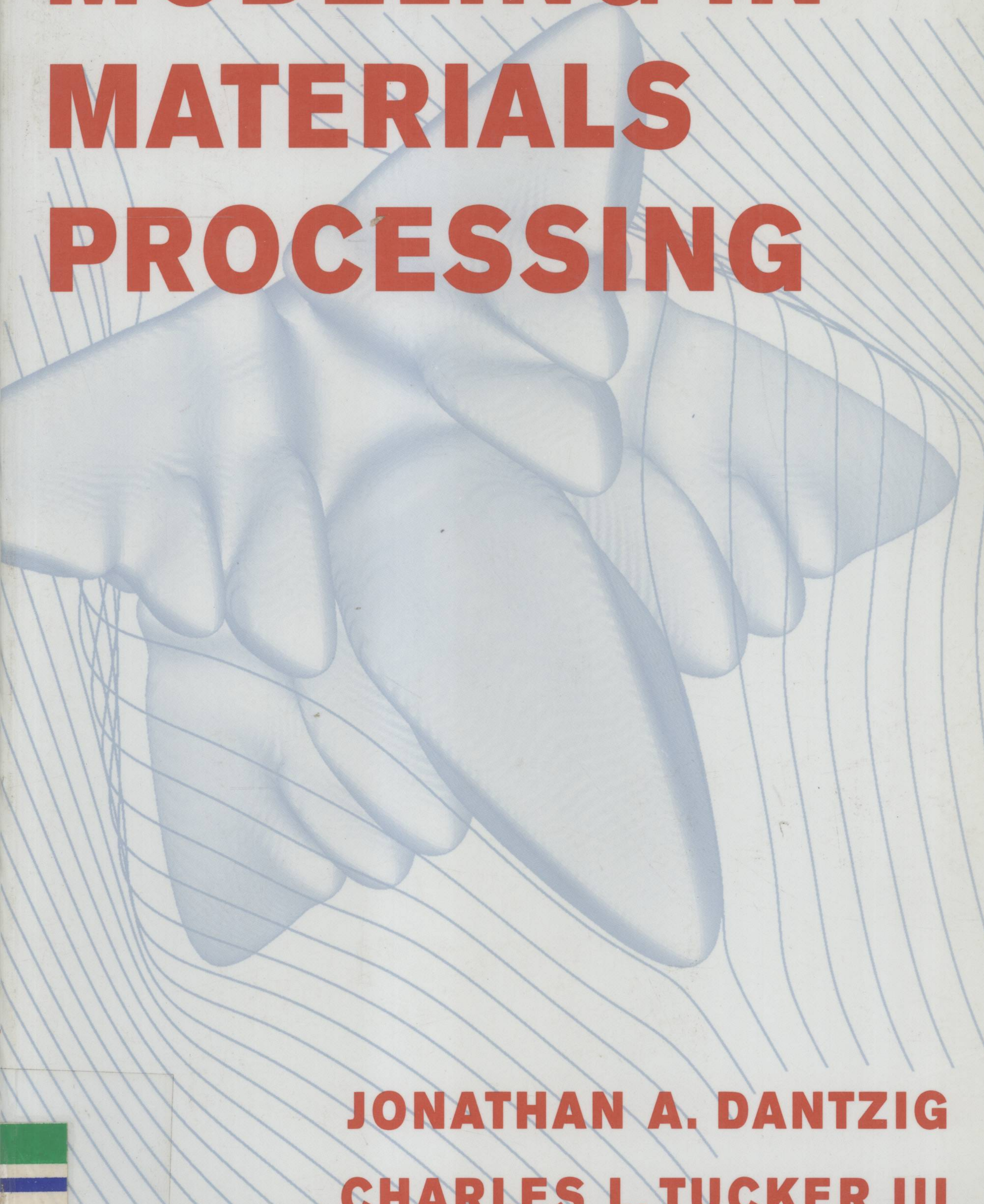
MODELING IN MATERIALS PROCESSING



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MODELING IN MATERIALS PROCESSING

Mathematical modeling and computer simulation have been widely embraced in industry as useful tools for improving materials processing. Although courses in materials processing have covered modeling, they have traditionally been devoted to one particular class of materials, that is, polymers, metals, or ceramics. This text offers a new approach, presenting an integrated treatment of metallic and nonmetallic materials. The authors show that a common base of knowledge – specifically, the fundamentals of heat transfer and fluid mechanics – provides a unifying theme for these seemingly disparate areas. Emphasis is placed on understanding basic physical phenomena and knowing how to include them in a model. Thus, chapters explain how to decide which physical phenomena are important in specific applications, and how to develop analytical models. A unique feature is the use of scaling analysis as a rational way to simplify the general governing equations for each individual process. The book also treats selected numerical methods, showing the relationship among the physical system, analytical solution, and the numerical scheme. A wealth of practical, realistic examples are provided, as well as homework exercises. Students, and practicing engineers who must deal with a wide variety of materials and processing problems, will benefit from the unified treatment presented in this book.

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Preface

After some years of teaching separate courses on metal solidification and polymer processing, we realized that the two subjects shared a substantial base of common material. All the models started with the same basic equations and were built by using the same general procedure. We began to teach a single course on materials processing, and we found that our unified treatment gave students a better overall perspective on modeling. We also discovered that we needed a new book, as existing texts were almost all devoted exclusively to polymers, or to metals, or to ceramics. In this book, we treat metal and polymer processing problems together, building around the transport equations as a unifying theme.

We were also dissatisfied with ad hoc model development, in which terms were arbitrarily dropped from the governing equations, or simplifications were made without a clear explanation. Simplifying the general governing equations is a critical step in modeling, but it is a skill, not an art. In this text we introduce scaling analysis as a systematic way to reduce the governing equations for any particular problem. Scaling provides a way for both novices and experts to simplify a model, while ensuring that all of the important phenomena are included.

After deriving the governing equations in their general form and introducing scaling analysis, we examine physical phenomena such as heat conduction and fluid flow. We work out many problems that include only a few of these phenomena – problems that can be solved analytically. One might call these "canonical problems." They allow the reader to study each phenomenon in isolation, and then to explore how that phenomenon interacts with others. Real processes frequently involve multiple physical phenomena, and the ability to isolate a single phenomenon and understand its role is one of the great benefits of modeling. Canonical problems help students place different phenomena in perspective, and give them the ability to anticipate which phenomena will be important in any particular process. We once overheard a student describe our materials processing course as "the place where you finally understand what they taught you in heat transfer and fluid mechanics." We hope so.

We present examples for many different materials and processes, including polymer extrusion and injection molding, as well as metal casting and microstructure development. In each example we begin with the governing equations, and we use scaling to arrive at the final set of equations to be solved. This systematic approach makes problems for many different materials accessible.

Of course, most practical materials processing models require a numerical solution, and any accomplished modeler knows a great deal about numerical methods. We chose not to say much about numerical methods, preferring to give solid coverage to the governing equations and physical phenomena. However, our canonical problems provide excellent test cases for numerical solution methods, and we use them to demonstrate some of the pitfalls of numerical modeling. By showing examples in which numerical schemes may be inaccurate or unstable, we help the reader become a more intelligent user of modeling software.

There is a lot to learn here, and many of the exercises at the end of each chapter go beyond the examples in the chapter. These exercises are written in a way that guides the student through the problem, step by step. This style emphasizes the overall pattern of problem solving, and it allows students to do more complex problems than they could otherwise attempt. A full set of solutions is available to instructors who adopt the book as a course text. Please contact the authors for the Solutions Manual.

We started writing this book to distill the important lessons from our own experience, one of us in polymer processing and the other in metal solidification. We eventually found that knowing more about modeling of all types of materials made us better at modeling the materials and processes we were so familiar with. We hope you will have the same experience.

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November 1, 2000

Principal Nomenclature

Symbol	*Quantity Represented*
A	area
a	parameter in exponential model for temperature-dependent viscosity
$\mathbf{b}$	vector of body force per unit mass
C_A	mass fraction of species A
C_ℓ	mass fraction of solute in liquid
C_s	mass fraction of solute in solid
$\hat{C}_A$	concentration (mass per unit volume) of species A
c_0, c_1, etc.	constants of integration
c_p	specific heat at constant pressure
c_v	specific heat at constant volume
D	mass diffusivity of solute; diameter
D_{AB}	intrinsic mass diffusivity of species A in B
$\tilde{D}$	interdiffusion coefficient of species A in B
$\mathbf{D}$	rate-of-deformation tensor $= (\mathbf{L} + \mathbf{L}^T)/2$
E	internal energy of a system
E_η, E_D	activation energies for viscosity, diffusion
$\mathbf{e}_1, \mathbf{e}_x$, etc.	unit vectors
$\mathbf{F}$	deformation gradient tensor, $F_{ij} = \partial X_i / \partial x_j$
f_ℓ	mass fraction of liquid
f_s	mass fraction of solid
g	acceleration that is due to gravity $= 9.82$ m/s^2
G	temperature gradient; magnitude of pressure gradient
h	heat transfer coefficient; height above a reference level; half-gap height
H	gap height; specific enthalpy
$\mathbf{I}$	unit tensor (identity tensor); the ij component is δ_{ij}
I_D, II_D, III_D	scalar invariants of the tensor $\mathbf{D}$
i	$\sqrt{-1}$
$\mathbf{J}_A$	mass fraction flux for species A, equal to $\hat{\mathbf{J}}_A/\rho$
$\hat{\mathbf{J}}_A$	mass flux vector for species A (mol/area $\times$ time)
J	Jacobian $= \det \mathbf{F}$

J_0, J_1	Bessel functions of the first kind, of order zero and one
$\mathbf{k}$	thermal conductivity (tensor)
k	thermal conductivity (scalar)
k_0	partition coefficient
L	length
L_d	primary dendrite arm length
L_f	latent heat of fusion
L_p	latent heat of pressure change
L_v	latent heat of volume change
$\mathbf{L}$	velocity gradient tensor, $L_{ij} = \partial v_i / \partial x_j$
ℓ	filled length of a mold
m	material constant in the power law model
m_ℓ, m_S	slopes of the liquidus and solidus lines
M	mass of a system; morphological number
n	power law index
$\mathbf{n}$	unit vector normal to a surface
P	power input to a system
p	pressure
$\hat{p}$	modified pressure $= p + \rho_0 g h$
$\mathbf{q}$	heat flux vector
Q	volume flow rate; power of a point heat source; heat input to a system
$\mathbf{Q}$	rotation matrix
R	radius; gas constant = 8.31 J/mol K
$\dot{R}$	specific heat generation rate
R_A	generation rate of species A
$\mathcal{R}$	thermal resistance
r, θ, z	cylindrical coordinates
r, θ, ϕ	spherical coordinates
S	bounding surface; specific entropy; flow conductance
s	inverse of power law index $= 1/n$
T	temperature; torque
T_m	melting temperature
T_L	liquidus temperature
T_S	solidus temperature
t	time
$\mathbf{t}$	surface traction vector
$\hat{\mathbf{t}}$	unit vector tangent to a curve
$\mathbf{v}$	velocity vector
V	volume; average velocity
$\hat{V}$	specific volume
W	width
$\mathbf{W}$	vorticity tensor $= (\mathbf{L} - \mathbf{L}^T)/2$
$\mathbf{X}$	material coordinate vector
$\mathbf{x}$	position vector
x, y, z	Cartesian coordinates; also x_1, x_2, x_3

α	thermal diffusivity = $k/(\rho c_p)$
β	volumetric thermal expansion coefficient
Γ	surface tension (interfacial tension)
$\dot{\gamma}$	scalar strain rate = $(2\mathbf{D} : \mathbf{D})^{1/2}$
δ	solidified layer thickness; boundary layer thickness
δ_{ij}	unit tensor in indicial notation (the Kronecker delta)
ε	specific internal energy
ϵ_{ijk}	permutation symbol
κ	curvature of a curve; ratio of an outer radius to inner radius
κ_m, κ_G	mean and Gaussian curvatures of a surface
Λ	magnitude of the pressure gradient
λ	dilatational viscosity, compressible Newtonian fluid
λ_2	secondary dendrite arm spacing
μ	viscosity, Newtonian fluid
ν	kinematic viscosity = μ/ρ
η	viscosity, non-Newtonian fluid
π	3.14159...
ρ	density
ρ_0	density at reference temperature and pressure
θ	dimensionless temperature; angular coordinate
$\boldsymbol{\sigma}$	total stress tensor
$\boldsymbol{\tau}$	extra stress tensor
τ	scalar magnitude of $\boldsymbol{\tau}$
τ_Y	yield stress
Ω	angular velocity
$\boldsymbol{\omega}$	vorticity vector = $\nabla \times \mathbf{v}$
ξ	scaled length within a boundary layer
ζ	similarity variable

Contents

CHAPTER ONE

Introduction

1.1 WHAT IS A MODEL?

In recent years, modeling has been embraced by the materials processing community as a tool for understanding and improving manufacturing processes. Models are often implemented in computer programs, but there are important differences between a model and the computer code that implements it. A model is a set of equations used to represent a physical process. Finite element or finite difference methods, and the computer programs that implement them, are techniques to *solve* the equations of the model, but they are not the model itself. Our main emphasis will be on creating models – on reducing a physical process to a set of equations – especially models whose solution accurately describes the behavior of the process. Occasionally we also will explore numerical solution methods, often to point out where unenlightened use can lead you astray.

Whenever we create a model, we make assumptions about what phenomena are important to the behavior of the physical process. This is both good and bad. Assumptions help define the mathematical model and make it amenable to analysis. However, incorrect assumptions and erroneous information become part of the model and may well distort the results. Sometimes assumptions greatly simplify the model and permit an easy solution, but they may also cause important physical phenomena to be misrepresented or overlooked. Limiting the number of assumptions helps to avoid this problem but may make the model overly complex. Then the solution becomes difficult, and important information may be obscured. Building a good model requires making careful and informed decisions about the assumptions.

In this book we describe a systematic approach to modeling. We start from the physical system and proceed through mathematical formulation to solution of the model equations. We pay particular attention to the issue of choosing what assumptions to make. Our goal is to ensure that the reduction of the physical system to a mathematical model is done correctly. We present the task of modeling as a series of steps.

1. Define the scope and goals of the model.
2. Make a conceptual sketch and define basic quantities.
3. Develop a mathematical description of the conceptual sketch.
4. Write fundamental equations that govern the primary variables.

5. Introduce constitutive relations between the primary variables.
6. Reduce the governing equations by making assumptions.
7. Scale the variables and governing equations.
8. Solve the remaining equations to infer the behavior of the system.

In the following sections we present two simple examples to illustrate this stepwise approach. The first example is a physical system whose mathematical model should be quite familiar to the reader: a simple pendulum. The second example, a model of traffic flow, examines a familiar physical situation, but it develops a mathematical representation that will be new to most readers. These two problems provide concrete examples of the overall approach, but they are simple enough to be easily followed. In later chapters we apply this same stepwise approach to problems in materials processing.

1.2 A SIMPLE PENDULUM

Consider the simple pendulum, constructed by connecting a mass to one end of a string and fixing the string at its opposite end. We will now construct a mathematical model of this system, following the procedure outlined above.

Step 1: Define the scope and goals of the model. The physical system is, of course, the pendulum. Defining the goals is not as easy as it might seem, because this requires us to decide what aspects of the system behavior are most important – at least to us. Let us assume that we are going to use this pendulum as a timepiece, so we are interested in computing its period of oscillation. Other aspects of the motion are secondary.

Step 2: Make a conceptual sketch and define basic quantities. A sketch of the pendulum is shown in Fig. 1.1. The figure defines some quantities that we will use to analyze the system. The suspended mass is m, and gravitational acceleration g is oriented vertically down the page. The distance from the fixed end of the string to the center of the mass is r, and we introduce the variable θ to represent the angular position of the pendulum at any time t. Note that m and g are *parameters* of the

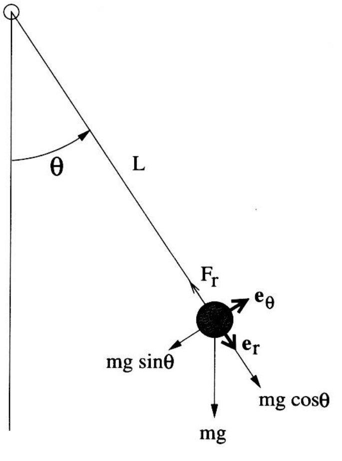

Figure 1.1: Conceptual sketch of a simple pendulum, showing forces and primitive variables; $\mathbf{e}_r$ and $\mathbf{e}_\theta$ are the unit vectors in the r and θ directions.

problems (i.e., they are constant for any specific pendulum), whereas r and θ are *variables*, because they may change as a function of time t; t itself is an independent variable.

Step 3: Develop a mathematical description of the conceptual sketch. As shown in Fig. 1.1, a force due to gravity with magnitude mg acts on the mass. It is convenient to resolve this force into radial and tangential components, as shown in the figure. The tension in the string also exerts a force, which has only a radial component F_r. We also will need the acceleration of the mass in terms of r, θ, and their derivatives. If both r and θ change with time, then the radial component of acceleration is $\ddot{r} - r\dot{\theta}^2$, and the tangential component is $r\ddot{\theta} + 2\dot{r}\dot{\theta}$; the dots indicate ordinary time derivatives.

Step 4: Write fundamental equations that govern the primary variables. We know that the motion of the mass will be governed by Newton's law, $\mathbf{f} = m\mathbf{a}$. We resolve the forces and accelerations into their r and θ components, and we get two equations:

$$\begin{aligned} m(\ddot{r} - r\dot{\theta}^2) &= mg\cos\theta - F_r \\ m(r\ddot{\theta} + 2\dot{r}\dot{\theta}) &= -mg\sin\theta \end{aligned} \tag{1.1}$$

We also need initial conditions on r, θ, and their first derivatives. For the moment we will just write the conditions for θ and $\dot{\theta}$, which we choose as

$$\begin{aligned} \theta(t = 0) &= \theta_0 \\ \dot{\theta}(t = 0) &= 0 \end{aligned} \tag{1.2}$$

The initial angle θ_0 is an additional parameter in the problem.

Step 5: Introduce constitutive relations between the primary variables. The governing equations are sufficient in this problem, and this step is not necessary. We will take it up in the next example.

Step 6: Reduce the governing equations by making assumptions. There are many reasons for making assumptions, each having its own inherent advantages and dangers. We will indicate some of these as we make various assumptions.

In fact, we have already made two important assumptions implicitly. Let us now state them explicitly.

- The mass of the string is negligible and the mass is concentrated at a point. The analysis is simplified because now we need only consider a point mass, and we can neglect such factors as the moment of inertia of the mass and string, and their angular acceleration. (A different model that includes these factors, called the *physical pendulum*, is well known.) Bear in mind, however, that we have introduced attributes into the model that may not necessarily match those of the real system.
- Friction has been neglected. Thus, our model represents a perpetual motion machine. Friction does play a role in determining the period of the pendulum, a phenomenon explored in one of the exercises.

We will now further assume that the string has constant length (independent of the tension F_r), so that $r = L$ for all time. Note that L is now another parameter of the problem. In the second of Eqs. (1.1), we replace r by the constant L and set $\dot{r} = 0$, which allows us to compute $\theta(t)$. The first of Eqs. (1.1) reduces to an equation to determine F_r once θ and $\dot{\theta}$ are known. The assumption of constant r reduces the dimensionality of the problem, greatly simplifying the solution. However, it further restricts the range of validity of our model.

Finally, we will limit our attention to small motions of the pendulum, that is, to small values of the angle θ. When using words like "small," one must define them carefully in the context of the present problem. Here we define small as that range of angles in which $\sin\theta \simeq \theta$. The error associated with this approximation is less than 1% for angles up to 14°. This assumption also greatly simplifies the problem, because the remaining equation is now linear:

$$L\ddot{\theta} = -g\theta \tag{1.3}$$

We have finally obtained an equation we can easily solve. Notice how simple our model of the pendulum has become in comparison to the real system.

Step 7: Scale the variables and governing equations. To *scale* a variable, one divides the variable by its characteristic value, expressed in terms of the parameters of the problem. This produces a new, dimensionless variable whose order of magnitude is one. For example, the angle θ has a characteristic value θ_0. Using this, we define a dimensionless variable ϕ as

$$\phi = \frac{\theta}{\theta_0} \tag{1.4}$$

Note that θ, while dimensionless, was not scaled to be of order one. The new variable ϕ is order one because, in the absence of external forces, $\phi \in [-1, 1]$.

The reasons for scaling and the methods for doing it will be discussed in Chapter 3. For the time being let us simply accept that it is convenient if all of the variables in the governing equation have been scaled to eliminate their dimensions and to make them of order one.

We also need to scale the time variable, though it is not obvious how to get a time scale from the problem parameters. We can deduce the time scale by going ahead and defining a scaled time variable τ as

$$\tau = \frac{t}{t_c} \tag{1.5}$$

where t_c is a characteristic time whose value we do not yet know. That is, we choose to measure time in units that are somehow related to our model system, but we still need to find how t_c depends on the known parameters of the problem.

Next we scale the governing equation by recasting it in terms of the scaled variables. Applying the chain rule for differentiation shows that

$$\frac{d}{dt} = \frac{d}{d\tau}\frac{d\tau}{dt} = \frac{1}{t_c}\frac{d}{d\tau} \tag{1.6}$$

Similarly, the second derivative is

$$\frac{d^2}{dt^2} = \frac{1}{t_c^2}\frac{d^2}{d\tau^2} \tag{1.7}$$

Substitution of this expression into Eq. (1.3) transforms the governing equation to

$$\left(\frac{L}{g}\right)\left(\frac{1}{t_c^2}\right)\frac{d^2\phi}{d\tau^2} = -\phi \tag{1.8}$$

Now because ϕ is of order one, the right-hand side of Eq. (1.8) is of order one, and thus the left-hand side of Eq. (1.8) side must be of order one as well. Because τ is of order one, we expect that $d^2\phi/d\tau^2$ on the left-hand side also will be of order one. The only way this can be true is for the collection of parameters on the left-hand side of Eq. (1.8) to equal one. From this we deduce that the characteristic time is

$$t_c = \sqrt{L/g} \tag{1.9}$$

This gives the characteristic value t_c in terms of known parameters L and g. Now all of our scaled variables are clearly defined, and the governing equation, Eq. (1.8), simplifies to

$$\frac{d^2\phi}{d\tau^2} = -\phi \tag{1.10}$$

Note that scaling has given us an estimate for the period for the pendulum, without ever solving a differential equation. This is one of the many benefits of scaling analysis.

The boundary conditions must also be scaled. Following the same procedure, we find that Eqs. (1.2) become

$$\begin{aligned} \phi(\tau = 0) &= 1 \\ \frac{d\phi}{d\tau}(\tau = 0) &= 0 \end{aligned} \tag{1.11}$$

Step 8: Solve the remaining equations to infer the behavior of the system. The solution of Eq. (1.10) is given by

$$\phi(\tau) = c_1 \sin\tau + c_2 \cos\tau \tag{1.12}$$

The two constants c_1 and c_2 are evaluated from the initial conditions, Eqs. (1.11). This gives the solution, in terms of the scaled dimensionless variables, to be

$$\phi = \cos\tau \tag{1.13}$$

If desired, one can substitute Eqs. (1.4) and (1.5) into Eq. (1.13) to express the solution in dimensional form.

$$\frac{\theta}{\theta_0} = \cos\left(\frac{t}{\sqrt{L/g}}\right) \tag{1.14}$$

Inspecting these equations shows that our *model* of the simple pendulum undergoes a simple harmonic motion of period $\tau = 2\pi$, or $t = 2\pi\sqrt{L/g}$. This is the result we were looking for.

At this point one might go back over the analysis, consider the validity of the various assumptions, and explore the sensitivity of the results to those assumptions. Usually this requires constructing and solving a new model without the assumptions, and comparing the results to the original model. The exercises at the end of