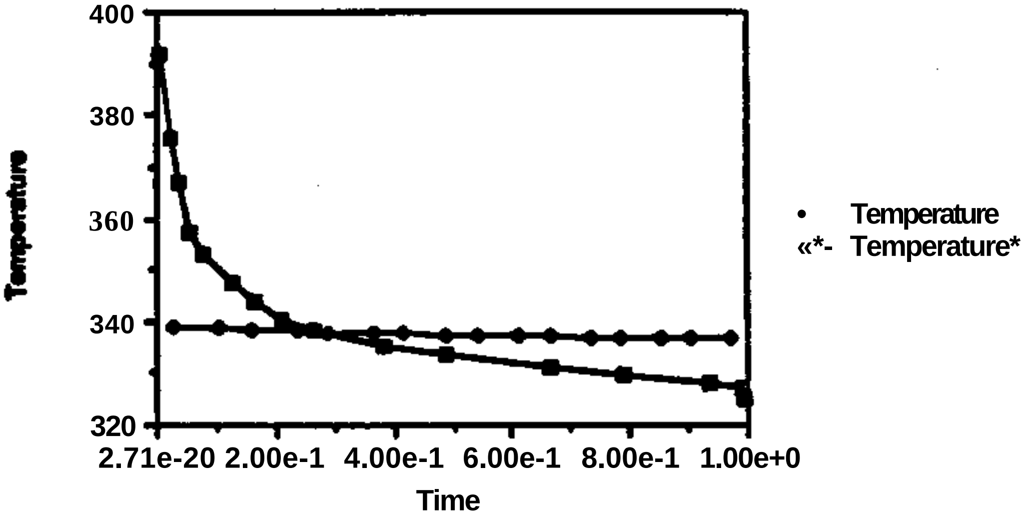


Figure 4. Comparison of Solution Levels
Example No. 2

The above example problems achieve good solutions with die error being controlled within the elements as a natural consequence of using orthogonal collocation at Gaussian roots. As discussed above, index 1 problems also pose no stability problems for our method.

62 Index Two Problems and Higher-Influence of Path Constraints

The next two systems art presented to illustrate that our method can handle path constraints. The first system is discussed by Neuman and Sen (1973), Mehra and Davis (1972), and Jacobson and Lele (1969). Here we consider two examples that become index two and index three when the path constraints are active. The first example is

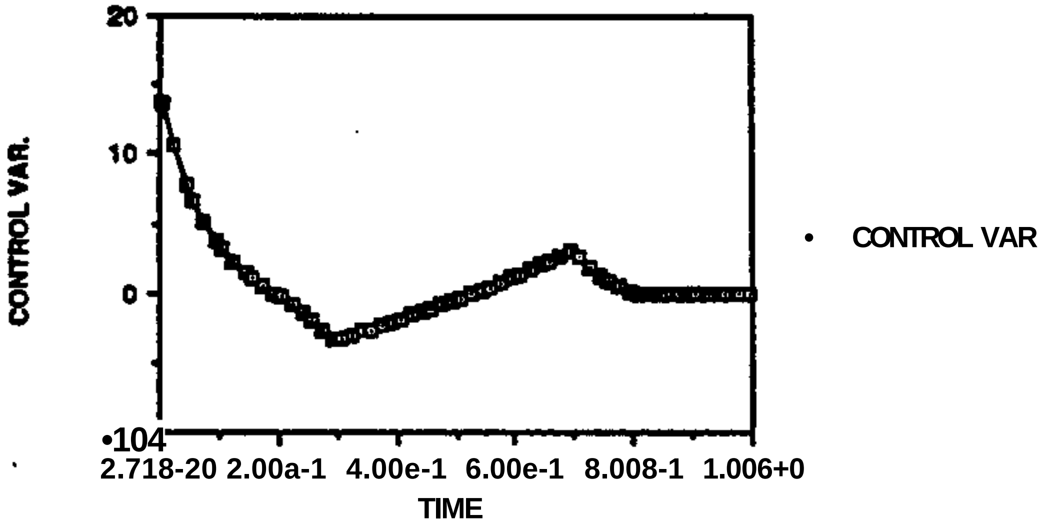
$$\min_{u(t)} J = \frac{1}{2}\int_0^1 \Big([x_1 \; x_2] \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \cdots$$

$$\text{s.t.} \quad \begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \end{bmatrix} u$$

$$x_2 \leq 8(t-0.5)^2-0.5$$

$$\begin{bmatrix} x_1(0) \\ x_2(0) \end{bmatrix} = \begin{bmatrix} 0 \\ -1 \end{bmatrix}$$

This system was solved by using three - point collocation and fixing the elements. The element length was kept small by using twenty equally spaced elements over the integration length. It was not necessary to allow the dements to float because there were no discontinuities in the profiles and the elements were sufficiently small to construct accurate profiles. Also, the control profile had an algebndc constraint included so that its 2nd derivative was less than a tolerance.The control profile and path oonstndnt profile are shown below.



FieuTt 5. Control Profile Exairrole #3

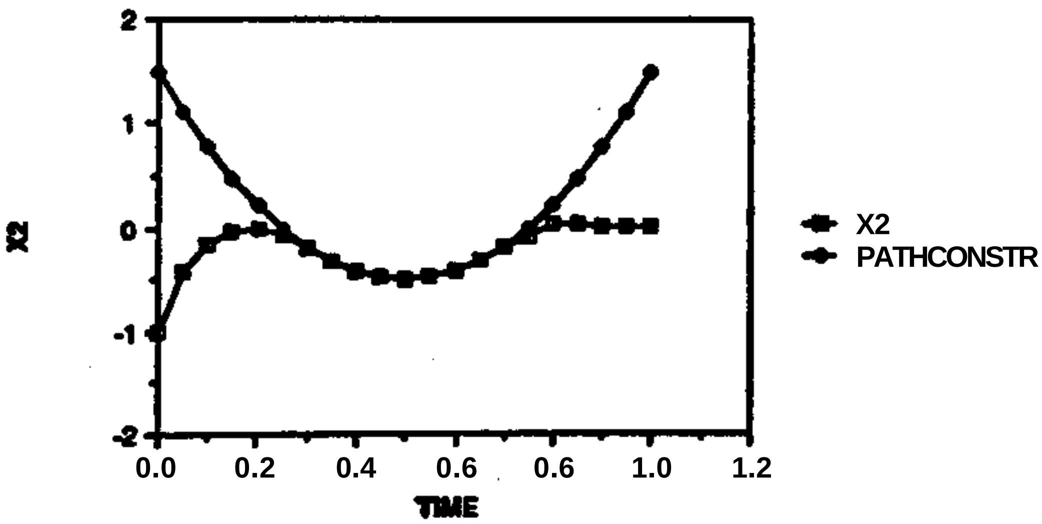


Figure 6. State Profile Exanrole # 3

Note from Figure 5 that the path constraint is active over eight of the elements, from time t=0.28 to t*0.70. The next example is based on the same problem formulation as above except that the inequality is substituted by the following index three path constraint:

$$x_x \quad £ \quad 8(t-0.5)^2-0.5$$

Again, the element lengths were fixed and three point collocation was used for the solution presented in Figures 7 and 8.

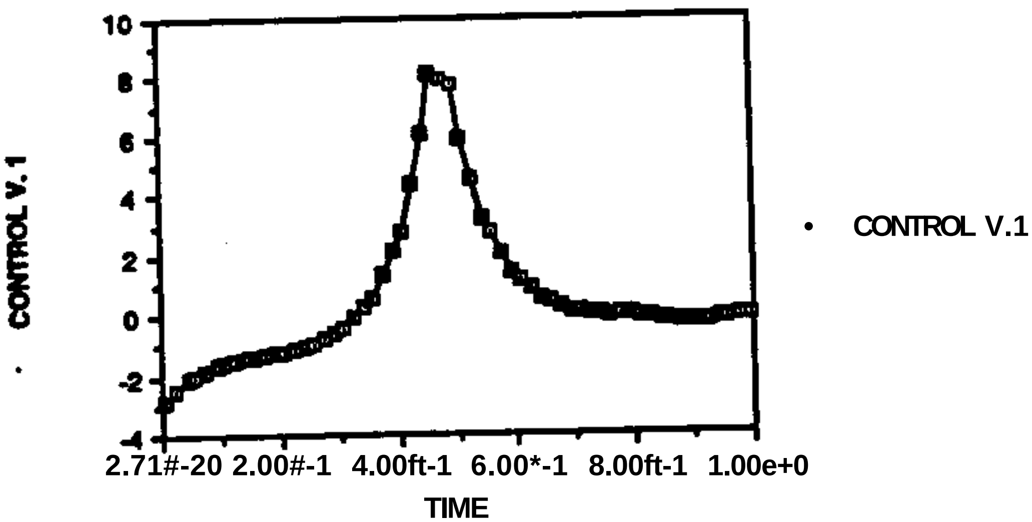


Figure 7. Control Profile Example # 4

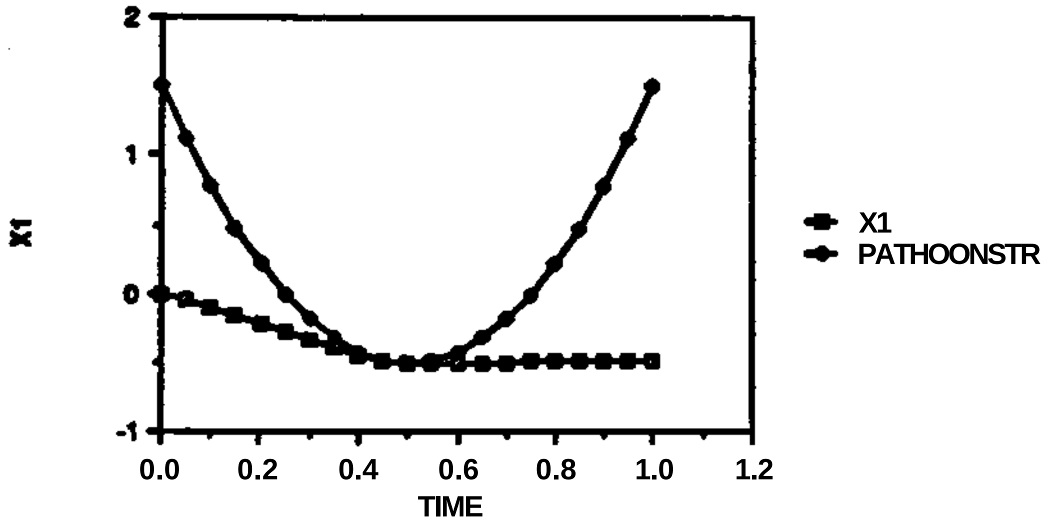


Figure 8. State Profile Example # 4

Note from Figure 8 that the path constraint is only active at one point of the trajectory (t=0.5). This allows three point collocation to find the solution because the higher index portion does not propagate into the index one portion of the system. The objective function values are summarized in Table 4.

Table 4 Minimum Values of Objective Function

Source	Index 2 Problem	Index 3 Problem
Jacobson and Lele (1969)	0.164	0.75
Mehra and Davis (1972)	0.178	0.79
Neuman and Sen (1973)	0.16946	0.6894
om* osetthOŏ	0.1696	0.7368

Neuman and Sen and lacobsen and Lele obtained lower objective function values because they found only approximate solutions and did not enforce error constraints for these profiles. On the other hand, by using the derivative constraint on the control profile, extrapolating the control variables to the initial and endpoints, and by bounding these points through inequality constraints, we were able to enforce die accuracy conditions over the entire trajectory.

For the second system, consider the problem of starting and stopping a car in minimum time for a fixed distance (300 units). The problem was described in Cuthrell and Biegler (1987) and is given by:

Min <Ktf)

s.t ij * z_1 MO) «0 , z_2(0) - 0

$\dot{z}_j$ - u $z_1(t_f)$ - 0 , zj(t^-300

-2 £ u £ 1

This problem is index 1 because one differentiation is needed to obtain an expression for $\dot{u}$ (from the active inequality constraint bounding u). The analytical solution is the expected bang-bang solution shown in Figures 9,10 and 11. Using a two point collocation method in the NLP formulation leads to a solution thai matches these results.

Next we place a path constraint on die problem by setting an upper bound on the speed of 10 units. When this speed limit comes into effect, the problem becomes index 2 for that portion of the solution trajectories. The problem is index 2 because the speed cannot exceed 10 units and the control has to be adjusted accordingly (note two differentiations are needed to obtain $\dot{u}$ from Z\ « 10). The analytic solution profiles for this problem are shown in Figures 12,13, and 14. Notice that the path constraint forces the control off of the bounds even though the problem is linear in the states and the control.

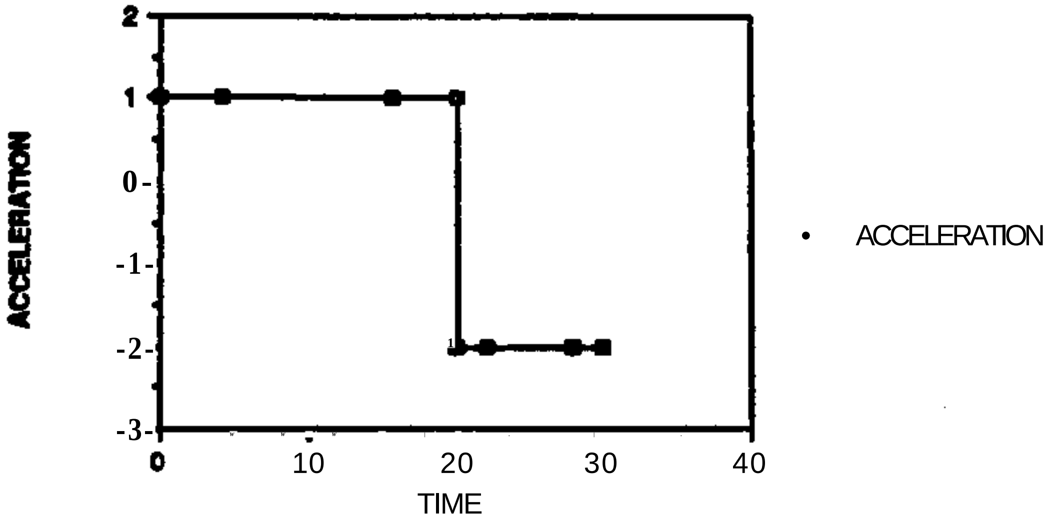


Figure 9. Analytical Acceleration - Unconstrained Case

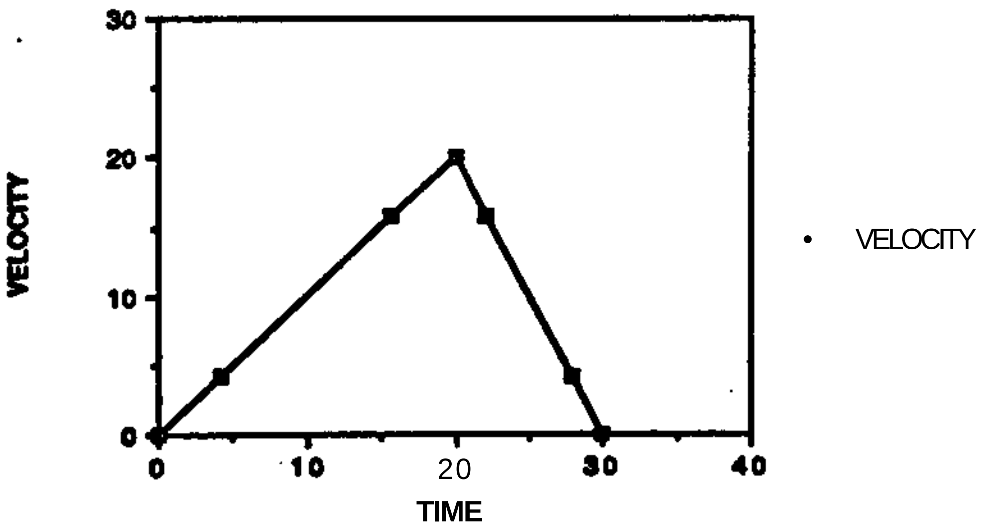


Figure 10. Analytical Velocity - Unconstrained Case

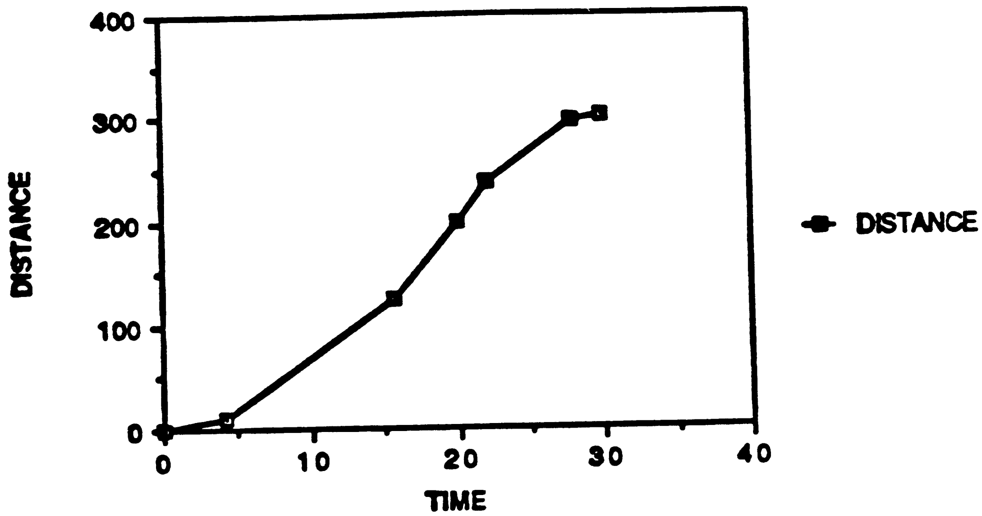


Figure 11. Analytical Distance - Unconstrained Case

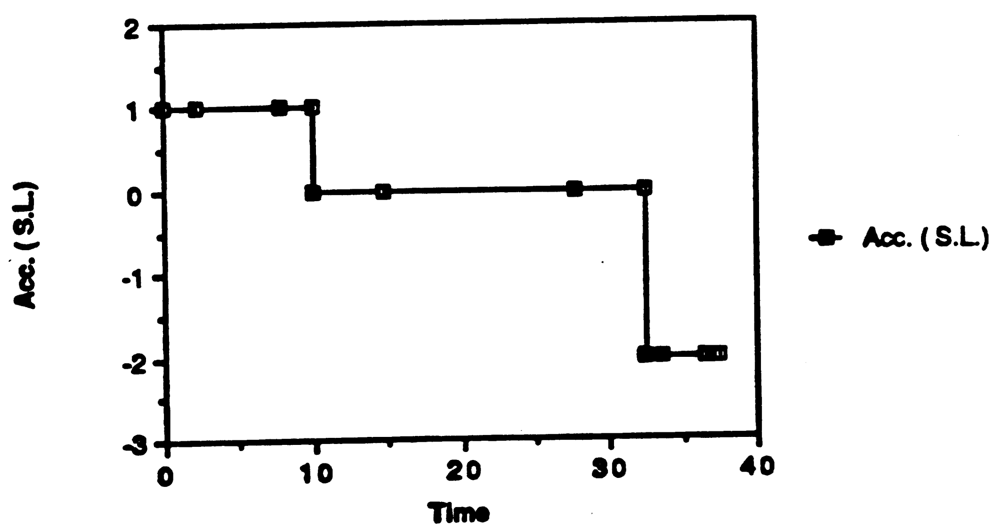
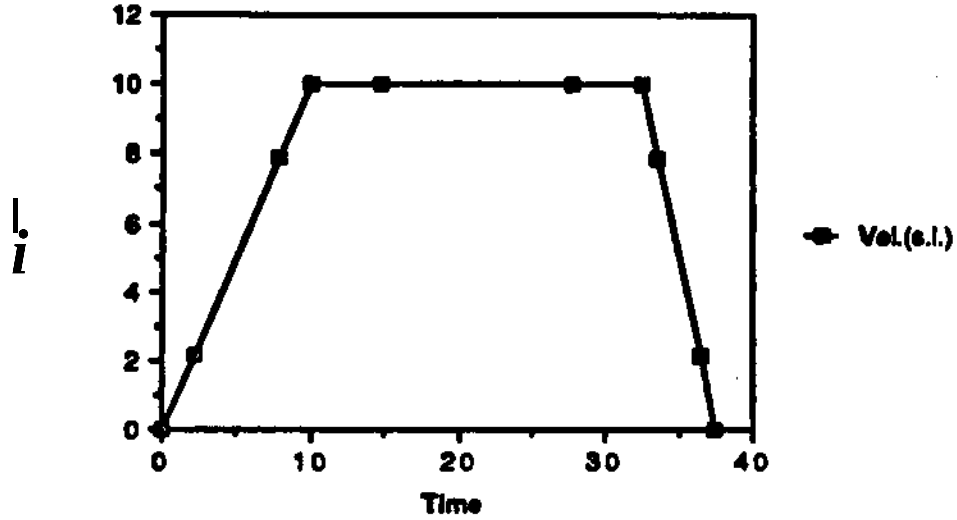


Figure 12. Analytical Acceleration - Constrained Case



Retire 13. Anaiytical Velocity - Constrained Case

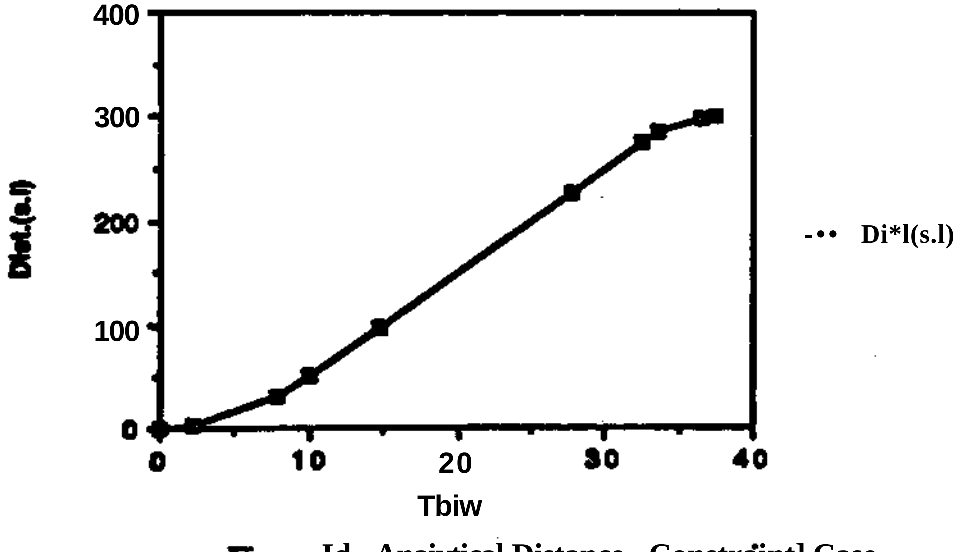


Figure Id. Anaiytical Distance - Constraintl Case

However, if a two point collocation formulation is used without controlling the residual error, one obtains the unsatisfactory profile as shown in Figure IS. Adding the residual constraints as inequalities to the formulation leads lo a numerical solution that matches the analytical result Note that we solved a mixed index 1 - index 2 system by enforcing error constraints using two point collocation, which does not have the stability properties for index 2 systems. The reason is that the analytical solution is approximated exactly by the polynomials . Thus, there is no error to propogate over the index two portion, which actually consists of only one element

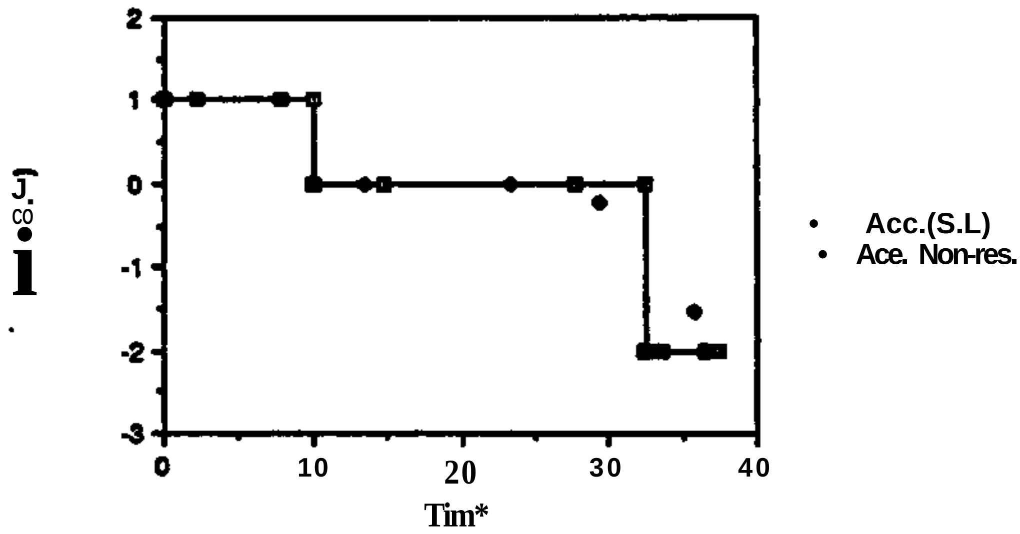


Figure 15. Acceleration Profile - Nonresidual case
Example No. 5

63 Index Three Problem • Singular Arc Example

The final example is a catalyst mixing problem of Ounn & Thomas (1964) that was solved analytically by Jackson (1968). For a sufficient reactor length, the system admits a singular arc segment to die optimal contitd profile. The problem description is:

$$\text{Max} \quad P(t) \quad « \quad 1-x(t^\wedge-y(t^\wedge \quad ,t_{(} \text{ specified}$$

$$\text{s.t.} \quad \frac{dx}{\text{-gj-}} \quad \bullet \quad u(k_2 y - k_1 x)$$

$$\frac{du}{\text{•g-}} \quad « \quad -u(k_2 y . k_1 x).(1-u)k_3 y$$

$$x(0) « 1.0$$

$$y(0) « 0.0$$

The Hamiltonian for this system is

$$H - X^\wedge C k j y - M) + X_2[(k_1 x - k_2 y) - (1- u)k_3 y]$$

and the adjoint equations are

$$\dot{X}_2 = -uk_2(X_1 - X^\wedge) \quad + (1-u)k_3 X_2$$

Taking the first time derivative yields

$$\frac{d}{dt}(\frac{\partial H}{\partial u}\text{J-katX-}^\wedge x - X^\wedge y) \; « \; 0$$

which does not exhibit any control dependence.

The second time derivative is

$$\frac{d^2}{dt^2}(\frac{\partial H}{du}) \quad .k_3 1 \dot{X}^\wedge x + X_2 k_x i \bullet (\dot{\lambda}_1 k_2 y + \lambda_1 k_2 \dot{y})].$$

from which one can obtain the control as in die general derivation$_9$ equation (20). The problem is index 3 over the singular arc section. The analytical solution is shown in Figure 16. The solution trajectory is comprised of mixed index portions with the first and last trajectories being the sections where the control is on the bounds. The middle section is a singular arc section with an index of three. This problem poses a severe test for the optimization code because of the index problems.

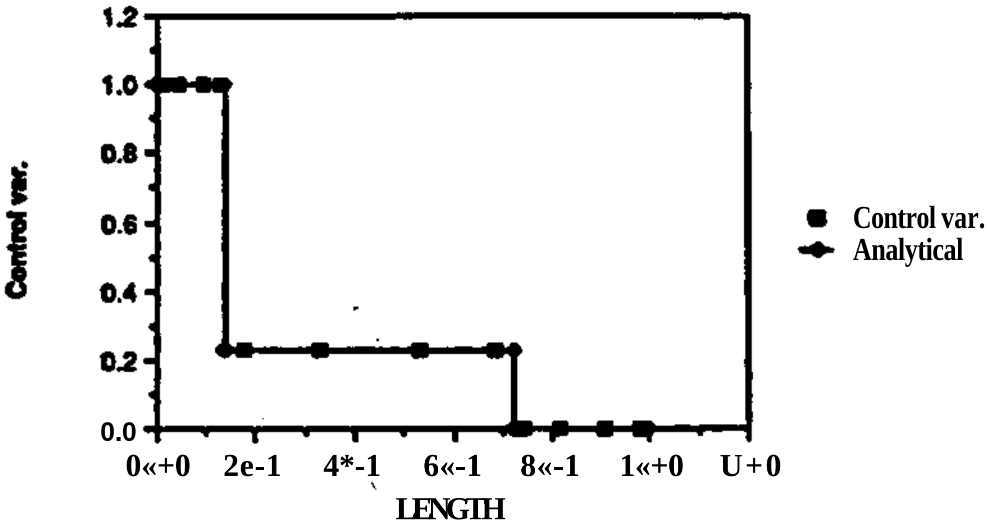


Figure 16. Ootimal Mixine Policy

Table 6.0 Mixed Catalyst Results

Elesnerit	Atti	Controls in element u_1	u_2	Final Residual	Error Tolerance
1	.07924	1.0	1.0	2.241e-5	2.5c-5
2	.05750	1.0	1.0	7.075e-7	9.0e-7
3	.29830	.2264	.2267	1.320e-10	9.0c-11
4	29311	.2252	2249	4.360e-ll	9.0e-ll
5	.27182	0.0	0.0	1.006e-8	L9e-8

Because the singular segment is of index thrte» a higher order collocation method should be applied to solve this problem. Moreover, if a large number of elements are required to describe the singular segment, this method shcwM be I^stabk in order to limit growth of the propagation error. To test these conditions, we attempted to solve this problem using only two point collocation and by controlling die integration error in each element As shown in Figure 16 and Table 6, we achieved a solution only by specifying different error tolerances in each element These were found by trial and error until the solution matched the analytical profile. Note that very tight enor tolerances needed to be specified for the singular segment Other attempts would either fail or converge to suboptimal solutions. Next, we considered four-point collocation using Gaussian roots (the A-stable case). Again, we enforced the error constraints in the formulation but failed to achieve the optimal solution. (Here we started with a flat profile of u « 0-2 and equally spaced elements over the integration length). Instead, we enforced an additional constraint on the control profile by requiring the third derivative oftiie control profile to be less than a tolerance. As discussed in section 5, this constraint was suggested in Russell and Christiansen (1978) and is directly related to the approximate error in the control profile. With die addition of this constraint, we achieved a numerical solution using the GAMS /MINOS optimization systems that matched the analytical profikta Figure 16. Note that by controlling the integration error on die control variable this is similar to DAE approaches that enforce different error control strategies for the higher index variables.

As with the index three path constraint problem, the singular segment was approximated only by a single element Thus the A-stable four point collocation method^ produced a solution because there was no propagation of error in the index 3 portion. An alternative approach would be to apply an L-stable collocation method to solve this problem. Four point collocation (using the three point orthogonal A-stable roots with the endpoint for die collocation points) was used to test the L-stable method The basis functions values were changed to reflect the L-stable roots, and the GAMS/MINOS system was used to achieve the solution matching the analytical. However, in order to obtain convergence, the error tolerance for the integration error enforced by die evaluation of a residual at a non-collocation point was relaxed This was necessary because the four point L-stable method is less accurate than the four point A-stable method

Finally, we converted die catalyst problem from an index three problem to an index zero problem by parameterizing die control profile as variable length piecewise constants. This approach is valid for this problem because die form of the optimal control profile is also piecewise constant In fact, if die numerical difficulties caused by higher index systems prevent die solution from cxmvcr^g for the general polynomial fbnn of the control profile outlined earlier, then one could always obtain a satisfactory feasible starting point for the gencndpolyiKmialfonn by par^erizing the control profile. The solution using this approach also matched the analytical solution within numerical tolerances (see Figure 16).

7. Conclusions

This paper presents a general method for obtaining optimal control profiles by numerical methods that are arbitrarily accurate and match analytical solutions wbcn tbcy can be found. This approach uses a math programming technique for the solution by discretizing the differential equations using orthogonal collocation on finite elements. Lagrange polynomials are used to construct the approximations to the continuous model and the resulting set of algebraic equations is solved as pan of the nonlinear program. This wofk is different from earlier weak using collocation to find these i^ofiles in that it directly uses the integration error information to construct accurate profiles.

Difficulties in solving sets of differential - algebraic equations that result from variational conditions can be classified by the index of the system to be solved These difficulties are associated with local error and stability properties of the integration method when higher index conditions exist in the system. Here collocation was shown to possess A-stable as well as L-stable properties* depending cm the location of die collocation points. Also, an appropriate number of collocation points needs to be used to overcome any potential order reduction from higher index systems. For optimal control problems, we show that these higher index conditions occur from active state variable constraints or singular arcs. Thus, by choosing an appropriate order for the collocation method, reformulation of the problem is not necessary when these higher index conditions become active in the system.

The method was demonstrated on index one, two, and three systems. For index one systems of batch reactors with nonlinear control profiles, die control profiles were continuous profiles. Thus, it was possible to let die element lengths vary slightly between upper and lower bounds rather than directly enforcing the residual constraints on die math program. The residuals were monitored as the element lengths varied to account for steep profiles. Implicit in this approach is a sufficient number of elements to allow for an accurate solution. Also, two path constraint problems of index two were considered The fim can be formulated as a simpteQP with the path constraint active over a large portion of die control profile. Here the solution was achieved with fixed element lengths. The second example considers movement of a vehicle in iraniimun tune to cover a fixed 4fi:gf fg>ft f with a speed limit path constraint This problem has two switching times (or two discontinuities in the control profile) as the path constraint was encountered. For successful solution, residual error constraints have to be directly enforced in the math program.

Finally, two index three systems were solved. Again, the first system was a simple QP with the index three system resulting from an active path constraint . However, the higher index constraint was active at only one point, and therefore the stability and error reduction issues were not a factor in the solution of the problem. The last example, finding the optimal mixing policy of catalyst for two reactions in a fixed length of a tubular reactor, was difficult to solve because of the existence of a singular arc in the optimal control profile. It was necessary to directly enforce the residual error constraints as well as an error constraint on the control profile, because of the higher index conditions due to the singular arc.

The above problems are small problems taken from the literature to demonstrate the validity of our approach. Future work will deal with larger chemical engineering systems (such as batch distillation systems) which will require decomposition techniques to obtain solutions. The Range and Null space decompositon technique (Vasantharajan and Biegler (1988)) for Successive Quadratic Programming will be exploited for this purpose.

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