1

Introduction

Our purpose in this opening chapter is to acquaint the reader with the class of mathematical problems discussed in this book. There are a number of general forms into which such problems are naturally cast. We consider these forms and discuss their relationships in Section 1.1. Then, in Section 1.2, a number of examples from various application areas are presented, which lead to instances of the general forms of Section 1.1. To a varying extent, we shall apply the general theory of Chapter 3 and the numerical methods of following chapters to these examples.

1.1 BOUNDARY VALUE PROBLEMS FOR ORDINARY DIFFERENTIAL EQUATIONS

We shall be concerned with *boundary value problems* (BVPs) for *ordinary differential equations* (ODEs). In this section several model problems and the most common general forms of BVPs are presented. Frequently, the special case of *initial value problems* (IVPs) will be discussed as well.

The treatment throughout deals almost exclusively with ODEs, so when we refer to IVPs or BVPs, "for ODEs" is to be implied.

1.1.1 Model problems

A boundary value problem consists of a differential equation (or equations) on a given interval and an explicit condition (or conditions) that a solution must satisfy at one or several points. The simplest instance of such explicit conditions is when they are all specified at one initial point. We refer to this as an initial value problem. Thus, a simple IVP would have the form

$$y' = f(x, y) \qquad x > a \tag{1.1a}$$

$$y(a) = \alpha \tag{1.1b}$$

where a is the initial point and α is a constant. Here, and throughout the book, we use the notation $y' \equiv \frac{dy}{dx}$. The IVP is called linear or nonlinear depending upon whether $f(x, y)$ is linear or nonlinear in y.

Frequently the variable x corresponds to time, and (1.1b) corresponds to the known initial position of the solution $y(x)$.

Example 1.1

If $y(x)$ represents the amount of the radioactive compound lead 210 present in a sample of ore at time x, then

$$\frac{dy}{dx} = \lambda y + r \qquad x > a$$

$$y(a) = \alpha$$

where α is the original amount present at the initial time $x = a$, the constant $\lambda \approx 22$ years is the half-life of lead 210, and $r(x)$ is the number of disintegrations of radium 226 (which produces lead 210) at time x. □

For a boundary value problem, information about a solution to the differential equation(s) may be generally specified at more than one point. Often there are two points, which correspond physically to the boundaries of some region, so that it is a *two-point boundary value problem.* A simple and common form for a two-point boundary value problem is

$$u'' = f(x, u, u') \qquad a < x < b \tag{1.2a}$$

$$u(a) = \beta_1, \qquad u(b) = \beta_2 \tag{1.2b}$$

where β_1 and β_2 are known constants and the known endpoints a and b may be finite or infinite. For the linear case of this BVP, (1.2a) takes the simpler form

$$u''(x) - c_1(x)u'(x) - c_0(x)u(x) = q(x) \qquad a < x < b \tag{1.2c}$$

Example 1.2

Consider a tightly stretched string with ends represented by the points $(0, 0)$ and $(b, 0)$ in the (x, u) plane. If it is hanging at rest under its own weight, the static displacement $u(x)$ satisfies

$$au'' - q = 0 \qquad 0 \le x \le b$$

$$u(0) = u(b) = 0$$

where a and q are constants dependent upon the material properties. □

1.1.2 General forms for the differential equations

Usually one assumes that general ordinary differential equations can be written as a first-order system

$$\mathbf{y}' = \mathbf{f}(x, \mathbf{y}) \qquad a < x < b \tag{1.3a}$$

where $\mathbf{y}(x) = (y_1(x), y_2(x), \ldots, y_n(x))^T$ is the unknown function and $\mathbf{f}(x, \mathbf{y}) = (f_1(x, \mathbf{y}), f_2(x, \mathbf{y}), \ldots, f_n(x, \mathbf{y}))^T$ is the (generally nonlinear) right-hand side. The interval ends a and b are finite or infinite constants. For linear problems, the ODE simplifies to

$$\mathbf{y}' = A(x)\mathbf{y} + \mathbf{q}(x) \qquad a < x < b \tag{1.4a}$$

where the matrix A and the vector $\mathbf{q}$ are functions of x, $A(x) \in \mathbf{R}^{n \times n}$ and $\mathbf{q}(x) \in \mathbf{R}^n$. The linear system (1.4a) is called *homogeneous* if $\mathbf{q} \equiv \mathbf{0}$, and it is *inhomogeneous* otherwise.

High-order ODEs can normally be converted to the first-order form (1.3a). Given any scalar differential equation

$$u^{(m)} = f(x, u, u', \ldots, u^{(m-1)}), \qquad a < x < b \tag{1.5}$$

let $\mathbf{y}(x) = (y_1(x), y_2(x), \ldots, y_m(x))^T$ be defined by

$$\begin{aligned} y_1(x) &= u(x) \\ y_2(x) &= u'(x) \\ &\vdots \\ y_m(x) &= u^{(m-1)}(x) \end{aligned} \tag{1.6}$$

Then the ODE can be converted to the equivalent first-order form

$$\begin{aligned} y_1' &= y_2 \\ y_2' &= y_3 \\ &\vdots \\ y_{m-1}' &= y_m \\ y_m' &= f(x, y_1, y_2, \ldots, y_m) \end{aligned}$$

This is in the form (1.3a).

Example 1.3

The equations for a three-body problem, such as a satellite moving under the influence of the earth and the moon in a coordinate system (u, v) and rotating so as to keep the positions of the earth and moon fixed, are

$$u'' = 2v + u - \frac{c_1(u + c_2)}{((u + c_2)^2 + v^2)^{1/2}} - \frac{c_2(u - c_1)}{((u - c_1)^2 + v^2)^{1/2}}$$

$$v'' = -2u + v - \frac{c_1 v}{((u + c_2)^2 + v^2)^{1/2}} - \frac{c_2 v}{((u - c_1)^2 + v^2)^{1/2}}$$

where c_1 is a given constant and $c_2 = 1 - c_1$. Letting $y_1 = u$, $y_2 = u'$, $y_3 = v$, and $y_4 = v'$, one obtains the first-order system

$$
\begin{aligned}
y_1' &= y_2 \\
y_2' &= 2y_3 + y_1 - \frac{c_1(y_1+c_2)}{((y_1+c_2)^2+y_3^2)^{1/2}} - \frac{c_2(y_1-c_1)}{((y_1-c_1)^2+y_3^2)^{1/2}} \\
y_3' &= y_4 \\
y_4' &= 2y_1 + y_3 - \frac{c_1 y_3}{((y_1+c_2)^2+y_3^2)^{1/2}} - \frac{c_2 y_3}{((y_1-c_1)^2+y_3^2)^{1/2}}
\end{aligned}
$$

□

In the linear case, the higher-order ODE (1.5) simplifies to

$$
u^{(m)} = \sum_{j=0}^{m-1} c_j(x) u^{(j)} + q(x), \qquad a < x < b \tag{1.7}
$$

The transformation (1.6) to a first-order system (1.4a) remains the same.

The most general form of a boundary value problem which we shall consider involves a system of differential equations which are of different orders. This is called a *mixed-order system.* It has the form

$$
\begin{aligned}
y_i^{(m_i)} &= f_i(x, y_1, \ldots, y_1^{(m_1-1)}, y_2, \ldots, y_d^{(m_d-1)}) && \text{(1.8a)} \\
&= f_i(x, \mathbf{z}(\mathbf{y})) \qquad 1 \le i \le d \qquad a < x < b
\end{aligned}
$$

where $\mathbf{y}(x) = (y_1(x), \ldots, y_d(x))^T$ and

$$
\mathbf{z}(\mathbf{y}(x)) := (y_1(x), y_1'(x), \ldots, y_1^{(m_1-1)}(x),\ y_2(x), \ldots, y_2^{(m_2-1)}(x), \ldots, y_d^{(m_d-1)}(x))^T
$$

The conversion of this system to a first-order form can proceed directly, as for one higher-order ODE. Letting $n := \sum_{i=1}^{d} m_i$, note that $\mathbf{z}(\mathbf{y}(x)) \in \mathbf{R}^n$ would be the vector of unknown functions of x in the first-order form.

1.1.3 General forms for the boundary conditions

A first-order system of ODEs like (1.3a) is normally supplemented by n boundary conditions (BC)

$$
\mathbf{g}(\mathbf{y}(a), \mathbf{y}(b)) = \mathbf{0} \tag{1.3b}
$$

where $\mathbf{g} = (g_1, \ldots, g_n)^T$ is a (generally nonlinear) vector function and 0 is a vector of n zeros. The simplest instance of $\mathbf{g}$ is the case for an IVP. Then the solution is given at the initial point; that is,

$$
\mathbf{y}(a) = \boldsymbol{\alpha} \tag{1.3c}
$$

where $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_n)^T \in \mathbf{R}^n$ is a known vector of initial conditions which uniquely determines $\mathbf{y}(x)$ near a .

Example 1.3 (continued)

For the three-body problem, typical boundary conditions would specify initial position and velocity of the body. If at time $x = 0$ the body is at $(u, v) = (1,0)$ with velocity -1 in the v direction then the initial conditions are

$$y_1(0) = 1$$
$$y_2(0) = 0$$
$$y_3(0) = 0$$
$$y_4(0) = -1$$

Note that these conditions have the form (1.3c). □

The relative simplicity of IVPs lies in the fact that the entire solution is known at a certain point. For the general BC (1.3b) this is not necessarily the case, as we have already seen in Example 1.2. Both analytic theory and numerical methods are considerably more involved in the general case. Correspondingly, there are a number of special cases of (1.3b) which will be considered.

The general form of linear two-point BC for a first-order system (or for a higher-order ODE) is

$$B_a \mathbf{y}(a) + B_b \mathbf{y}(b) = \boldsymbol{\beta} \tag{1.4b}$$

Here B_a and $B_b \in \mathbf{R}^{n \times n}$ and $\boldsymbol{\beta} \in \mathbf{R}^n$. In Chapter 3 we shall see that for the linear BVP (1.4a, b) to have a unique solution, it is necessary but not sufficient that these BC be linearly independent; that is, that the matrix (B_a, B_b) have n linearly independent columns, or simply *rank* $(B_a, B_b) = n$. BC of the general form (1.4b) are called *non-separated BC,* since each involves information about $\mathbf{y}(x)$ at both endpoints.

It is worthwhile to distinguish cases when some BC information is given at only one point. If rank $(B_a) < n$ or rank $(B_b) < n$, then the BC are called *partially separated.* In the case rank $(B_b) = q < n$, the BVP can be transformed to one where the BC have the form

$$B_{a1}\mathbf{y}(a) = \boldsymbol{\beta}_1$$
$$B_{a2}\mathbf{y}(a) + B_{b2}\mathbf{y}(b) = \boldsymbol{\beta}_2 \tag{1.4c}$$

where $B_{a1} \in \mathbf{R}^{p \times n} (p := n-q)$, B_{a2} and $B_{b2} \in \mathbf{R}^{q \times n}$, $\boldsymbol{\beta}_1 \in \mathbf{R}^p$, and $\boldsymbol{\beta}_2 \in \mathbf{R}^q$. The case *rank* $(B_a) < n$ is of course similar. Details of the transformation from (1.4b) to (1.4c) are given in Chapter 4.

The BC are called *separated* if they simplify further to

$$B_{a1}\mathbf{y}(a) = \boldsymbol{\beta}_1$$
$$B_{b2}\mathbf{y}(b) = \boldsymbol{\beta}_2 \tag{1.4d}$$

The nonlinear BC (1.3b) can also occur in partially separated or separated form. Thus, the boundary conditions are separated if they are of the form

$$\mathbf{g}_1(\mathbf{y}(a)) = \mathbf{0}_1$$
$$\mathbf{g}_2(\mathbf{y}(b)) = \mathbf{0}_2 \tag{1.3d}$$

where $\mathbf{g}_1$, $\mathbf{0}_1 \in \mathbf{R}^p$ and $\mathbf{g}_2$, $\mathbf{0}_2 \in \mathbf{R}^q$ with $n = p + q$. This latter case turns out to be particularly pleasant, both theoretically and practically. In fact, a significant portion of the currently available software for BVPs assumes that the BC are separated. Fortunately, a BVP with nonseparated or partially separated BC can be converted to one with separated BC (but with more ODEs), as we show next.

Consider the BVP with partially separated BC (1.4a, c) (which contains the nonseparated case (1.4b) as a special case with $p = 0$). Adding the $q = n - p$ trivial ODEs

$$\mathbf{z}' = \mathbf{0}$$

(implying $\mathbf{z}(a) = \mathbf{z}(b)$, *not* through the BC), we have an augmented system of order $n + q$ with separated BC which can be written as

$$\begin{pmatrix} \mathbf{y} \\ \mathbf{z} \end{pmatrix}' = \begin{pmatrix} A & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \mathbf{y} \\ \mathbf{z} \end{pmatrix} + \begin{pmatrix} \mathbf{q} \\ \mathbf{0} \end{pmatrix} \tag{1.9a}$$

$$\begin{bmatrix} B_{a1} & 0 \\ B_{a2} & -I \end{bmatrix} \begin{pmatrix} \mathbf{y} \\ \mathbf{z} \end{pmatrix}(a) = \begin{bmatrix} \boldsymbol{\beta}_1 \\ \mathbf{0} \end{bmatrix}, \qquad (B_{b2} \;\; I) \begin{pmatrix} \mathbf{y} \\ \mathbf{z} \end{pmatrix}(b) = \boldsymbol{\beta}_2 \tag{1.9b}$$

A demonstration of this trick is provided later on, in Example 1.10. Its validity is further discussed in Chapter 6. Note, however, that the enlarged size of the augmented system (1.9) is a disadvantage.

A general linear *multipoint* BVP consists of the ODE (1.4a) and multipoint BC

$$\sum_{j=1}^{J} B_j \, \mathbf{y}(\zeta_j) = \boldsymbol{\beta} \tag{1.4e}$$

where $B_1, \ldots, B_J \in \mathbf{R}^{n \times n}$, $\boldsymbol{\beta} \in \mathbf{R}^n$, and $a = \zeta_1 < \zeta_2 < \cdots < \zeta_J = b$. A multipoint BVP can be converted to a two-point problem by transforming each of the subintervals $[\zeta_j, \zeta_{j+1}]$ onto the interval [0,1], say, and writing the ODEs (1.4a) for the independent variable

$$t = \frac{x - \zeta_j}{\zeta_{j+1} - \zeta_j}$$

for each j, $1 \le j \le J-1$. The obtained $(J-1)n$ ODEs are then subject to the n BC of (1.4e) which are now specified at the interval ends, plus $n(J-2)$ additional BC resulting from the requirement that the solution $\mathbf{y}(x)$ should be continuous at the interior break points $\zeta_j, j = 2, \ldots, J-1$. Obviously, this transformation is not without a cost, but it helps to justify an analysis for only two-point BVPs. This we do throughout most of the book.

The most general form of a boundary value problem which we shall consider involves a mixed-order system (1.8a) subject to separated, multipoint boundary conditions

$$g_j(\mathbf{z}(\mathbf{y}(\zeta_j))) = 0 \qquad 1 \le j \le n \tag{1.8b}$$

$a = \zeta_1 \le \zeta_2 \le \ldots \le \zeta_n = b$. Again there is a transformation which brings this BVP into one with separated two-point BC, at the cost of increased system size.

Typically, the theoretical and numerical treatment of initial value problems is done by assuming they are in the first-order form (1.3a, c) or (1.4a), (1.3c). It is also common to treat BVPs in the form of first-order systems (1.3a, b) or (1.4a, b). Occasionally we will also consider BVPs expressed in terms of high-order equations (1.5) or (1.7) because (a) problems usually arise in this form, (b) numerical methods can be easier to motivate and describe for these equations, and (c) these methods can be more efficient if applied directly to the high-order equations instead of the corresponding first-order systems. Nevertheless, the basic properties and definitions for BVPs will be given just for first-order systems, as they can then be related to a general BVP by applying them to its equivalent first-order formulation.

1.2 BOUNDARY VALUE PROBLEMS IN APPLICATIONS

In this section we have collected 22 instances of BVPs which arise in a variety of application areas. The reader can therefore have an appreciation of the types of problems and difficulties encountered in practice. These examples can be used in order to test proposed methods and codes for the numerical solution of BVPs. When presenting numerical techniques in later chapters, we will use some of the examples listed here to illustrate the discussion, and the reader will be invited to try and solve other examples. Reading this section is, however, *not a prerequisite* to any other part of the book.

We do not insist on a uniform notation here; in some cases the notation is natural to the application. In each case, the formulation of the BVP is brought into one of the usual general forms discussed in the previous section, which we shall refer to as a "standard form."

For the background, and sometimes the detailed derivation of the application, we rely on the literature cited in the notes and references at the end of the book, and our intention here is not to go into too much detail about the physical origins of each problem. (Many of the formulations originate as PDEs which by various techniques are reduced to ODEs.) Additional papers which discuss applications not included here are mentioned in the bibliography of the chapter. The list is certainly not complete, but the collection forms a significant test-bed for any code.

Example 1.4 Flow in a Channel

Consider the problem of fluid injection through one side of a long vertical channel. The Navier-Stokes and the heat transfer equations can be reduced to the following system:

$$f''' - R\,[(f')^2 - ff''] + RA = 0 \tag{1.10a}$$

$$h'' + R\,fh' + 1 = 0 \tag{1.11a}$$

$$\theta'' + Pf\,\theta' = 0 \tag{1.12a}$$

$$f(0) = f'(0) = 0, \qquad f(1) = 1, \qquad f'(1) = 0 \tag{1.10b}$$

$$h(0) = h(1) = 0 \tag{1.11b}$$

$$\theta(0) = 0, \qquad \theta(1) = 1 \tag{1.12b}$$

Here f and h are two potential functions, θ is a temperature distribution function, and A is an undetermined constant. There are two parameters with known values, R = Reynolds number and P = Peclet number (e.g., take $P = 0.7R$).

At first, note that the subproblem (1.10a, b) is separated from the rest and thus can be solved separately. Suppose that this is done. Then (1.11a, b) and (1.12a, b) are two separated, *linear* second-order problems in standard form. The original problem is thus effectively broken into three subproblems.

Now consider (1.10a, b). We have a nonlinear third-order ODE for f, with the constant A determined by the requirement that the *four* BC (1.10b) be satisfied. One way to bring this into standard form is to differentiate (1.10a), obtaining

$$f'''' = R\,[f'f'' - ff'''] \tag{1.10c}$$

The problem (1.10c, b) is now in standard form (and no longer explicitly involves A). Another, more general, trick is to treat the constant A as another dependent variable, adding the ODE

$$A' = 0 \tag{1.10d}$$

The problem (1.10a, b, d) is again in standard form.

The difficulty in solving the nonlinear problem (1.10) numerically depends, in a typical way, on the Reynolds number R. For moderate values of R, say $R = 10$, the problem is easy, but it gets tougher as R increases and for $R = 10{,}000$ there is a fast change in some solution values near $x = 0$. This is called a *boundary layer.* □

Example 1.5 Particle Diffusion and Reaction

The ODEs governing the reaction are

$$T'' + \frac{2}{x}T' = -\phi^2\beta C e^{\gamma(1-T^{-1})} \tag{1.13a}$$

$$0 < x < 1$$

$$C'' + \frac{2}{x}C' = \phi^2 C e^{\gamma(1-T^{-1})} \tag{1.13b}$$

where x is time, C is the concentration, and T is the temperature. The constants ϕ, γ and β are known (they are the Thiele modulus, thermicity, and activation energy parameter, respectively). Representative values are $\phi = 14.44$, $\gamma = 20$, $\beta = 0.02$.

The BC at $x = 0$ are

$$T'(0) = C'(0) = 0 \tag{1.13c}$$

Note that the coefficient $\frac{2}{x}$ in (1.13a, b) is unbounded as $x \to 0$. This singularity typically comes from a reduction, due to cylindrical or spherical symmetry, of a partial differential equation to an ODE and is an artificial singularity: The solution is smooth near $x = 0$. The BC (1.13c) imply that

$$\frac{2}{x}T' \to 2T'', \qquad \frac{2}{x}C' \to 2C'' \;\; as \;\; x \to 0 \tag{1.14}$$

In a numerical implementation, an expression giving $\frac{0}{0}$ should not be evaluated, of course, so (1.13a, b) should be modified by (1.14) if we intend to evaluate the ODE at the boundary.

At $x = 1$ we may have two types of BC:

(i) Dirichlet type

$$T(1) = C(1) = 1 \tag{1.13d}$$

The resulting BVP (1.13a, b, c, d) is not very difficult, numerically.

(ii) Mixed type

$$-T'(1) = B(T(1) - 1), \qquad -C'(1) = B_m(C(1) - 1) \tag{1.13e}$$

with (for instance) $B = 5$, $B_m = 250$. Here we get a thin boundary layer near $x = 1$ and the BVP (1.13a, b, c, e) is significantly more difficult to solve numerically. □

Example 1.6 Soil Problem

The problem is to determine moisture (water) transport in dessicated soil. The numerical BVP is tough to solve for dry desert soil, and the difficulty is enhanced as the soil becomes drier. The original problem is a PDE in time t and one space variable ξ. However, using the similarity transformation for small times

$$x = \frac{\xi}{\sqrt{t}}$$

one obtains the BVP

$$(K_r P')' = \frac{1}{2}x(-\frac{dS}{dP})P' \qquad 0 < x < \infty \tag{1.15a}$$

$$P(0) = \beta_0, \qquad P(\infty) = \beta_1 \qquad (\text{e.g., } \beta_0 = 0, \qquad \beta_1 = -1) \tag{1.15b}$$

where P is the water pressure, K_r is the relative permeability, and S is the saturation. The latter two are given in terms of P by

$$\frac{S - S_r}{1 - S_r} = \frac{1}{1 + (-PL/A)^{\eta}}, \qquad K_r = \frac{1}{1 + (-PL/B)^{\lambda}} \qquad 0 < x < \infty \tag{1.15c}$$

where, typically,

$$S_r = 0.32, \quad A = 231, \quad B = 146, \quad \eta = 3.65, \quad \lambda = 6.65, \quad L = 100 \tag{1.15d}$$

The problem gets tougher for larger L (up to $L = 1000$ may be desired).

Note that the BVP is defined on an infinite interval. Here, however, this does not cause practical difficulties. Simply replace ∞ by a large enough value b, e.g., $b = 10$, and solve the BVP with

$$P(b) = \beta_1 \tag{1.15e}$$

We will have much more to say about infinite intervals later on (see Example 8.1, Section 11.4, and Examples 1.8 and 1.12). □

Example 1.7 Seismic Ray Tracing

The problem of determining when and where a relatively minor earthquake has occurred can sometimes be dealt with through ray theory. Suppose that the origin of the earthquake (in cartesian coordinates) is at the hypocenter (x_0, y_0, z_0) somewhere underneath the earth's surface ($z = 0$) and that the time at which the explosion has occurred is T_0. The explosion generates waves that propagate in all directions from the hypocenter; the time that a seismograph, located at a point (x_i, y_i, z_i) (with $z_i = 0$ if the seismograph is not buried underground), registers the earthquake, is equal to T_0 plus the time t_i it takes the wave front to travel from (x_0, y_0, z_0) to (x_i, y_i, z_i). Let t_i^0 be the actually observed time of tremor at the station located at (x_i, y_i, z_i). Then theoretically

$$T_0 + t_i = t_i^0$$

In practice, of course, t_i cannot be found exactly, but it can be calculated approximately, depending on the unknown (x_0, y_0, z_0). Thus, if we have N seismographs, $N \geq 4$, located at (x_i, y_i, z_i) and observing times t_i^0, $i = 1, \ldots, N$, then we can solve the nonlinear least squares problem

$$\text{minimize} \sum_{i=1}^{N} F_i^2 \tag{1.16a}$$

with

$$F_i = F_i(x_0, y_0, z_0, T_0) = T_0 + t_i - t_i^0 \tag{1.16b}$$

The question is then, how to calculate t_i.

Now, it can be shown that the normal to the wave front at any point (x, y, z) behaves, as a function of time t, like an optical ray and satisfies the following differential equations

$$\frac{dx}{ds} = v\xi, \qquad \frac{dy}{ds} = v\eta, \qquad \frac{dz}{ds} = v\zeta \tag{1.17a}$$

$$0 < s < S$$

$$\frac{d\xi}{ds} = u_x, \qquad \frac{d\eta}{ds} = u_y, \qquad \frac{d\zeta}{ds} = u_z$$

where s is the arclength along the path, S is the (unknown) total arclength, $(x(s), y(s), z(s))$ are the coordinates of the ray, $v = v(x, y, z)$ is the velocity of a sound wave at a point (x, y, z) of the earth and $u \equiv 1/v$ is the slowness. The notation u_x stands for $\frac{\partial u}{\partial x}$, etc. How to obtain the velocity structure $v(x, y, z)$ of the medium is a nontrivial practical question, but we assume here that it is given; we note in passing that this velocity structure, or an approximation to it, can be obtained from a set of velocity measurements using three-dimensional interpolation.

Now, the time t_i it takes the ray to reach the i^{th} seismograph is

$$t_i = \int_0^S u(s)\,ds \tag{1.17b}$$

and we can integrate this knowing the ray path, which we obtain by solving the differential equations (1.17a) subject to the boundary conditions

$$x(0) = x_0, \qquad y(0) = y_0, \qquad z(0) = z_0 \tag{1.17c}$$

$$\frac{dx}{ds}(0)^2 + \frac{dy}{ds}(0)^2 + \frac{dz}{ds}(0)^2 = 1 \tag{1.17d}$$

$$x(S) = x_i, \qquad y(S) = y_i, \qquad z(S) = z_i \tag{1.17e}$$

Here, the boundary conditions (1.17c, e) are obvious and (1.17d) comes from ray theory. Since S is a free parameter, it makes sense to have seven boundary conditions for six differential equations.

We now reformulate the problem (1.17) in standard form. For this we have to convert the interval of integration from a free-ended to a specified one, which we do by scaling the independent variable

$$\tau = s/S$$

and having S as a dependent variable, specifying

$$\frac{dS}{d\tau} \equiv S' = 0$$

Then, to incorporate (1.17b) we write

$$t_i = T(1)$$

where $T' = Su$ and T(0) = 0. The converted system is then

$$\begin{aligned} x' &= Sv\xi, & y' &= Sv\eta, & z' &= Sv\zeta & & \\ \xi' &= Su_x, & \eta' &= Su_y, & \zeta' &= Su_z & 0 < \tau < 1 \\ T' &= Su, & S' &= 0 & & \end{aligned} \tag{1.18a}$$

subject to the boundary conditions

$$\begin{aligned} &x(0) = x_0, && y(0) = y_0, && z(0) = z_0 \\ &T(0) = 0, && \xi(0)^2 + \eta(0)^2 + \zeta(0)^2 = u(x(0), y(0), z(0))^2 \\ &x(1) = x_i, && y(1) = y_i, && z(1) = z_i \end{aligned} \tag{1.18b}$$

The problem (1.18a, b) is now a nonlinear BVP in standard form.

To summarize, the location and origin time of the earthquake are determined by solving the minimization problem (1.16a), where for each i, $1 \le i \le N$, and each trial location (x_0, y_0, z_0) and origin time T_0, the function F_i of (1.16b) is evaluated by solving the boundary value problem (1.18a, b) and using $t_i = T(1)$. Since there are many boundary value problems to be solved, the code used for their solution should be very efficient.

The difficulty in solving (1.18) depends on the smoothness of the velocity structure v. For a constant v (a uniform medium) the problem is trivial, the ray being a straight line. However, if there are abrupt changes in the medium, then the problem may be difficult to solve numerically. □

Example 1.8 Theoretical Seismograms

This is another seismological application, where one attempts to calculate the ground displacements caused by a point moment seismic source. Assuming that the material properties of the medium (the earth) are a function of depth z only, we apply a Fourier-Bessell transform to the governing PDE (which is linear, in four independent variables), obtaining two uncoupled ODE systems of the form

$$\frac{d\mathbf{y}}{dz} \equiv \mathbf{y}' = A(z; \omega, k)\mathbf{y} \qquad 0 < z < b \tag{1.19}$$

Here the angular frequency ω and the horizontal wave number k are parameters, $-\infty < \omega < \infty, 0 \le k < \infty$. For each depth z, the solution of (1.19), under appropriate BC to be discussed below, is a function of k and ω. A double integral on k and ω is then taken to obtain the solution in terms of space and time. Thus, there are a very large number of BVPs to be solved.

We next specify these BVPs. Consider a half-space $0 < z < \infty$ in which P-wave velocity $\alpha(z)$, S-wave velocity $\beta(z)$, and density $\rho(z)$ are given piecewise continuous functions, which are constant for $z \ge b$. The first ODE system, called the SH equations, is given by (1.19) with

$$A = A_H = \begin{pmatrix} 0 & 1/\mu \\ \mu k^2 - \rho\omega^2 & 0 \end{pmatrix} \qquad \mu = \rho\beta^2 \tag{1.20a}$$

while the second, more complex ODE system, called the P-SV equations, is given by (1.19) with

$$A = A_P = \begin{pmatrix} 0 & \dfrac{1}{\rho\alpha^2} & k(1-2\beta^2/\alpha^2) & 0 \\ -\omega^2\rho & 0 & 0 & k \\ -k & 0 & 0 & 1/\mu \\ 0 & -k(1-2\beta^2/\alpha^2) & 4\mu k^2(1-\beta^2/\alpha^2)-\rho\omega^2 & 0 \end{pmatrix} \tag{1.21a}$$

The BC at $z = b$ are derived from a radiation condition, that is, the requirement that only downgoing waves exist for $z \geq b$. This gives for the SH problem

$$\nu_\beta y_1 + \mu^{-1} y_2 = 0 \qquad \text{at } z = b \tag{1.20b}$$

and for the P-SV problem

$$(\rho\omega^2 - 2\mu k^2) y_1 + 2\mu k \nu_\alpha y_3 - \nu_\alpha y_2 + k y_4 = 0 \tag{1.21b}$$

$$\text{at } z = b$$

$$2\mu k \nu_\beta y_1 + (\rho\omega^2 - 2\mu k^2) y_3 + k y_2 - \nu_\beta y_4 = 0 \tag{1.21c}$$

(When $\omega = 0$, (1.21b) and (1.21c) become linearly dependent and (1.21c) is then replaced by

$$(\rho\alpha^2)^{-1} y_2 + 2k(1-\beta^2/\alpha^2) y_3 + \mu^{-1} y_4 = 0 \qquad \text{at } z = b) \tag{1.21d}$$

Here, $\pm\nu_\beta$ and $\pm\nu_\beta$, $\pm\nu_\alpha$ are the eigenvalues of A_H and A_P, respectively:

$$\nu_\beta = (k^2 - \frac{\omega^2}{\beta^2})^{1/2}, \qquad \nu_\alpha = (k^2 - \frac{\omega^2}{\alpha^2})^{1/2}$$

with the sign choice $\mathrm{Re}(\nu) \geq 0$; $\mathrm{Im}(\nu) \leq 0$ when $\mathrm{Re}(\nu) = 0$. When $\mathrm{Re}(\nu) > 0$, we have a decaying solution in z (a surface wave), while if $\mathrm{Re}(\nu) = 0$, $\nu \neq 0$, we have an oscillatory solution (body wave). The rate of decay or oscillation increases as ω increases and the problem then gets tougher.

To complete the specification of the BVPs, solution values are given at the earth surface, viz.

$$y_2(0) = \beta_1 \tag{1.20c}$$

for the SH problem and

$$y_2(0) = \beta_1, \qquad y_4(0) = \beta_2 \tag{1.21e}$$

for the P-SV problem. The problem actually appears in two flavors in the seismology literature. One is where $\beta_1 \neq 0$ and/or $\beta_2 \neq 0$, corresponding to including an inhomogeneous source term, and a unique solution to (1.20) and (1.21) is sought. In the other approach, $\beta_1 = \beta_2 = 0$, and one solves for the eigenvalues and eigenfunctions of the (linear) problem. The double integral over ω and k then becomes a sum of residues at poles.

The large number of BVPs to be solved and their drastically different character for different (large) values of ω and k make this problem challenging, despite its linearity. A saving grace is the high degree of parallelism possible in these computations. □

Example 1.9 Meniscus in a Cylinder

Consider the equilibrium-free surface of a liquid inside a vertical cylinder of circular cross section (e. g., a capillary). The surface $f(r)$ satisfies the BVP

$$\frac{1}{r}\left[\frac{rf'(r)}{(1+(f'(r))^2)^{1/2}}\right]' - Bf(r) - 2\lambda = 0 \qquad 0 < r < 1 \tag{1.22a}$$

$$f(0) = 0, \qquad f'(0) = 0 \tag{1.22b}$$

$$f'(1) = \cot\theta \tag{1.22c}$$

The independent variable r runs from the middle of the cylinder ($r = 0$) to its boundary $r = 1$, where the angle θ of contact with the fluid is given. There are two other parameters: The Bond number B is given, while the mean curvature λ of the surface at $r = 0$ is unknown, accounting for the three BC (1.22b, c). A straightforward reformulation of (1.22a) is then (cf. Example 1.4)

$$\lambda' = 0 \tag{1.22d}$$

$$f'' = (1+(f')^2)^{3/2}(Bf + 2\lambda) - \frac{1}{r}((f')^3 + f') \tag{1.22e}$$

The problem (1.22d, e, b, c) is in standard form. The ranges of interest for the parameters are $B_{cr} < B \le 1000$, where B_{cr} is a critical parameter, $-10 < B_{cr} < 0$, and $0 \le \theta \le \pi/2$ (wetting fluid). Unless $\theta \approx 0$, this BVP is not particularly difficult numerically. When $\theta = 0$, however, the end value in (1.22c) blows up, and another formulation is needed. This is done by letting x, the angle between the surface and the horizontal line, be the independent variable. From the relation

$$\tan x = f'(r)$$

we get

$$\dot{\lambda} = 0 \tag{1.23a}$$

$$\dot{f} = D \sin x \qquad 0 < x < \pi/2 - \theta \tag{1.23b}$$

$$\dot{r} = D \cos x \tag{1.23c}$$

$$f(0) = r(0) = 0, \qquad r(\pi/2 - \theta) = 1 \tag{1.23d}$$

where $(\dot{\ }) \equiv \frac{d}{dx}$ and

$$D = D(x) = [Bf(x) - r^{-1}\sin x + 2\lambda]^{-1} \tag{1.23e}$$

This latter formulation (1.23) is now good even when $\theta = 0$. □

Example 1.10 Measles

Consider the following epidemiology model. Assume that a given population of constant size N can be divided into four categories: Susceptibles, whose number at time t is $S(t)$, infectives $I(t)$, latents $L(t)$, and immunes $M(t)$. We have

$$S(t) + I(t) + L(t) + M(t) = N \qquad t \in [0,1]$$

Under certain assumptions on the disease, its dynamics can be expressed as

$$y_1' = \mu - \beta(t)y_1y_3 \tag{1.24a}$$

$$y_2' = \beta(t)y_1y_3 - y_2/\lambda \qquad 0 < t < 1 \tag{1.24b}$$

$$y_3' = y_2/\lambda - y_3/\eta \tag{1.24c}$$

where $y_1 = S/N$, $y_2 = L/N$, $y_3 = I/N$, $\beta(t) = \beta_0(1+\cos 2\pi t)$ and representative values of the appearing constants are μ=0.02, λ=0.0279, η=0.01, and β_0 = 1575.

The solution sought is periodic; that is, the BC are

$$\mathbf{y}(1) = \mathbf{y}(0) \tag{1.24d}$$

The BC (1.24d) are not separated. We can separate them by the general trick introduced in the previous section. Thus, let $\mathbf{c} = (c_1, c_2, c_3)^T$ be a vector of constants. We augment (1.24a, b, c) and replace (1.24d) by

$$\mathbf{c}' = \mathbf{0} \tag{1.24e}$$

$$\mathbf{y}(0) = \mathbf{c}(0), \qquad \mathbf{y}(1) = \mathbf{c}(1) \tag{1.24f}$$

The BVP (1.24a, b, c, e, f) now has separated BC. However, the size of the problem has doubled — a significant expense. The problem is not very difficult numerically. □

Example 1.11 Kidney Model

This problem is not only larger, but also much tougher than the previous two. The model describes mass and energy balance of the renal counterflow system. With F_{iv} the axial volume flow in the i^{th} tube, J_{iv} the outward transmural volume flux, $F_{iv}C_{ik}$ the axial flow of the k^{th} solute in the i^{th} tube and J_{ik} the outward transmural flux per unit length of the k^{th} solute from the i^{th} tube, the ODEs for the steady state problem are

$$\frac{dF_{iv}}{dx} + J_{iv} = 0, \qquad 1 \le i \le 6 \tag{1.25a}$$

$$\frac{d}{dx}(F_{iv}C_{ik}) + J_{ik} = 0, \qquad 1 \le i \le 6, \qquad 1 \le k \le 2 \tag{1.25b}$$

and $0 < x < 1$.

Boundary conditions are as follows:

$$\begin{array}{lll}
F_{1v}(0) = 1 & F_{5v}(0) = 5 & \\
C_{11}(0) = 1 & C_{51}(0) = 1 & \\
C_{12}(0) = 0.05 & C_{52}(0) = 0.05 & \\
F_{2v}(1) = -F_{1v}(1) & & \\
C_{2k}(1) = C_{1k}(1) & \text{for } k = 1,2 & \\
F_{6v}(0) = -F_{2v}(0) & & \\
C_{6k}(0) = C_{2k}(0) & \text{for } k = 1,2 & \\
F_{3v}(0) = F_{6v}(1) & & \\
C_{3k}(0) = C_{6k}(1) & \text{for } k = 1,2 & \\
F_{4v}(1) = -F_{5v}(1) & & \\
C_{4k}(1) = C_{5k}(1) & \text{for } k = 1,2 &
\end{array} \tag{1.25c}$$

This gives 18 BC for the 18 ODEs (1.25a, b). But we still have to specify the functions J_{i1}, J_{i2}, and J_{iv}, $1 \le i \le 6$. Transmural volume fluxes are defined as follows:

$$J_{iv} = h_{iv}\sum_{k=1}^{2}(C_{4k} - C_{ik}), \qquad i = 1,2,3,5$$

$$J_{4v} = -\sum_{i \neq 4,6} J_{iv}$$

$$J_{6v} = (1.0 - C_{61}) + (0.05 - C_{62})$$

where $h_{1v} = h_{3v} = 10$ and $h_{iv} = 0$ for i=2, 5.

Transmural solute fluxes are

$$\begin{aligned} J_{i1} &= 0, && i = 1,3 \\ &= 0.75\, C_{i1}/(1. + C_{i1}), && i = 6 \\ &= 1000(C_{i1} - C_{41}), && i = 5 \end{aligned}$$

$$J_{21}(x) = \begin{cases} 1.8, & 0. \le x \le 0.4 \\ 1.8 + [-18. + 100(C_{21}(x) - C_{41}(x))]\cdot(x - 0.4), & 0.4 < x < 0.5 \\ 10[C_{21}(x) - C_{41}(x)], & 0.5 \le x \le 1 \end{cases}$$

$$\begin{aligned} J_{i2} &= 0, && i = 1,2,6 \\ &= 1000(C_{i2} - C_{42}), && i = 5 \end{aligned}$$

$$J_{32}(x) = \begin{cases} 0., & 0. \le x \le 0.4 \\ 0.1[C_{32}(x) - C_{42}(x)]\cdot(x - 0.4), & 0.4 < x < 0.5 \\ 0.01[C_{32}(x) - C_{42}(x)], & 0.5 \le x \le 1 \end{cases}$$

$$J_{4k}(x) = -\sum_{i \neq 4,6} J_{ik}(x), \qquad 0. \le x \le 1, \qquad 1 \le k \le 2$$

This completes the specification of the problem. However, some simplification is possible. The reader can verify that the following BVP of order 13 is equivalent to (1.25).

$$C_{12}' = 20h_{1v}(C_{12})^2[C_{41} + C_{42} - 21C_{12}] \tag{1.26a}$$

$$C_{11} = 20C_{12}, \quad F_{1v} = \frac{0.05}{C_{12}}, \quad F_{2v} = -\frac{0.05}{C_{22}}$$

$$C_{21}' = 20C_{22}J_{21}, \quad C_{22}' = 0 \tag{1.26b}$$

$$C_{31}' = \frac{h_{3v}}{K_1}(C_{31})^2[C_{41} + C_{42} - C_{31} - C_{32}] \tag{1.26c}$$

$$C_{32}' = \frac{C_{31}}{K_1}[J_{3v}C_{32} - J_{32}] \tag{1.26d}$$

$$K_1' = 0, \quad F_{4v}' = -J_{4v} \tag{1.26e}$$

$$K_1 = \frac{C_{31}(0)}{20C_{32}(0)}, \quad F_{3v} = \frac{K_1}{C_{31}}, \quad F_{5v} = 5, \quad F_{6v} = \frac{0.05}{C_{62}}$$

$$C_{41}' = \frac{1}{F_{4v}}[J_{4v}C_{41} - J_{41}] \tag{1.26f}$$

$$C_{42}' = \frac{1}{F_{4v}}[J_{4v}C_{42} - J_{42}] \tag{1.26g}$$

$$C'_{51} = -200(C_{51} - C_{41}), \qquad C'_{52} = -200(C_{52} - C_{42}) \tag{1.26h}$$

$$C'_{61} = 20C_{62}[J_{6v} C_{61} - J_{61}] \tag{1.26i}$$

$$C'_{62} = 20(C_{62})^2 J_{6v} \tag{1.26j}$$

$$C_{12}(0) = 0.05, \quad C_{51}(0) = 1, \qquad C_{52}(0) = 0.05, \qquad F_{4v}(1) = -5 \tag{1.26k}$$

$$C_{31}(0) - 20K_1(0)C_{32}(0) = 0, \qquad C_{22}(0) = C_{62}(0), \qquad C_{61}(0) = C_{21}(0) \tag{1.26l}$$

$$C_{12}(1) = C_{22}(1), \qquad C_{21}(1) = 20C_{12}(1), \qquad C_{41}(1) = C_{51}(1) \tag{1.26m}$$

$$C_{42}(1) = C_{52}(1), \qquad C_{61}(1) - 20K_1(1)C_{62}(1) = 0$$

$$C_{31}(0) = C_{61}(1) \tag{1.26n}$$

This BVP has one nonseparated BC. An equivalent problem of order 14 can be formed which has only separated BC, using the trick introduced in the previous section. □

Example 1.12 Magnetic Monopoles

The standard laws of electromagnetism (Maxwell's equations) forbid the possibility of magnetic monopoles. But classical solutions having the properties of monopoles can be found in the more general Yang-Mills theory. The governing equations are nonlinear partial differential equations, but an ODE over an infinite interval can be obtained in some special cases involving symmetry.

After mapping the independent variable onto the interval (0, 1), the obtained BVP reads

$$y_1'' = \frac{2y_1'}{1-x} + \frac{y_1}{x^2(1-x)^2}[y_1^2 - 1 + \frac{y_3^2 - y_2^2}{(1-x)^2}] \tag{1.27a}$$

$$y_2'' = \frac{2y_2 y_1^2}{x^2(1-x)^2} \qquad 0 < x < 1 \tag{1.27b}$$

$$y_3'' = \frac{y_3}{x^2(1-x)^2}[2y_1^2 + \frac{\beta(y_3^2 - x^2)}{(1-x)^2}] \tag{1.27c}$$

$$y_1(0) = 1, \qquad y_2(0) = y_3(0) = 0 \tag{1.27d}$$

$$y_1(1) = 0, \qquad y_2(1) = \eta, \qquad y_3(1) = 1 \tag{1.27e}$$

where β and η are given constants. The mass for a monopole can be expressed in terms of an integral of these quantities.

Typically, one may want solutions of this BVP for a number of parameter values in the range $0 \le \beta \le 20$, $0 < \eta < 1$. For an efficient numerical solution procedure it then makes sense to use information obtained when solving for one pair of parameter values to expedite solving a neighboring problem. Such a neighboring problem would be the same BVP (1.27) with a slightly different pair of values for β and η. This leads to ideas of *continuation,* applicable in a natural way to many of the examples presented here, and discussed in Section 8.3.

The BVP (1.27) is not very difficult numerically. □

Example 1.13 Solitary Wave

The Fitzhugh-Nagumo equations are a simple mathematical model for the propagation of action potentials down the giant axon of the squid, Loligo:

$$V_t = V_{\xi\xi} + V - \frac{1}{3}V^3 - R + S$$

$$(t,\xi) \in D \subset \mathbf{R}^2$$

$$R_t = \phi(V + a - bR)$$

where t is time, ξ is distance, V is membrane potential, R is recovery variable, S is prescribed stimulating current and ϕ, a, b are given constants. Subscripts denote partial derivatives with respect to ξ and t.

Looking for travelling wave solutions, we introduce a single variable $x = \xi + ct$, $c > 0$, and obtain the problem

$$v'' - cv' - (V_R^2-1)v - r - V_R v^2 - \frac{1}{3}v^3 = 0 \qquad (1.28a)^*$$

$$r' - \frac{\phi}{c}(v - br) = 0 \qquad (1.28b)$$

$$v(-\infty) = v(\infty) = r(\infty) = 0 \qquad (1.28c)$$

$$r(-\infty) = 0 \qquad (1.28d)$$

Here, V_R is a given constant (rest state) and c is an unknown constant. Representative values for the constants are $a = 0.7$, $b = 0.8$, $\phi = 0.08$, $V_R = 1.1994080352440$. The sought solution is a single pulse solitary wave, but note that equations (1.28a, b, c, d) pin it down only to within a translation in x. Thus, to get a unique solution we treat c as another dependent variable and add the equation

$$c' = 0 \qquad (1.28e)$$

and the boundary condition

$$v(0) = v_0 \neq 0 \qquad (1.28f)$$

where v_0 is some nonzero value in the range of v.

Now, however, we have too many BC. The BC (1.28c, d) need to be replaced by three independent ones. Analysis (see Section 11.4.2) yields that one possible way to proceed is to drop (1.28d) (this is a redundant BC). The remaining BVP (1.28a, b, c, e, f) can then be solved for $-L \le x \le L$, with, say, $L = 70$. Note that we have here a *3-point* BVP. The BC are given at three points -L, 0, and L. □

Example 1.14 Nonlinear Elastic Beams

The deformation of a beam under the action of axial and transverse loading which is also resting on a nonlinear foundation is governed by the equations

$$x' = (1+e)\cos\theta \qquad (1.29a)$$

$$y' = (1+e)\sin\theta \qquad (1.29b)$$

$$s' = 1 + e \qquad (1.29c)$$

$$\theta' = (1+e)\kappa \qquad 0 < t < L \qquad (1.29d)$$

$$Q' = (1+e)[(ky - P)\cos\theta - \kappa T] \qquad (1.29e)$$

$$M' = (1+e)Q \qquad (1.29f)$$

$$T' = (1+e)[(ky-P)\sin\theta + \kappa Q] \tag{1.29g}$$

with $e = T/EA$, $\kappa = M/EI$, $P(t)$ and $k(y)$ are given functions and E, I, A are constants. Possible boundary conditions are

(i) Simple supports

$$y(0) = y(L) = 0,\ x(0) = 0,\ M(0) = M(L) = 0,\ s(0) = 0,\ T(0) = x_0 \tag{1.30a}$$

(with x_0 given)

(ii) Clamped ends

$$y(0) = y(L) = 0,\quad x(0) = 0,\quad \theta(0) = \theta(L) = 0,\quad s(0) = 0,\quad T(0) = x_0 \tag{1.30b}$$

(iii) Elastic support at the left end

$$Q(0) = K_L y(0),\quad x(0) = 0,\quad M(0) = -K_T\theta(0),\quad s(0) = 0,\quad T(0) = x_0 \tag{1.30c}$$

[with BC at $x = L$ as in (ii)].

This defines one BVP with three types of BC. Now, assuming that the deformation is inextensional, i. e., $e \equiv 0$ but $T \neq 0$ (which makes sense only after introducing appropriate scaling and taking appropriate limits) and introducing dimensionless variables

$$t := t/L,\qquad y := y/L,\qquad M := ML/EI,\qquad T := T/X_0,\qquad k := k/k_0$$

$$P := PL/x_0,\qquad \lambda := \sqrt{k_0L^2/x_0},\qquad \varepsilon := \sqrt{EI/x_0L^2},\qquad Q := Q/\varepsilon x_0$$

we get (1.29) in the form

$$x' = \cos\theta \tag{1.31a}$$

$$y' = \sin\theta \tag{1.31b}$$

$$\theta' = M \qquad\qquad 0 < t < 1 \tag{1.31c}$$

$$\varepsilon M' = -Q \tag{1.31d}$$

$$\varepsilon Q' = (\lambda^2 ky - P)\cos\theta - MT \tag{1.31e}$$

$$T' = (\lambda^2 ky - P)\sin\theta + \varepsilon MQ \tag{1.31f}$$

The last equation (1.31f) can be replaced by

$$T = \sec\theta + \varepsilon Q\tan\theta \tag{1.31g}$$

Note that the first equation (1.31a) is not coupled with the rest and may be integrated after we solve a 4th order system (1.31b, c, d, e) for y, θ, M and Q, using (1.31g) to substitute for T.

The BC are extracted, in an obvious way, from (1.30a), (1.30b) or (1.30c). For instance, the simple support BC are

$$y(0) = y(1) = 0,\qquad M(0) = M(1) = 0$$

Also, for simplicity one can take $\lambda^2 k = P = 1$ in (1.31e).

When extension dominates bending, $\varepsilon \ll 1$ and boundary layers at $t = 0$ and at $t = 1$ appear in the solution. A first approximation to the solution corresponding to the boundary conditions (1.30a) which does not contain the boundary layers [they are, incidentally, of width $O(\sqrt{sec\ \theta_0})$] is given by the system

$$
\begin{aligned}
x_0' &= \cos\theta_0 \\
y_0' &= \sin\theta_0 \\
\theta_0' &= M_0 \\
M_0 &= (\lambda^2 k y_0 - P)\cos^2\theta_0 \\
Q_0 &= 0 \\
x_0(0) = 0, &\qquad y_0(0) = y_0(1) = 0
\end{aligned}
\tag{1.32}
$$

The BVP (1.32) is easy to solve numerically, whereas the full BVP (1.31) is not. □

Example 1.15 Semiconductors

One popular mathematical model for a semiconductor device in steady state consists of three second order differential equations. These are Poisson's equation for the potential ψ, a continuity equation for the electron current J_n, and a continuity equation for the hole current J_p. In one dimension they can be written as

$$\psi'' = \frac{q}{\varepsilon}(n-p-C(x)) \tag{1.33a}$$

$$J_n' = q\hat{R}(n,p) \qquad -l < x < l \tag{1.33b}$$

$$J_p' = -q\hat{R}(n,p) \tag{1.33c}$$

where n and p are the unknown electron and hole densities (of negative and positive charges, respectively), q, ε and l are known constants, $C(x)$ is a known doping profile function and $\hat{R}(n,p)$ is a given generation-recombination rate. The continuity equations (1.33b, c) become second-order ODEs for $n(x)$ and $p(x)$ upon use of the electron and hole current relations

$$J_n = q(D_n n' - \mu_n n \psi') \tag{1.33d}$$

$$J_p = -q(D_p p' + \mu_p p \psi') \tag{1.33e}$$

where D_n, D_p, μ_n and μ_p are additional diffusion and mobility functions, which we assume for simplicity to be known constants, satisfying $D_n/\mu_n = D_p/\mu_p = U_T$, with U_T a thermal voltage.

These ODEs for ψ, n and p are subject to boundary conditions

$$\psi(-l) = U_T \ln\frac{n_i}{p(-1)} + U \tag{1.33f}$$

$$\psi(l) = U_T \ln\frac{n(1)}{n_i} \tag{1.33g}$$

$$n(\pm l)p(\pm l) = n_i^2 \tag{1.33h}$$

$$n(\pm l) - p(\pm l) = C(\pm l) \tag{1.33i}$$

where U is the applied bias and n_i is an intrinsic number.

The BVP (1.33) is not well-scaled, because the doping profile may have values in a rather wide range, say $[-10^{14}, 10^{20}]$. Use of the scaling

$$D(x) := C(x)/\bar{C}, \qquad \bar{C} := \max|C(x)|, \qquad x := x/l, \qquad U := U/U_T$$

$$\lambda^2 := \frac{U_T \varepsilon}{l^2 \bar{C} q}, \qquad (\lambda > 0), \qquad \gamma := \frac{n_i}{\bar{C}}$$

and an appropriate scaling of the dependent variables gives

$$\lambda^2 \psi'' = n - p - D(x) \tag{1.34a}$$

$$(n' - n\psi')' = R(n,p) \tag{1.34b}$$

$$(p' + p\psi')' = R(n,p) \tag{1.34c}$$

One choice for R is the Shockley-Read-Hall term, which yields

$$R(n,p) = \frac{1}{4}\,\frac{np - \gamma^2}{n + p + 2\gamma} \tag{1.34d}$$

Typical values for the constants appearing in (1.34a, d) are $\lambda^2 = 0.4 \cdot 10^{-6}$, $\gamma = 10^{-7}$, and they can get as low as 10^{-10}. The BC are now

$$\psi(-1) = \ln \frac{\gamma}{p(-1)} + U, \qquad \psi(1) = \ln \frac{n(1)}{\gamma} \tag{1.34e}$$

$$n(\pm 1) p(\pm 1) = \gamma^2 \tag{1.34f}$$

$$n(\pm 1) - p(\pm 1) = D(\pm 1) \tag{1.34g}$$

In a typical situation, we may consider $D(x)$ to be piecewise smooth. Locations of discontinuities in the doping profile are called pn- or np- junctions. Since λ is small, we may expect that sharp layers develop in the solution near the junctions. However, it is important to note that these are essentially boundary-type layers, unlike those in Examples 1.17, 1.23, and 1.24 below. In particular, there are no turning points here, despite the appearance of internal layers (cf. Chapter 10). The location of these junction layers is known, and a simple transformation of the independent variable can be used to transform them to the boundary. Thus suppose, for simplicity, that there is one discontinuity in $D(x)$ at $x = 0$. Then we may transform $[-1, 0] \to [0, 1]$ by $x := -x$. This yields three second-order ODEs in addition to the original (1.34a, b, c), obtaining a BVP of order 12 on (0, 1), with a boundary layer at $x = 0$.

The BVP (1.34) may be cautiously treated as a singular perturbation problem (cf. Chapter 10), but note that the boundary values in (1.34e) slowly blow up when $\lambda \to 0$ (i.e., when $\bar{C} \to \infty$, which also implies $\gamma \to 0$).

Due to the special form of the continuity equations (1.34b, c), some special transformations can be applied, which have proven useful for both theoretical and practical purposes. One such transformation is

$$n = \gamma e^{\psi - \phi_n}, \qquad p = \gamma e^{\phi_p - \psi} \tag{1.35a}$$

The unknowns ϕ_n and ϕ_p replacing n and p are called (scaled) quasi-Fermi levels. This transformation yields in place of (1.34b, c),

$$\gamma (e^{\psi - \phi_n} \phi_n')' = R \tag{1.35b}$$

$$\gamma (e^{\phi_p - \psi} \phi_p')' = R \tag{1.35c}$$

The BVP in the new dependent variables turns out to have nicer properties for numerical approximation. A slight disadvantage is, however, that ϕ_n and ϕ_p do not appear linearly in (1.35b, c). A related transformation which yields linear forms (useful for analysis) is

$$n = \gamma e^{\psi} u, \qquad p = \gamma e^{-\psi} v \tag{1.36a}$$

This gives

$$(e^{\Psi}u')' = R \tag{1.36b}$$

$$(e^{-\Psi}v')' = R \tag{1.36c}$$

The latter transformation is not without fault either, because it turns out that u and v are not sufficiently well-scaled for numerical use, and overflow often occurs in (1.36a).

The BVP in any of the forms (1.34) or (1.35) is numerically difficult, but not extremely so. It becomes much more computationally challenging in several independent variables. □

Example 1.16 Electron-Irradiated Silicon

Here is another BVP from semiconductor theory,

$$\varepsilon n' = (n+\beta p)[\alpha n \tilde{f} - \sum_{i=1}^{N_A} \hat{f}_i - \sum_{j=1}^{N_D} \bar{f}_j] \tag{1.37a}$$

$$0 < x < 1$$

$$\varepsilon p' = (n+\beta p)[\alpha p \tilde{f} + \frac{1}{\beta}\sum_{i=1}^{N_A} \hat{f}_i + \frac{1}{\beta}\sum_{j=1}^{N_D} \bar{f}_j] \tag{1.37b}$$

$$n(0) = 1, \qquad p(1) = 0 \tag{1.37c}$$

Here $n(x)$ and $p(x)$ are as in the previous example and ε is a normalized current density. Values of interest for ε range from 1 to 10^{-12}. The functions and constants appearing on the right-hand sides of (1.37a, b) are given by

$$\tilde{f} = 1-n+p-\sum_{i=1}^{N_A} a_i(x)\frac{n+\alpha_i u_i}{n+v_i+\alpha_i(u_i+p)}+\sum_{j=1}^{N_D} d_j(x)\frac{z_j+\delta_j p}{n+z_j+\delta_j(y_j+p)} \tag{1.37d}$$

$$\hat{f}_i = \alpha_i A_i a_i(x)\frac{np-v_i u_i}{n+v_i+\alpha_i(u_i+p)} \qquad \bar{f}_j = \delta_j D_j d_j(x)\frac{np-y_j z_j}{n+z_j+\delta_j(y_j+p)} \tag{1.37e}$$

$$\beta = 1/3, \qquad N_A = 2, \qquad N_D = 1, \qquad \alpha = 0.05162 \tag{1.37f}$$

$$\alpha_i = \delta_j = 1, \qquad A_i = D_j = 2.222\cdot 10^{-3} \qquad \text{all } i, j$$

$$a_1(x) = 15, \qquad a_2(x) = 10, \qquad d_1(x) = 400$$

$$u_1 = 1.854\cdot 10^{-4}, \qquad u_2 = 0.1021, \qquad v_1 = 21.47, \qquad v_2 = 3.899\cdot 10^{-2}$$

$$y_1 = 2.902\cdot 10^3, \qquad z_1 = 1.371\cdot 10^{-6}$$

For ε small, this BVP has a boundary layer at $x = 0$ and an interior (turning point) layer near $x = 1$. □

Example 1.17 Shock Wave

Consider a shock wave in a one-dimensional nozzle flow. The steady state Navier-Stokes equations give

$$\varepsilon A(x)uu'' - [\frac{1+\gamma}{2} - \varepsilon A'(x)]uu' + u'/u + \frac{A'(x)}{A(x)}(1 - \frac{\gamma-1}{2}u^2) = 0 \quad 0 < x < 1 \tag{1.38a}$$

where x is the normalized downstream distance from the throat, u is a normalized velocity, $A(x)$ is the area of the nozzle at x, e. g., $A(x) = 1+x^2$, $\gamma = 1.4$, and ε is essentially the inverse of Reynolds number, e. g., $\varepsilon = 4.792\cdot 10^{-8}$. The BC are

$$u(0) = 0.9129 \qquad \text{(supersonic flow in throat)} \tag{1.38b}$$

$$u(1) = 0.375 \tag{1.38c}$$

Given its simple appearance, the BVP (1.38a, b, c) turns out to be a surprisingly difficult nut to crack numerically. An $O(\sqrt{\varepsilon})$-wide shock develops, whose location depends on ε. Singular-perturbation-type problems usually require a *continuation method* to solve them; i. e., the problem is solved successively for a decreasing sequence of values of ε, thereby permitting a methodical refinement of the solution profile (and adjustment of certain parameters of the numerical method). For this BVP, however, many ε-steps need to be taken. (This, of course, depends also on the particular numerical method used.) □

Example 1.18 Swirling Flow I

Consider the steady flow of a viscous, incompressible axisymmetric fluid ("swirling" flow) above an infinite rotating disk. Using a cylindrical coordinate system (r, ϕ, z), the disk is rotating at $z=0$ with angular velocity Ω, and the fluid has angular velocity $\gamma\Omega$ at $z=\infty$. Defining

$$x = \sqrt{\Omega/\nu}\, z$$

where ν is viscosity, we find that the Navier-Stokes equations yield by similarity transformation,

$$f''' + 2ff'' - (f')^2 + g^2 = \gamma^2 \tag{1.39a}$$

$$0 < x < \infty$$

$$g'' + 2fg' - 2f'g = 0 \tag{1.39b}$$

with the velocity field of the fluid given by $(\Omega r f'(x), \Omega r g(x), -2\sqrt{\nu\Omega} f(x))$. The BC are

$$f(0) = 0, \qquad f'(0) = 0, \qquad g(0) = 1 \tag{1.39c}$$

$$f'(\infty) = 0, \qquad g(\infty) = \gamma \tag{1.39d}$$

The task at hand is to find solutions to (1.39) as γ, called the Rossby number, varies. The value $\gamma=0$ is of particular interest.

It turns out that there are (possibly infinitely) many solutions to this problem for $\gamma=0$. To find many solutions to a BVP, parameter continuation techniques are used (see Chapter 8). □

Example 1.19 Swirling Flow II

We consider again a swirling flow over an infinite disk, but now the azymuthal velocity behaves like r^{-n} (so $n=-1$ corresponds to a solid body rotation and $n=1$ corresponds to a potential vortex) and a magnetic field is applied in the direction of the axis of rotation. The disk is stationary. The resulting BVP is

$$f''' + \tfrac{1}{2}(3-n)ff'' + n(f')^2 + g^2 - sf' = \gamma^2 \tag{1.40a}$$

$$0 < x < \infty$$

$$g'' + \tfrac{1}{2}(3-n)fg' + (n-1)gf' - s(g-1) = 0 \tag{1.40b}$$

$$f(0) = f'(0) = g(0) = 0, \quad f'(\infty) = 0, \quad g(\infty) = \gamma \tag{1.40c}$$

Note that the ODEs (1.39a, b) are a special case of (1.40a, b) with $n=-1$, $s=0$. Let us take $\gamma=1$. Whereas a numerical solution of (1.39) is not difficult to obtain (the difficulty there is of a different kind, namely, obtaining *many* solutions for $\gamma=0$), the BVP (1.40) becomes tough as $n \uparrow 1$ and $s \downarrow 0$. In fact, it can be shown that when $s = 0$ no solution exists for $n = 1$, and it is believed that no solution exists if $n > n_0 \approx 0.1217$.

Determining n_0, as well as solving (1.40) for values like $s = 0.05$, $n = 0.3$ lead to difficult numerical tasks. □

Example 1.20 Swirling Flow III

This time we consider the swirling flow between two rotating, coaxial disks, located at $x = 0$ and at $x = 1$. The BVP is

$$\varepsilon f'''' + f f''' + g g' = 0 \qquad (1.41a)$$

$$0 < x < 1$$

$$\varepsilon g'' + f g' - f' g = 0 \qquad (1.41b)$$

$$f(0) = f(1) = f'(0) = f'(1) = 0 \qquad (1.41c)$$

$$g(0) = \Omega_0, \qquad g(1) = \Omega_1 \qquad (1.41d)$$

where Ω_0, Ω_1 are the angular velocities of the infinite disks, $|\Omega_0| + |\Omega_1| \neq 0$, and ε is a viscosity parameter, $0 < \varepsilon \ll 1$. Thus we have an interesting singular perturbation problem, which becomes numerically difficult for ε small (say $\varepsilon \leq 10^{-4}$), i.e., for large Reynolds numbers. Multiple solutions are possible. Taking, e.g., $\Omega_1 = 1$, we obtain different cases for different values of Ω_0. If $\Omega_0 < 0$ (with a special symmetry when $\Omega_0 = -1$) then the disks are counter-rotating; if $\Omega_0 = 0$ then one disk is at rest, while if $\Omega_0 > 0$ then the disks are corotating. □

Example 1.21 Re-entry of a Space Vehicle

In this optimal control problem, a control $u(t)$ has to be chosen as a function of time t, to minimize the heating

$$\int_0^T 10\, v^3 \sqrt{\rho}\, dt$$

which a space vehicle experiences during the flight through the earth's atmosphere on the way back from outer space. In this functional, T is an unspecified final time, v is velocity and $\rho = \rho_0 e^{-\beta R \xi}$ is atmospheric density, $\rho_0 = 2.704 \cdot 10^3$, $R = 209$, $\beta = 4.26$. The minimization of the functional is subject to the equations of state

$$\frac{dv}{dt} \equiv \dot{v} = -s \rho v^2 C_D(u) - \frac{g \sin \gamma}{(1+\xi)^2} \qquad (1.42a)$$

$$\dot{\gamma} = s \rho v C_L(u) + \frac{v \cos \gamma}{R(1+\xi)} - \frac{g \cos \gamma}{v(1+\xi)^2} \qquad (1.42b)$$

$$\dot{\xi} = \frac{v \sin \gamma}{R} \qquad (1.42c)$$

$$v(0) = 0.36, \qquad \gamma(0) = -8.1 \cdot \pi/180, \qquad \xi(0) = 4/R \qquad (1.42d)$$

$$v(T) = 0.27, \qquad \gamma(T) = 0, \qquad \xi(T) = 2.5/R \qquad (1.42e)$$

where γ is the flight-path angle, ξ is a normalized altitude, $s = 26{,}600$, $g = 3.2172 \cdot 10^{-4}$, $C_D(u) = 1.174 - 0.9 \cos u$, $C_L(u) = 0.6 \sin u$.

To solve the optimization problem we use three adjoint variables (Lagrange multipliers) λ_v, λ_γ and λ_ξ (which are functions of t) and form the Hamiltonian

$$H = 10v^3\sqrt{\rho} + \lambda_v\dot{v} + \lambda_\gamma\dot{\gamma} + \lambda_\xi\dot{\xi}$$

where for $\dot{v}$, $\dot{\gamma}$ and $\dot{\xi}$ we use the right-hand sides of (1.42a, b, c). Then by calculus of variations we have the ODEs

$$\dot{\lambda}_v = -\frac{\partial H}{\partial v} \tag{1.42f}$$

$$\dot{\lambda}_\gamma = -\frac{\partial H}{\partial \gamma} \tag{1.42g}$$

$$\dot{\lambda}_\xi = -\frac{\partial H}{\partial \xi} \tag{1.42h}$$

and a terminal BC

$$H = 0 \qquad \text{at } t = T \tag{1.42i}$$

In (1.42) we have a *free* BVP (free flight time T) with 6 ODEs and 7 BC. To obtain the problem in standard form we can transform the independent variable

$$x = t/T$$

and treat T as another dependent variable, adding the ODE

$$\frac{dT}{dx} \equiv T' = 0 \tag{1.43a}$$

Using the already defined right-hand sides we write the remaining equations of the BVP as

$$v' = \dot{v}T, \qquad \gamma' = \dot{\gamma}T, \qquad \xi' = \dot{\xi}T \tag{1.43b}$$

$$\lambda_v' = \dot{\lambda}_vT, \quad \lambda_\gamma' = \dot{\lambda}_\gamma T, \quad \lambda_\xi' = \dot{\lambda}_\xi T \tag{1.43c}$$

The BVP is then the ODEs (1.43) subject to the BC (1.42d, e, i) (with $x = 1$ replacing $t = T$).

The numerical difficulty in this problem is of a somewhat different character than that of the previous example. Here there is no strong singular perturbation feature, however the nonlinear problem is sensitive. Convergence of a numerical technique using some variant of Newton's method can be expected only if the initial iterate (i. e., an initial solution profile which a user has to guess in a — we hope — educated way) is fairly close to the solution. □

Example 1.22 Optimal Harvesting

This problem arises in the optimal harvesting of a randomly fluctuating resource. The objective is to choose a harvesting effort function $y = y(x)$, $y_- \le y \le y_+$, so as to maximize the present value, $v(x)$, of the resource. The maximum principle gives that

$$y(x) = \begin{cases} y_- & n(x) < v'(x) \\ y_+ & n(x) > v'(x) \end{cases} \tag{1.44a}$$

where, e. g., $n(x) = e^x$. The present value v satisfies

$$\varepsilon v'' + (f(x) - y(x))v' - \gamma v + n(x)y(x) = 0 \qquad -\infty < x < \infty \tag{1.45a}$$

where $f(x) = 1 - e^x$ and the discount rate γ is a parameter, $0<\gamma<1$. The BC for (1.45a) are that the solution v be bounded as $|x| \to \infty$.

The problem may at a first glance look linear, but in fact it is not, because even though the values of $y(x)$ are known, the *switching points* s, where

$$n(s) = v'(s) \tag{1.44b}$$

are not. Assume further that there is only one switching point s and that $-\infty < y_- < y_+ < \infty$ (other cases may be similarly treated). Then the BC are

$$(f(-L)-y_-)v'(-L) - \gamma v(-L) + n(-L)y_- = 0 \tag{1.45b}$$

$$(f(L)-y_+)v'(L) - \gamma v(L) + n(L)y_+ = 0 \tag{1.45c}$$

with $L > 0$, sufficiently large (e. g., $L = 10$).

One may attempt to solve the BVP (1.45a, b, c) numerically, but this is not simple because of the jump in $y(x)$ at the unknown point s (where v and v' are continuous!). Thus, it is preferable to transform s to a known location, say 0,

$$x := x - s$$

This yields

$$\varepsilon v'' + (f(x+s)-y)v' - \gamma v + n(x+s)y = 0 \tag{1.46a}$$

$$y = \begin{cases} y_- & x < 0 \\ y_+ & x > 0 \end{cases} \tag{1.46b}$$

$$s' = 0 \tag{1.46c}$$

$$v'(0) = n(s(0)) \tag{1.46d}$$

and (1.45b, c). The obtained three-point BVP may now be solved, e.g. by a finite difference technique with a mesh point at $x = 0$ (cf. Chapter 5). It is not very difficult anymore.

□

Example 1.23 Spherical Shells

Consider a homogeneous, isotropic, thin spherical shell of constant thickness, subject only to an axisymmetric normal distributed surface load. With ξ the angle between the meridional tangent at a point of the midsurface of the undeformed shell and the base plane, ϕ the meridional angle change of the deformed middle surface, $\beta = \xi - \phi$, and ψ a stress function, the following BVP governs the deformation elastostatics of the shell,

$$\mu[\psi'' + \cot\xi\,\psi' + (\nu - \cot^2\xi)\psi] - \frac{1}{\sin\xi}(\cos\beta - \cos\xi) \tag{1.47a}$$

$$= \mu[\nu P' + (1+\nu)P\cot\xi - \frac{1}{\sin\xi}(\gamma\sin^2\xi)' - \nu\gamma\cos\xi] \qquad 0 \le \xi \le \pi/2$$

$$\varepsilon^4/\mu[\phi'' + \cot\xi\,\phi' + \frac{\cos\beta}{\sin^2\xi}(\sin\beta - \sin\xi) - \frac{\nu}{\sin\xi}(\cos\beta - \cos\xi)] + \frac{\sin\beta}{\sin\xi}\psi = \frac{\cos\beta}{\sin\xi}P \tag{1.47b}$$

$$\phi(0) = \psi(0) = \phi(\pi/2) = \psi(\pi/2) = 0 \tag{1.47c}$$

Here

$$P(\xi) = -\int_0^{\xi}(1 - \delta\sin\eta)\cos\beta\,\sin\eta\,d\eta, \qquad \gamma = -\sin\beta(1 - \delta\sin\xi)$$

and $\delta > 1$ a constant, say $\delta = 1.2$ (we have assumed a particular load distribution). Also $\nu = 0.3$ is a typical value.

To evaluate $P(\xi)$ we introduce the simple trick of incorporating it as another ODE and BC

$$P' = -(1 - \delta \sin \xi)\cos \beta \sin \xi \tag{1.47d}$$

$$P(0) = 0 \tag{1.47e}$$

The BVP (1.47) is now in standard form.

The parameters ε and μ are positive and small (they relate to the thickness vs radius of the shell). The solution sought has an interior layer in ϕ (i.e., a narrow region in ξ, away from the boundaries, where ϕ varies fast), corresponding to a *dimpling* of the spherical shell.

Numerically, the problem gets tougher as ε and μ get smaller. Some representative (ε, μ)-values for which the problem is fairly difficult are (0.01, 0.0001), (0.001, 0.001), (0.0001, 0.01). □

Example 1.24 Shallow Cap Dimpling

This is another example from the theory of shells of revolution. The ODEs are

$$\varepsilon^2 [\psi'' + \frac{1}{x}\psi' - \frac{1}{x^2}\psi] - \frac{1}{x}\phi(\phi_0 - \frac{1}{2}\phi) = 0 \tag{1.48a}$$

$$0 < x < 1$$

$$\varepsilon^2 [\phi'' + \frac{1}{x}\phi' - \frac{1}{x^2}\phi] + \frac{1}{x}\psi(\phi_0 - \phi) = 2\kappa P(x) \tag{1.48b}$$

with ϕ and ψ essentially as in the previous example; $\phi_0(x)$ is ϕ of the undeformed shell (for a spherical shell $\phi_0(x) = x$, but consider also $\phi_0(x) = x^m$, $m = 2, 3$), and

$$P(x) = x(1 - \gamma + \frac{\gamma}{2}x^2)$$

$\gamma = 1.2$, $\nu = 0.3$, $\kappa = 1$. The BC are

$$\phi(0) = \psi(0) = 0, \qquad \phi(1) = \psi'(1) - \nu\psi(1) = 0 \tag{1.48c}$$

As in the previous example, the BVP gets tough as ε gets small, and an interior layer (corresponding to dimpling) forms in a solution for ϕ. There is an additional boundary layer at $x = 1$, and more than one solution exist. The value $\varepsilon = 10^{-4}$ (which gives a rather thin shell) yields a challenging numerical problem. □

Example 1.25 Burner-Stabilized Flame

A simple, two-stage, unimolecular, one-dimensional flame may be represented by the mechanism

$$Y_r \rightarrow Y_i \rightarrow Y_p$$

Here Y_r and Y_i are the mass fraction concentrations of the reactant and intermediate, respectively. The product concentration Y_p is determined from conservation of mass by

$$Y_p = 1.0 - Y_r - Y_i$$

After appropriate coordinate transformations and nondimensionalizations, the system can be described under steady-state conditions by the BVP

$$M_0 \frac{dY_r}{dx} = \frac{1}{Le_r} \frac{d^2Y_r}{dx^2} - k_{ri} Y_r \exp(-E_r/T) \tag{1.49a}$$

$$M_0 \frac{dY_i}{dx} = \frac{1}{Le_i} \frac{d^2Y_i}{dx^2} + k_{ri} Y_r \exp(-E_r/T) - k_{ip} Y_i \exp(-E_i/T), \qquad 0 < x < \infty \tag{1.49b}$$

$$M_0 \frac{dT}{dx} = \frac{d^2T}{dx^2} + k_{ri}(h_r - h_i) Y_r \exp(-E_r/T) + k_{ip} h_i Y_i \exp(-E_i/T) \tag{1.49c}$$

$$Y_r(0) - \frac{1}{M_0 Le_r} \frac{dY_r}{dx}(0) = \varepsilon_r \tag{1.49d}$$

$$Y_i(0) - \frac{1}{M_0 Le_i} \frac{dY_i}{dx}(0) = \varepsilon_i \tag{1.49e}$$

$$T(0) = T_0 \tag{1.49f}$$

$$\frac{dY_r}{dx}(\infty) = \frac{dY_i}{dx}(\infty) = \frac{dT}{dx}(\infty) = 0 \tag{1.49g}$$

where T denotes the temperature. Typical values for the problem constants are as follows: the preexponential constants $k_{ri} = 5 \times 10^8$ and $k_{ip} = 10^2$, the activation energies $E_r = 80$ and $E_i = 10$, the Lewis numbers $Le_r = 0.75$ and $Le_i = 1.25$, the specific enthalpy differences between the reactant and the product $h_r = 4.4$ and between the intermediate and product $h_i = 4.5$, the mass flux fractions $\varepsilon_r = 1$ and $\varepsilon_i = 0$, the burner temperature $T_0 = 1.25$, and the initial mixture flow rate $M_0 = 0.985$. Quantities such as the thermal conductivity and the specific heat capacity do not appear explicitly in the model, because they are contained in the other nondimensionalized variables. In practice the solution domain is truncated at a large value of $x = L$ such that the zero gradient boundary conditions are "satisfied" (cf. Section 11.4.2); for the given parameter values, $L = 10$ is sufficient.

Asymptotic analyses of this reaction-diffusion system can be performed and resulting analytical expressions for the flame velocity and species concentrations obtained for various values of activation energies, preexponential constants, and Lewis numbers. Although the three-species model is rather schematic and has limited ability to account for the behavior of real complex flames, it still contains terms that represent the main processes occurring in larger, many-species, reaction-diffusion systems. □