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Uri M. Ascher   Linda R. Petzold

Computer Methods for Ordinary Differential Equations and Differential-Algebraic Equations

常微分方程和微分代数方程的计算机方法

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Part I: Introduction

Chapter 1

Ordinary Differential Equations

Ordinary differential equations (ODEs) arise in many instances when using mathematical modeling techniques for describing phenomena in science, engineering, economics, etc. In most cases the model is too complex to allow one to find an exact solution or even an approximate solution by hand: an efficient, reliable computer simulation is required.

Mathematically, and computationally, a first cut at classifying ODE problems is with respect to the additional or side conditions associated with them. To see why, let us look at a simple example. Consider

$$u''(t) + u(t) = 0, \qquad 0 \le t \le b,$$

where t is the independent variable (it is often, but not always, convenient to think of t as "time"), and $u = u(t)$ is the unknown, dependent variable. Throughout this book we use the notation

$$u' = \frac{du}{dt}, \qquad u'' = \frac{d^2u}{dt^2},$$

etc. We shall often omit explicitly writing the dependence of u on t.

The general solution of the ODE for u depends on two parameters α and β,

$$u(t) = \alpha \sin(t + \beta).$$

We can therefore impose two side conditions.

- ***Initial value problem*** (IVP): Given values $u(0) = c_1$ and $u'(0) = c_2$, the pair of equations

$$\alpha \sin \beta = u(0) = c_1,$$
$$\alpha \cos \beta = u'(0) = c_2$$

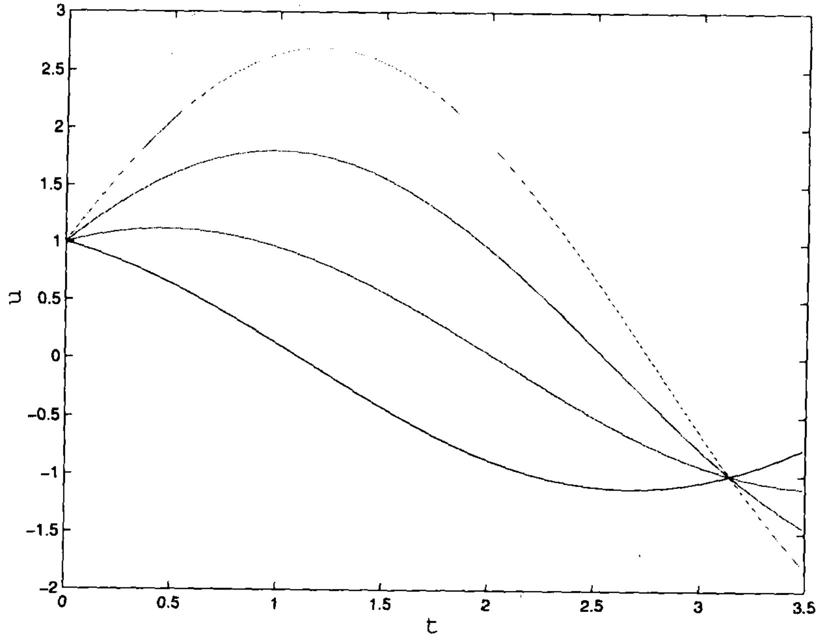

Figure 1.1: *u vs. t for* $u(0) = 1$ *and various values of* $u'(0)$.

can always be solved uniquely for $\beta = \tan^{-1}\frac{c_1}{c_2}$ and $\alpha = \frac{c_1}{\sin\beta}$ (or $\alpha = \frac{c_2}{\cos\beta}$; at least one of these is well defined). The IVP has a unique solution for any initial data $\mathbf{c} = (c_1, c_2)^T$. Such solution curves are plotted for $c_1 = 1$ and different values of c_2 in Figure 1.1.

- ***Boundary value problem*** (BVP): Given values $u(0) = c_1$ and $u(b) = c_2$, it appears from Figure 1.1 that for $b = 2$, say, if c_1 and c_2 are chosen carefully then there is a unique solution curve that passes through them, just like in the initial value case. However, consider the case where $b = \pi$: now different values of $u'(0)$ yield the same value $u(\pi) = -u(0)$ (see again Figure 1.1). So, if the given value of $u(b) = c_2 = -c_1$ then we have infinitely many solutions, whereas if $c_2 \neq -c_1$ then no solution exists.

This simple illustration already indicates some important general issues. For IVPs, one starts at the initial point with all the solution information and marches with it (in "time")—the process is *local.* For BVPs the entire solution information (for a second-order problem this consists of u and u') is not locally known anywhere, and the process of constructing a solution is *global* in t. Thus we may expect many more (and different) difficulties with the latter, and this is reflected in the numerical procedures discussed in this book.

1.1 IVPs

The general form of an IVP that we shall discuss is

$$\begin{aligned} \mathbf{y}' &= \mathbf{f}(t, \mathbf{y}), \qquad 0 \le t \le b, \\ \mathbf{y}(0) &= \mathbf{c} \ \ \text{(given)}. \end{aligned} \tag{1.1}$$

Here $\mathbf{y}$ and $\mathbf{f}$ are vectors with m components, $\mathbf{y} = \mathbf{y}(t)$, and $\mathbf{f}$ is in general a nonlinear function of t and $\mathbf{y}$. When $\mathbf{f}$ does not depend explicitly on t, we speak of the *autonomous* case. When describing general numerical methods we shall often assume the autonomous case simply in order to carry less notation around. The simple example from the beginning of this chapter is in the form (1.1) with $m = 2$, $\mathbf{y} = (u, u')^T$, $\mathbf{f} = (u', -u)^T$.

In (1.1) we assume, for simplicity of notation, that the starting point for t is 0. An extension of everything which follows to an arbitrary interval of integration $[a, b]$ is obtained without difficulty.

Before proceeding further, we give three examples which are famous for being very simple on one hand and for representing important classes of applications on the other hand.

Example 1.1 (simple pendulum)
Consider a tiny ball of mass 1 attached to the end of a rigid, massless rod of length 1. At its other end the rod's position is fixed at the origin of a planar coordinate system (see Figure 1.2).

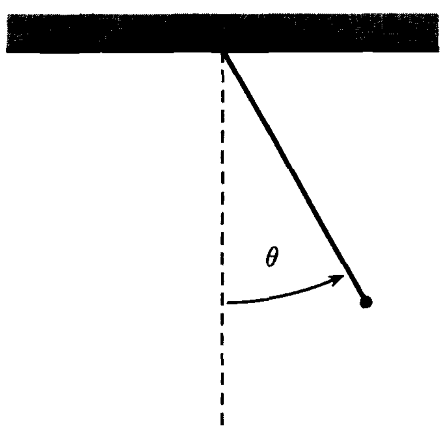

Figure 1.2: *Simple pendulum.*

Denoting by θ the angle between the pendulum and the y-axis, the friction-free motion is governed by the ODE (cf. Example 1.5 below)

$$\theta'' = -g \sin \theta, \tag{1.2}$$

where g is the (scaled) constant of gravity. This is a simple, nonlinear ODE for θ. The initial position and velocity configuration translates into values for $\theta(0)$ and $\theta'(0)$. The linear, trivial example from the beginning of this chapter can be obtained from an approximation of (a rescaled) (1.2) for small displacements θ. ♦

The pendulum problem is posed as a second-order scalar ODE. Much of the software for IVPs is written for first-order systems in the form (1.1). A scalar ODE of order m,

$$u^{(m)} = g(t, u, u', \ldots, u^{(m-1)}),$$

can be rewritten as a first-order system by introducing a new variable for each derivative, with $y_1 = u$:

$$\begin{aligned} y_1' &= y_2, \\ y_2' &= y_3, \\ &\vdots \\ y_{m-1}' &= y_m, \\ y_m' &= g(t, y_1, y_2, \ldots, y_m). \end{aligned}$$

Example 1.2 (predator-prey model)
Following is a basic, simple model from population biology which involves differential equations. Consider an ecological system consisting of one prey species and one predator species. The prey population would grow unboundedly if the predator were not present, and the predator population would perish without the presence of the prey. Denote

- $y_1(t)$—the prey population at time t;
- $y_2(t)$—the predator population at time t;
- α—prey's birthrate minus prey's natural death rate ($\alpha > 0$);
- β—probability of a prey and a predator coming together;
- γ—predator's natural growth rate (without prey; $\gamma < 0$);
- δ—increase factor of growth of predator if prey and predator meet.

Typical values for these constants are $\alpha = .25$, $\beta = .01$, $\gamma = -1.00$, $\delta = .01$.
Writing

$$\mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}, \qquad \mathbf{f} = \begin{pmatrix} \alpha y_1 - \beta y_1 y_2 \\ \gamma y_2 + \delta y_1 y_2 \end{pmatrix}, \tag{1.3}$$

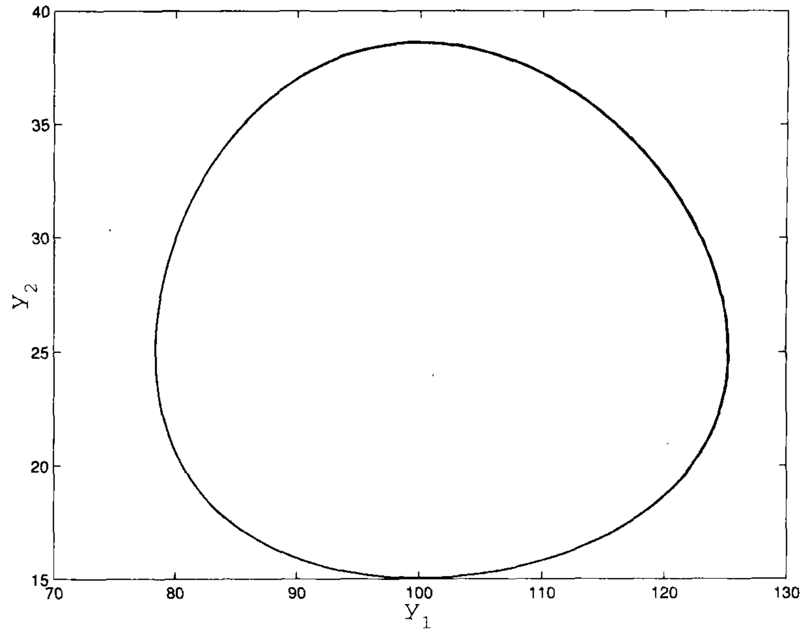

Figure 1.3: *Periodic solution forming a cycle in the $y_1 \times y_2$ plane.*

we obtain an ODE in the form (1.1) with $m = 2$ components, describing the time-evolution of these populations.

The qualitative question here is, starting from some initial values $\mathbf{y}(0)$ out of a set of reasonable possibilities, will these two populations survive or perish in the long run? As it turns out, this model possesses periodic solutions: starting, say, from $\mathbf{y}(0) = (80, 30)^T$, the solution reaches the same pair of values again after some time period T, i.e., $\mathbf{y}(T) = \mathbf{y}(0)$. Continuing to integrate past T yields a repetition of the same values, $\mathbf{y}(T + t) = \mathbf{y}(t)$. Thus, the solution forms a cycle in the phase plane (y_1, y_2) (see Figure 1.3). Starting from any point on this cycle, the solution stays on the cycle for all time. Other initial values not on this cycle yield other periodic solutions with a generally different period. So, under these circumstances the populations of the predator and prey neither explode nor vanish for all future times, although their number never becomes constant.[1] ♦

[1] In other examples, such as the Van der Pol equation (7.13), the solution forms an attracting *limit cycle*: starting from any point on the cycle the solution stays on it for all time, and starting from points near the solution, it tends in time towards the limit cycle.

The neutral stability of the cycle in our current example, in contrast, is one reason why this predator-prey model is discounted among mathematical biologists as being too simple.

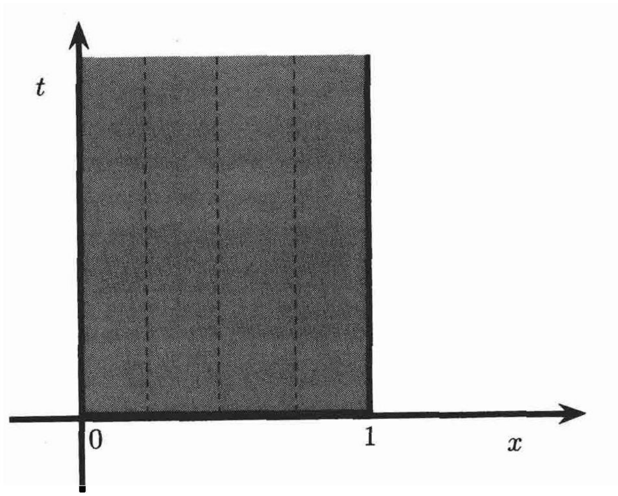

Figure 1.4: *Method of lines. The shaded strip is the domain on which the diffusion PDE is defined. The approximations $y_i(t)$ are defined along the dashed lines.*

Example 1.3 (a diffusion problem)
A typical diffusion problem in one space variable x and time t leads to the partial differential equation (PDE)

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(p\frac{\partial u}{\partial x}\right) + g(x,u),$$

for an unknown function $u(t,x)$ of two independent variables defined on a strip $0 \le x \le 1$, $t \ge 0$. For simplicity, assume that $p = 1$ and g is a known function. Typical side conditions which make this problem well posed are

$$\begin{aligned} u(0,x) &= q(x),\ 0 \le x \le 1 && \text{(initial conditions)},\\ u(t,0) &= \alpha(t),\ u(t,1) = \beta(t),\ t \ge 0 && \text{(boundary conditions)}. \end{aligned}$$

To solve this problem numerically, consider discretizing in the space variable first. For simplicity assume a uniform mesh with spacing $\Delta x = 1/(m+1)$, and let $y_i(t)$ approximate $u(x_i,t)$, where $x_i = i\Delta x$, $i = 0,1,\dots,m+1$. Then replacing $\frac{\partial^2 u}{\partial x^2}$ by a second-order central difference, we obtain

$$\frac{dy_i}{dt} = \frac{y_{i+1} - 2y_i + y_{i-1}}{\Delta x^2} + g(x_i, y_i), \qquad i = 1,\dots,m,$$

with $y_0(t) = \alpha(t)$ and $y_{m+1}(t) = \beta(t)$ given. We have obtained an initial value ODE problem of the form (1.1) with the initial data $c_i = q(x_i)$.

This technique of replacing spatial derivatives by finite difference approximations and solving an ODE problem in time is referred to as the *method of lines*. Figure 1.4 illustrates the origin of the name. Its more general form is discussed further in Example 1.7 below. ♦

We now return to the general IVP for (1.1). Our intention in this book is to keep the number of theorems down to a minimum: the references which we quote have them all in great detail. But we will nonetheless record those which are of fundamental importance, and the one just below captures the essence of the (relative) simplicity and locality of initial value ODEs. For the notation that is used in this theorem and throughout the book, we refer to Section 1.6.

Theorem 1.1 *Let* $\mathbf{f}(t, \mathbf{y})$ *be continuous for all* $(t, \mathbf{y})$ *in a region* $\mathcal{D} = \{0 \le t \le b,\ |\mathbf{y}| < \infty\}$. *Moreover, assume Lipschitz continuity in* $\mathbf{y}$*: there exists a constant* L *such that for all* $(t, \mathbf{y})$ *and* $(t, \hat{\mathbf{y}})$ *in* $\mathcal{D}$,

$$|\mathbf{f}(t, \mathbf{y}) - \mathbf{f}(t, \hat{\mathbf{y}})| \le L|\mathbf{y} - \hat{\mathbf{y}}|. \tag{1.4}$$

Then

1. *For any* $\mathbf{c} \in \Re^m$ *there exists a unique solution* $\mathbf{y}(t)$ *throughout the interval* $[0, b]$ *for the IVP* (1.1). *This solution is differentiable.*
2. *The solution* $\mathbf{y}$ *depends continuously on the initial data: if* $\hat{\mathbf{y}}$ *also satisfies the ODE (but not the same initial values) then*

$$|\mathbf{y}(t) - \hat{\mathbf{y}}(t)| \le e^{Lt}|\mathbf{y}(0) - \hat{\mathbf{y}}(0)|. \tag{1.5}$$

3. *If* $\hat{\mathbf{y}}$ *satisfies, more generally, a perturbed ODE*

$$\hat{\mathbf{y}}' = \mathbf{f}(t, \hat{\mathbf{y}}) + \mathbf{r}(t, \hat{\mathbf{y}}),$$

where $\mathbf{r}$ *is bounded on* $\mathcal{D}$, $\|\mathbf{r}\| \le M$, *then*

$$|\mathbf{y}(t) - \hat{\mathbf{y}}(t)| \le e^{Lt}|\mathbf{y}(0) - \hat{\mathbf{y}}(0)| + \frac{M}{L}(e^{Lt} - 1). \tag{1.6}$$

Thus we have solution existence, uniqueness, and continuous dependence on the data—in other words, a *well-posed problem*—provided that the conditions of the theorem hold. Let us check these conditions: if $\mathbf{f}$ is differentiable in $\mathbf{y}$ (we shall automatically assume this throughout), then the constant L can be taken as a bound on the first derivatives of $\mathbf{f}$ with respect to $\mathbf{y}$. Denote by $\mathbf{f_y}$ the *Jacobian matrix*,

$$(\mathbf{f_y})_{ij} = \frac{\partial f_i}{\partial y_j}, \qquad 1 \le i, j \le m.$$

We can write

$$\begin{aligned}\mathbf{f}(t,\mathbf{y}) - \mathbf{f}(t,\hat{\mathbf{y}}) &= \int_0^1 \frac{d}{ds}\mathbf{f}(t,\hat{\mathbf{y}} + s(\mathbf{y}-\hat{\mathbf{y}}))\,ds \\ &= \int_0^1 \mathbf{f}_{\mathbf{y}}(t,\hat{\mathbf{y}} + s(\mathbf{y}-\hat{\mathbf{y}}))\,(\mathbf{y}-\hat{\mathbf{y}})\,ds.\end{aligned}$$

Therefore, we can choose $L = \sup_{(t,\mathbf{y})\in\mathcal{D}} \|\mathbf{f}_{\mathbf{y}}(t,\mathbf{y})\|$.

In many cases we must restrict $\mathcal{D}$ in order to be assured of the existence of such a (finite) bound L. For instance, if we restrict $\mathcal{D}$ to include bounded $\mathbf{y}$ such that $|\mathbf{y}-\mathbf{c}| \le \gamma$, and on this $\mathcal{D}$ both the Lipschitz bound (1.4) holds and $|\mathbf{f}(t,\mathbf{y})| \le M$, then a unique existence of the solution is guaranteed for $0 \le t \le \min(b, \gamma/M)$, giving the basic existence result a more local flavor.

For further theory and proofs, see, for instance, Mattheij and Molnaar [67].

Note: Before continuing our introduction, let us remark that a reader who is interested in getting to the numerics of IVPs as soon as possible may skip the rest of this chapter and the next, at least on first reading.

1.2 BVPs

The general form of a BVP which we consider is a nonlinear first-order system of m ODEs subject to m independent (generally nonlinear) boundary conditions,

$$\mathbf{y}' = \mathbf{f}(t,\mathbf{y}), \tag{1.7a}$$

$$\mathbf{g}(\mathbf{y}(0),\mathbf{y}(b)) = \mathbf{0}. \tag{1.7b}$$

We have already seen in the beginning of the chapter that in those cases where solution information is given at both ends of the integration interval (or, more generally, at more than one point in time), nothing general like Theorem 1.1 can be expected to hold. Methods for finding a solution, both analytically and numerically, must be global, and the task promises to be generally harder than for IVPs. This basic difference is manifested in the current status of software for BVPs, which is much less advanced or robust than what is available for IVPs.

Of course, well-posed BVPs do arise on many occasions.

Example 1.4 (vibrating spring)
The small displacement u of a vibrating spring obeys a linear differential equation

$$-(p(t)u')' + q(t)u = r(t),$$

where $p(t) > 0$ and $q(t) \geq 0$ for all $0 \leq t \leq b$. (Such an equation also describes many other physical phenomena in one space variable t.) If the spring is fixed at one end and is left to oscillate freely at the other end, then we get the boundary conditions

$$u(0) = 0, \qquad u'(b) = 0.$$

We can write this problem in the form (1.7) for $\mathbf{y} = (u, u')^T$. Better still, we can use

$$\mathbf{y} = \begin{pmatrix} u \\ pu' \end{pmatrix},$$

obtaining

$$\mathbf{f} = \begin{pmatrix} p^{-1}y_2 \\ qy_1 - r \end{pmatrix}, \qquad \mathbf{g} = \begin{pmatrix} y_1(0) \\ y_2(b) \end{pmatrix}.$$

This BVP has a unique solution (which gives the minimum for the energy in the spring), as shown and discussed in many books on finite element methods, e.g., Strang and Fix [90]. ♦

Another example of a BVP is provided by the predator-prey system of Example 1.2, if we wish to find the periodic solution (whose existence is evident from Figure 1.3). We can specify $\mathbf{y}(0) = \mathbf{y}(b)$. However, note that b is unknown, so the situation is more complex. Further treatment is deferred to Chapter 6 and Exercise 7.5. A complete treatment of the topic of finding periodic solutions for ODE systems falls outside the scope of this book.

What can generally be said about existence and uniqueness of solutions to a general BVP (1.7)? We may consider the associated IVP (1.1) with the initial values $\mathbf{c}$ as a parameter vector to be found. Denoting the solution for such an IVP by $\mathbf{y}(t; \mathbf{c})$, we wish to find the solution(s) for the nonlinear algebraic system of m equations

$$\mathbf{g}(\mathbf{c}, \mathbf{y}(b; \mathbf{c})) = \mathbf{0}. \tag{1.8}$$

However, in general, there may be one, many, or no solutions for a system like (1.8). We delay further discussion to Chapter 6.

1.3 Differential-Algebraic Equations

Both the prototype IVP (1.1) and the prototype BVP (1.7) refer to an *explicit ODE* system

$$\mathbf{y}' = \mathbf{f}(t, \mathbf{y}). \tag{1.9}$$

A more general form is an *implicit ODE*

$$\mathbf{F}(t, \mathbf{y}, \mathbf{y}') = \mathbf{0}, \tag{1.10}$$

where the Jacobian matrix $\frac{\partial \mathbf{F}(t,\mathbf{u},\mathbf{v})}{\partial \mathbf{v}}$ is assumed to be nonsingular for all argument values in an appropriate domain. In principle, it is then often possible to solve for $\mathbf{y}'$ in terms of t and $\mathbf{y}$, obtaining the explicit ODE form (1.9). However, this transformation may not always be numerically easy or cheap to realize (see Example 1.6 below). Also, in general there may be additional questions of existence and uniqueness; we postpone further treatment until Chapter 9.

Consider next another extension of the explicit ODE, that of an *ODE with constraints*:

$$\mathbf{x}' = \mathbf{f}(t, \mathbf{x}, \mathbf{z}), \tag{1.11a}$$
$$\mathbf{0} = \mathbf{g}(t, \mathbf{x}, \mathbf{z}). \tag{1.11b}$$

Here the ODE (1.11a) for $\mathbf{x}(t)$ depends on additional algebraic variables $\mathbf{z}(t)$, and the solution is forced in addition to satisfy the algebraic constraints (1.11b). The system (1.11) is a *semi-explicit* system of *differential-algebraic equations* (DAEs). Obviously, we can cast (1.11) in the form of an implicit ODE (1.10) for the unknown vector $\mathbf{y} = \binom{\mathbf{x}}{\mathbf{z}}$; however, the obtained Jacobian matrix

$$\frac{\partial \mathbf{F}(t, \mathbf{u}, \mathbf{v})}{\partial \mathbf{v}} = \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix}$$

is no longer nonsingular.

Example 1.5 (simple pendulum revisited)
The motion of the simple pendulum of Figure 1.2 can be expressed in terms of the Cartesian coordinates (x_1, x_2) of the tiny ball at the end of the rod. With $z(t)$ a Lagrange multiplier, Newton's equations of motion give

$$x_1'' = -z x_1,$$
$$x_2'' = -z x_2 - g,$$

and the fact that the rod has a fixed length 1 gives the additional constraint

$$x_1^2 + x_2^2 = 1.$$

After rewriting the two second-order ODEs as four first-order ODEs, we obtain a DAE system of the form (1.11) with four equations in (1.11a) and one in (1.11b).

In this very simple case of a multibody system, the change of variables $x_1 = \sin\theta$, $x_2 = -\cos\theta$ allows elimination of z by simply multiplying the ODE for x_1 by x_2 and the ODE for x_2 by x_1 and subtracting. This yields the simple ODE (1.2) of Example 1.1. Such a simple elimination procedure is usually impossible in more general situations, though. ♦

The difference between an implicit ODE (with a nonsingular Jacobian matrix) and a DAE is fundamental. Consider the simple example

$$x' = z,$$
$$0 = x - t.$$

Clearly, the solution is $x = t$, $z = 1$, and no initial or boundary conditions are needed. In fact, if an arbitrary initial condition $x(0) = c$ is imposed, it may well be inconsistent with the DAE (unless $c = 0$, in which case this initial condition is just superfluous). We refer to Chapter 9 for more on this. Another point to note is that even if consistent initial values are given, we cannot expect a simple, general existence and uniqueness theorem like Theorem 1.1 to hold for (1.11). The nonlinear equations (1.11b) alone may have any number of solutions. Again we refer the reader to Chapter 9 for more details.

1.4 Families of Application Problems

Initial and boundary value problems for ODE and DAE systems arise in a wide variety of applications. Often an application generates a family of problems which share a particular system structure and/or solution requirements. Here we briefly mention three families of problems from important applications. The notation we use is typical for these applications and is not necessarily consistent with (1.1) or (1.11).

> **Note:** You *don't need* to understand the details given in this section in order to follow the rest of the text; this material is supplemental.

Example 1.6 (mechanical systems)
A fast, reliable simulation of the dynamics of multibody systems is needed in order to simulate the motion of a vehicle for design or to simulate safety

tests in physically based modeling in computer graphics, and in a variety of instances in robotics. The system considered is an assembly of rigid bodies (e.g., comprising a car suspension system). The kinematics define how these bodies are allowed to move with respect to one another. Using generalized position coordinates $\mathbf{q} = (q_1, \ldots, q_n)^T$ for the bodies, with m (so-called holonomic) constraints $g_j(t, \mathbf{q}(t)) = 0$, $j = 1, \ldots, m$, the equations of motion can be written as

$$\frac{d}{dt}\left(\frac{\partial L}{\partial q_i'}\right) - \frac{\partial L}{\partial q_i} = 0, \;\; i = 1, \ldots, n,$$

where $L = T - U - \sum \lambda_j g_j$ is the Lagrangian, T is the kinetic energy, and U is the potential energy. See almost any book on classical mechanics, for example, Arnold [1] or the lighter Marion and Thornton [65]. The resulting equations of motion can be written as

$$\mathbf{q}' = \mathbf{v}, \tag{1.12a}$$

$$M(t, \mathbf{q})\mathbf{v}' = \mathbf{f}(t, \mathbf{q}, \mathbf{v}) - G^T(t, \mathbf{q})\boldsymbol{\lambda}, \tag{1.12b}$$

$$\mathbf{0} = \mathbf{g}(t, \mathbf{q}), \tag{1.12c}$$

where $G = \frac{\partial \mathbf{g}}{\partial \mathbf{q}}$, M is a positive definite generalized mass matrix, $\mathbf{f}$ are the applied forces (other than the constraint forces), and $\mathbf{v}$ are the generalized velocities. The system sizes n and m depend on the chosen coordinates $\mathbf{q}$. Typically, using relative coordinates (describing each body in terms of its near neighbor) results in a smaller but more complicated system. If the topology of the multibody system (i.e., the connectivity graph obtained by assigning a node to each body and an edge for each connection between bodies) does not have closed loops, then with a minimal set of coordinates one can eliminate all the constraints (i.e., $m = 0$) and obtain an implicit ODE in (1.12). For instance, Example 1.1 uses a minimal set of coordinates for a particular multibody system without loops, while Example 1.5 does not. If the multibody system contains loops (e.g., a robot arm, consisting of two links, with the path of the "hand" prescribed, as in Example 10.9), then the constraints cannot be totally eliminated in general, and a DAE must be considered in (1.12) even if a minimal set of coordinates is employed. ♦

Example 1.7 (method of lines)
The diffusion equation of Example 1.3 is an instance of a time-dependent PDE in one space dimension,

$$\frac{\partial u}{\partial t} = f\left(t, u, \frac{\partial u}{\partial x}, \frac{\partial^2 u}{\partial x^2}\right) \tag{1.13}$$

Time-dependent PDEs naturally arise in more than one space dimension as well, with higher-order spatial derivatives and as systems of PDEs. The