Numerical Solution of Initial-Value Problems in Differential-Algebraic Equations

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Preface

Differential-algebraic equations (DAE's) arise naturally in many applications, but present numerical and analytical difficulties which do not occur with ordinary differential equations. The numerical solution of these types of systems has been the subject of intense research activity in the past few years. A great deal of progress has been made in the understanding of the mathematical structure of DAE's, the analysis of numerical methods applied to DAE systems, the development of robust and efficient mathematical software implementing the numerical methods, and the formulation and solution of DAE systems arising from problems in science and engineering. Many of the results of this research effort are scattered throughout the literature. Our objective in writing this monograph has been to bring together these developments in a unified way, making them more easily accessible to the engineers, scientists, applied mathematicians and numerical analysts who are solving DAE systems or pursuing further research in this area. We have tried not only to present the results on the analysis of numerical methods, but also to show how these results are relevant for the solution of problems from applications and to develop guidelines for problem formulation and effective use of the available mathematical software.

As in every effort of this type, time and space constraints made it impossible for us to address in detail all of the recent research in this field. The research which we have chosen to describe is a reflection of our hope of leaving the reader with an intuitive understanding of those properties of DAE systems and their numerical solution which would in our opinion be most useful in the modeling of problems from science and engineering. In cases where a more extensive description can be found in the literature, we have given references.

Much of our research on this subject has benefitted from collaboration. The DASSL code would never have reached its present state of development without the encouragement of Bob Kee and Bill Winters, whose problems provided us with numerical difficulties that we couldn't possibly have dreamed up ourselves. The direction of our research and the development of DASSL have both benefitted enormously from the many users of DASSL who were generous, or in early versions desperate, enough to share with us their expe-

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riences and frustrations. We would like to thank John Betts for introducing us to the difficult nonlinear higher index trajectory problems which inspired much of our research on the solution of higher index systems. Our thinking on the analysis of numerical methods for DAE's has been influenced through our collaborations with Kevin Burrage, Ken Clark, Bill Gear, Björn Engquist, Ben Leimkuhler and Per Lötstedt, with whom we have shared a great many happy hours discussing this subject.

Our friends and colleagues have made many useful suggestions and corrected a large number of errors in early versions of the manuscript. We would like to thank Peter Brown, George Byrne, Alan Hindmarsh, Bob Kee, Michael Knorrenschild, Ben Leimkuhler, Quing Quing Fu and Clement Ulrich for their comments and constructive criticism on various chapters. Claus Führer provided us with such excellent and extensive comments on Section 6.2 that he can virtually be considered a coauthor of that section.

We are grateful to our management at Lawrence Livermore National Laboratory and at The Aerospace Corporation for their support of this project, and for their confidence and patience when it became clear that the effort would take longer to complete than we had originally planned. Very special thanks are due to Don Austin of the Applied Mathematical Sciences Subprogram of the Office of Energy Research, U. S. Department of Energy, and to Lt. Col. James Crowley of the Air Force Office of Scientific Research for their funding and support not only of this project but also of much of the research upon which this monograph is based. Part of this work was performed under the auspices of the U. S. Department of Energy by the Lawrence Livermore National Laboratory under Contract W-7405-Eng-48. Fran Karmitz and Auda Motschenbacher provided much needed expert assistance in typesetting various sections of the manuscript and its revisions.

March 31, 1989

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Chapter 1

Introduction

1.1 Why DAE's?

Most treatments of ordinary differential equations (ODE's), both analytical and numerical, begin by defining the first order system

$$F(t, y(t), y'(t)) = 0,$$
 (1.1.1)

where F and y are vector valued. An assumption that (1.1.1) can be rewritten in the *explicit*, or *normal* form

$$y'(t) = f(t, y(t))$$
 (1.1.2)

is then typically invoked. Thereafter, the theorems and numerical techniques developed concern only (1.1.2). While (1.1.2) will continue to be very important, there has been an increasing interest in working directly with (1.1.1). This monograph will describe the current status of that effort.

Our emphasis is on the numerical solution of (1.1.1) in those cases where working directly with (1.1.1) either has proved, or may prove to be, advantageous. This perspective has affected our choice of techniques and applications. We assume that the reader has some knowledge of traditional numerical methods for ordinary differential equations, although we shall review the appropriate information as needed. We confine ourselves to initial value problems.

If (1.1.1) can, in principle, be rewritten as (1.1.2) with the same state variables y, then it will be referred to as a system of *implicit* ODE's. In this monograph we are especially interested in those problems for which this rewriting is impossible or less desirable. In a system of differential-algebraic equations, or DAE's, there are algebraic constraints on the variables. The constraints may appear explicitly as in (1.1.3b) of the system

$$F(x',x,y,t) = 0 ag{1.13a}$$

$$G(x,y,t) = 0, (1.1.3b)$$

where the Jacobian of F with respect to x' (denoted by $\partial F/\partial x' = F_{x'}$) is nonsingular, or they may arise because $F_{y'}$ in (1.1.1) is singular. In the latter case, we assume that the Jacobian is always singular. In the problems considered here, difficulties arise from a lower dimensional solution manifold and the dependence of the solution on derivatives of other terms, rather than from the existence of turning or singular points.

There are several reasons to consider (1.1.1) directly, rather than to try to rewrite it as an ODE. First, when physical problems are simulated, the model often takes the form of a DAE depicting a collection of relationships between variables of interest and some of their derivatives. These relationships may even be generated automatically by a modeling or simulation program. The variables usually have a physical significance. Changing the model to (1.1.2) may produce less meaningful variables. In the case of computer-generated or nonlinear models, it may be time consuming or impossible to obtain an explicit model. Parameters are present in many applications. Changing parameter values can alter the relationships between variables and require different explicit models with solution manifolds of different dimensions. If the original DAE can be solved directly, then it becomes easier for the scientist or engineer to explore the effect of modeling changes and parameter variation. It also becomes easier to interface modeling software directly with design software. These advantages enable researchers to focus their attention on the physical problem of interest. There are also numerical reasons for considering DAE's. The change to explicit form, even if possible, can destroy sparsity and prevent the exploitation of system structure. These points will be examined more carefully in later chapters.

The desirability of working directly with DAE's has been recognized for over twenty years by scientists and engineers in several areas. Depending on the area, DAE's have been called singular, implicit, differential-algebraic, descriptor, generalized state space, noncanonic, noncausal, degenerate, semistate, constrained, reduced order model, and nonstandard systems. In the 1960's and early 1970's there was a study of the analytical theory of linear constant coefficient and some nonlinear systems [174,227]. This work was based on coordinate changes, reductions, and differentiations. The first practical numerical methods for certain classes of DAE's were the backward differentiation formulas (BDF) of [113]. Beginning in the late 1970's, there was a resurgence of interest in DAE's in both the scientific and mathematical literature. New and more robust codes, such as DASSL [200] and LSODI [143] have recently become available. The theoretical understanding of when to expect these codes to work, and what to do when they do not, has improved. There has been increasing computational experience with a wider variety of applications. This monograph deals with these recent developments, many of which have reached a degree of maturity only within the last two or three years.

1.2 Basic Types of DAE's

None of the currently available numerical techniques work for all DAE's. Some additional conditions, either on the structure of the DAE and/or the numerical method, need to be satisfied. One approach to developing a theory for numerical methods is to make technical assumptions that can be hard to verify or understand but enable proofs to be carried out. We prefer, as much as possible, to consider DAE's under various structural assumptions. This approach is more directly related to problem formulation, makes the assumptions easier to verify in many applications, and has proven useful in deriving new algorithms and results. This structural classification will be begun in this section and is continued in more detail in Chapter 2.

Linear constant coefficient DAE's are in the form

$$Ax'(t) + Bx(t) = f(t),$$
 (1.2.1)

where A, B are square matrices of real or complex numbers and t is a real variable. We shall usually assume vectors are real for notational convenience but the results are the same for the complex case. The case of rectangular coefficients has been studied [49,111] but we shall not consider it. The general analytical and numerical behavior of (1.2.1) is well understood. However, there is still some research being done on applications of (1.2.1) in the control literature and in the numerical problem of computing the structure of matrix pencils [126,149,242].

While most applications that we have seen have led to either linear constant coefficient or nonlinear DAE's, linear time varying DAE's

$$A(t)x'(t) + B(t)x(t) = f(t)$$
 (1.2.2)

with A(t) singular for all t, exhibit much of the behavior which distinguishes general DAE's from linear constant coefficient DAE's. At this time, there are techniques and results which seem appropriate for nonlinear systems, but for which complete and rigorous proofs exist only for linear time varying systems. Hence, (1.2.2) represents an important class of DAE's which we will study in order to gain an understanding of general DAE's. We shall also see that in occurs in some applications.

System (1.2.2) is the general, or fully-implicit linear time varying DAE. An important special case is the semi-explicit linear DAE

$$x'_1(t) + B_{11}(t)x_1(t) + B_{12}(t)x_2(t) = f_1(t)$$

$$B_{21}(t)x_1(t) + B_{22}(t)x_2(t) = f_2(t).$$

The general (or fully-implicit) nonlinear DAE

$$F(t,y(t),y'(t))=0$$

may be linear in the derivative

$$A(t, y(t))y'(t) + f(t, y(t)) = 0. (1.2.3)$$

This system is sometimes referred to as linearly implicit. A special case of (1.2.3) is the semi-explicit nonlinear DAE

$$x'_1(t) = f_1(x_1(t), x_2(t), t)$$

0 = $f_2(x_1(t), x_2(t), t)$.

Depending on the application, we shall sometimes refer to a system as semi-explicit if it is in the form

$$F(x'(t), x(t), y(t), t) = 0$$

$$G(x(t), y(t), t) = 0$$

where $F_{x'}$ is nonsingular. Many problems, such as variational problems, lead to semi-explicit systems. We shall see that such systems have properties which may be exploited by some numerical algorithms. However, since it is always possible to transform a fully-implicit linear constant coefficient DAE to a semi-explicit linear constant coefficient DAE by a constant coordinate change, these two cases are not considered separately. While in Chapter 2 we will discuss what type of operations, such as coordinate transformations or premultiplications by nonsingular matrices, may be safely applied to a DAE without altering the behavior of a numerical method, it is important to note here that constant coordinate changes are permitted.

1.3 Applications

In this section we will briefly describe several classes of problems where DAE's frequently arise. The categories overlap to some extent, but there are essentially four types of applications that we consider. Our grouping of these applications is based on how the equations are derived rather than on the type of equations that result. Throughout the remainder of this monograph we shall make reference to these problems in order to illustrate the relevance of key concepts. The numerical solution of several specific applications involving DAE's will be developed in more detail in Chapter 6.

1.3.1 Constrained Variational Problems

Variational problems subject to constraints often lead to DAE's. For example, in a constrained mechanical system with position x, velocity u, kinetic energy T(x,u), external force f(x,u,t) and constraint $\phi(x)=0$, the Euler-Lagrange formulation yields [121]

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where $G = \partial \phi / \partial x$, and λ is the Lagrange multiplier. This system can be rewritten as

$$\frac{\partial^2 T}{\partial u^2} u' = g(x, u, t) + G^T \lambda$$

$$x' = u$$

$$0 = \phi(x).$$
(1.3.1a)
$$(1.3.1b)$$

$$(1.3.1c)$$

$$x' = u \tag{1.3.1b}$$

$$0 = \phi(x). \tag{1.3.1c}$$

This DAE system in the unknown variables u, x, and λ is linear in the derivatives. If, as is often the case, $\partial^2 T/\partial u^2$ is a positive definite matrix, then multiplication of (1.3.1a) by $(\partial^2 T/\partial u^2)^{-1}$ converts (1.3.1) to a semi-explicit DAE.

As a classical example of a DAE arising from a variational problem, consider the equations of motion describing a pendulum of length L. If g is the gravitational constant, λ the force in the bar, and (x,y) the cartesian coordinates of the infinitesimal ball of mass one at the end, we obtain the DAE

$$x'' = \lambda x$$

$$y'' = \lambda y - g$$

$$0 = x^2 + y^2 - L^2$$

Several problems in robotics have been formulated as DAE's utilizing this variational approach [187]. One example is a robot arm moving with an end point in contact with a surface. Using joint coordinates; the motion of this object may be modeled as the DAE

$$M(x)x'' + G(x,x') = u + B^{T}(x)\lambda$$
$$0 = \phi(x)$$

with $B = \phi_x, x \in \mathbb{R}^n, \lambda \in \mathbb{R}^m, u \in \mathbb{R}^n$. M is the mass matrix, G characterizes the Coriolis, centrifugal and gravitational effects of the robot, u is the input (control) torque vector at the joints, c defines the contact surface, and $B^T \lambda$ is the contact force vector. This system can be converted using the standard substitution x' = v to a DAE which is linear in the derivative. Other variations such as two robots, inertial loads, and moving contact surfaces also fall into this framework [187].

Other examples of DAE's arising from constrained variational problems include optimal control problems with unconstrained controls. In these problems, there is a process given by

$$x' = f(x, u, t) \tag{1.3.2}$$

and a cost

$$J[x,u] = \int_{t_0}^{t_1} g(x,u,s)ds.$$
 (1.3.3)

The problem is to choose the control u in order to minimize the cost (1.3.3) subject to (1.3.2) and certain specified initial or boundary conditions. The variational equations for (1.3.2), (1.3.3) for the fixed time, fixed endpoint problem yield the semi-explicit DAE system

$$x' = f(x, u, t)$$

$$\lambda' = -g_x(x, u, t) - f_x^T \lambda$$

$$0 = g_u(x, u, t) + f_u^T \lambda.$$

One of the most studied special cases of this DAE is the quadratic regulator problem with process and cost

$$x' = Ax + Bu$$

 $J[x, u] = \int_{t_0}^{t_1} x^T Qx + u^T Ru \, ds,$ (1.3.4)

where A, B, Q, R are matrices with Q, R positive (semi-)definite. In this case, the variational equations become the linear time varying semi-explicit DAE system

$$x' = Ax + Bu$$

$$\lambda' = -Qx + A^{T}\lambda$$

$$0 = Ru + B^{T}\lambda.$$
(1.3.5)

Often the matrices A, B, Q, and R are constant. Depending on the initial conditions, boundary conditions, and information sought, these DAE's are frequently boundary value problems. Many other variations on these control problems can be found in [12,37].

1.3.2 Network Modeling

In this approach, one starts with a collection of quantities and known, or desired, relationships between them. Electrical circuits are often modeled this way. The circuit is viewed as a collection of devices such as sources, resistors, inductors, capacitors (and more exotic elements such as gyrators, diodes, etc.) lying on branches connected at nodes. The physical quantities of interest are usually taken to be the currents in the branches and the voltages at the nodes (or voltage drops on the branches). These quantities are related by the device laws which are usually in the form of v-i characteristics and Kirchoff's node (current) and loop (voltage) laws. These DAE models are often called descriptor or semistate [191] systems in the electrical engineering literature. In an RLC circuit with linear capacitors, resistors, and inductors, the equations will be semi-explicit and often linear constant coefficient. They will be nonlinear if such devices as diodes or nonlinear resistors are included.

Many of these systems can be written in the form of a DAE which is linear in the derivative [191]

$$Ax' + B(x) = Du$$
$$y = F(x)$$

where A may be singular, u is the vector of inputs, and y is the vector of outputs or observations.

Earlier we discussed constrained variational equations. A somewhat related problem is that of prescribed path control. In prescribed path control, one considers the process (or plant) to be given by

$$x' = f(x, u, t) \tag{1.3.6}$$

where x are the state variables and u are the control variables. The goal is to pick u so that the trajectory x follows some prescribed path

$$0 = g(x, u, t). (1.3.7)$$

Frequently u is absent from (1.3.7). As we shall see later, this can impose numerical difficulties in solving the semi-explicit DAE (1.3.6), (1.3.7).

To illustrate the relationship between this problem and our earlier constrained optimization problem, consider a robotic control problem. If a contact point is moving along a surface, then the constraint is imposed by the surface. The surface exerts forces on the robot and the problem would most likely be modeled by the variational approach. If, however, the robot were moving freely through the workspace and the prescribed path (1.3.7) was being specified to avoid collision with fixed objects, then the problem would most likely be modeled by taking the free dynamics (1.3.6) and imposing the constraint (1.3.7). In Chapter 2 we shall define a fundamental concept called the index of a DAE. Generally, the higher the index, the more difficult the problem is numerically. The prescribed path control of robot arms with flexible joints [88,90] leads to the highest index problems we have seen to date.

In trajectory prescribed path control problems, the DAE system models a vehicle flying in space when algebraic path constraints are imposed on its trajectory. A particular example of this type of DAE concerned the design of a safe reentry profile for the space shuttle [32]. In order to insure the shuttle is able to survive the reentry, mission restrictions concerning heating constraints and structural integrity requirements must be evaluated with respect to the forces acting on the vehicle. A particular trajectory profile is selected inside an acceptable corridor of trajectories which has been determined by analyzing numerous physical constraints such as the vehicle's maximum load factors, maximum surface temperature constraints at a set of control points, and equilibrium glide boundaries. The equations modeling the shuttle flying along this reentry profile describe a DAE system in the form (1.3.6),(1.3.7). The differential equations (1.3.6) include the vehicle's translational equations of motion.

The trajectory profile is described by one additional algebraic equation of the form

$$g(x,t) = 0, (1.3.8)$$

where the state variables x describe the vehicle's position and velocity. The bank angle β is selected as the control variable u. The semi-explicit DAE (1.3.6),(1.3.8) exhibits several features that will be discussed in Chapters 2 and 6. Note that because of the many nonlinearities involved in this model problem, it is not easy to convert this DAE into an explicit ODE, even locally.

Another type of prescribed path control problem arises when there are invariants (i.e., relations which hold along any solution trajectory) present in the solution to a system of ODE's. For example, these invariants may be equalities (or inequalities in general) describing the conservation of total energy, mass, or momentum of a system. Maintaining solution invariants in the numerical solution of ODE's can pose difficulties for numerical ODE methods [223], but may be essential to the stability of the system. Problems of this type may be formulated as systems of DAE's where the invariants are imposed as algebraic constraints [117].

There is a large engineering literature devoted to the properties of the system

$$x' = Ax + Bu$$
$$y = Cx + Du$$

where A, B, C, D are constant matrices, x is the state, u is the control or input, and y is the output or vector of observations. Notice that if we consider a desired y as known and want to find x or u, then this system can be viewed as the linear constant coefficient DAE in x and u

$$\left[\begin{array}{cc} I & 0 \\ 0 & 0 \end{array}\right] \left[\begin{array}{c} x \\ u \end{array}\right]' = \left[\begin{array}{cc} A & B \\ C & D \end{array}\right] \left[\begin{array}{c} x \\ u \end{array}\right] + \left[\begin{array}{c} 0 \\ -y \end{array}\right].$$

Our final network example is derived from the equations describing a chemical reactor [199]. A first-order isomerisation reaction takes place and the heat generated is removed from the system through an external cooling circuit. The relevant equations are

$$C' = K_1(C_0 - C) - R (1.3.9a)$$

$$T' = K_1(T_0 - T) + K_2R - K_3(T - T_C)$$
 (1.3.9b)

$$0 = R - K_3 \exp\left(\frac{-K_4}{T}\right) C \tag{1.3.9c}$$

$$0 = C - u. \tag{1.3.9d}$$

Here C_0 and T_0 are the (assumed) known feed reactant concentration and feed temperature, respectively. C and T are the corresponding quantities in the product. R is the reaction rate per unit volume, T_C is the temperature of the

cooling medium (which can be varied), and the K_i are constants. We shall consider two variations of this problem later. The simpler one is (1.3.9a)-(1.3.9c) with T_C known and the state variables C, T, R. The more interesting one is (1.3.9a)-(1.3.9d) where (1.3.9d) is a specified desired product concentration and we want to determine the T_C (control) that will produce this C. In this case, we obtain a semi-explicit DAE system with state variables C, T, R, T_C . Even though these two problems turn out to be different in several respects (for example, in the dimension of their solution manifolds), they can be studied from the same DAE model. This example again illustrates the flexibility of working with a problem which is formulated as a DAE.

1.3.3 Model Reduction and Singular Perturbations

In a given model, there may be various small parameters. In an attempt to simplify the model or obtain a first order approximation to its behavior, these parameters may be set equal to zero. The resulting system is often a DAE.

In the classical singular perturbation problem (1.3.10) with $0 < \epsilon \ll 1$,

$$x' = f(x, y, t, \epsilon)$$

$$\epsilon y' = g(x, y, t, \epsilon)$$
(1.3.10)

setting $\epsilon = 0$ leads to the reduced order model

$$x' = f(x, y, t, 0)$$

0 = $g(x, y, t, 0)$. (1.3.11)

This semi-explicit DAE may be used if parasitics are to be ignored. Even if the solution of (1.3.10) is sought for all $t \ge 0$, the DAE (1.3.11) can often be solved and the solution added to a boundary layer correction term corresponding to a fast time scale to obtain a solution.

In general, there may be several small parameters, and the original equations may also be a DAE. As an example, consider the circuit (known as a loaded degree-one Hazony section under small loading) described in [51,102]. This circuit has time-invariant linear resistors, capacitors, a current source, and a gyrator. A gyrator is a 2-port device for which the voltage and current at one port are multiples of the current and voltage at the other port. The resistances R_i are large since they model parasitic terms, and similarly the capacitances are small. Letting $G_i = 1/R_i$, G = 1/R, g the gyration conductance, $g = i_s$ the current source, $g = v_s$, $g = v_s$, g =

$$\begin{bmatrix} C_1 & 0 & 0 \\ 0 & C_2 & 0 \\ C & -C_2 & 0 \end{bmatrix} x' + \begin{bmatrix} G_1 & g & 1 \\ g & G + G_2 & -1 \\ G_3 & -G_3 & -1 \end{bmatrix} x = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} u.$$
 (1.3.12a)

$$y = \begin{bmatrix} 0 & 1 & 0 \end{bmatrix} x. \tag{1.3.12b}$$

Here we assume that $G \ge 0$, g > 0, C > 0. In this problem there are five small parasitic parameters G_1 , G_2 , G_3 , C_2 , C_1 and one small model parameter G. The state dimension changes with G but all variations are easily examined within the one DAE model (1.3.12) [51].

Another example of DAE's arising from singular perturbation problems appears in cheap control problems. A simple example is the quadratic regulator problem mentioned earlier, where the control weighting matrix R depends on a small parameter $R(\epsilon)$ and R(0) is either singular or of lower rank.

Problems such as (1.3.10) are often referred to as stiff differential equations. It is well known that the solution of stiff differential equations, even for explicit ODE's, requires a special choice of numerical method. For example, explicit methods require exceedingly small stepsizes for stability reasons, so implicit methods are generally employed. The $\epsilon=0$ problem results when the stiffness is pushed to the limit. It is not surprising then that parallels will be found in the following chapters between the theory for the numerical solution of DAE's and that for stiff differential equations.

1.3.4 Discretization of PDE's

Solving partial differential equations (PDE's) can lead to DAE's. We shall consider the method of lines and moving grids.

Numerical methods for solving PDE's usually involve the replacement of all derivatives by discrete difference approximations. The method of lines (MOL) does this also, but in a special way that takes advantage of existing software. For parabolic PDE's, the typical MOL approach is to discretize the spatial derivatives, for example by finite differences, and thus convert the PDE system into an ODE initial value problem.

There are two important advantages to the MOL approach. First, it is computationally efficient. The ODE software takes on the burden of time discretization and of choosing the time steps in a way that maintains accuracy and stability in the evolving solution. Most production ODE software is written to be robust and computationally efficient. Also, the person using a MOL approach has only to be concerned with discretizing spatial derivatives, thus reducing the work required to write a computer program.

Many MOL problems lead, either initially or with slight modification, to an explicit ODE. However, many well posed problems of practical interest are more easily handled as a DAE. As a simple first example of the MOL consider the heat equation

$$\frac{\partial y}{\partial t} = \frac{\partial^2 y}{\partial x^2}$$

defined on the region $t \geq 0$, $0 \leq x \leq 1$ with boundary conditions given for y(t,0) and y(t,1), and initial conditions given for y(0,x). Taking a uniform spatial mesh of Δx , and mesh points $x_j = (j+1)\Delta x$, $1 \leq j \leq (1/\Delta x) - 1 = N$, and using centered differences, we obtain the semi-explicit DAE in the variables