CHAPTER

1

Modeling and Mathematical Concepts

A system is a big black box
Of which we can't unlock the locks,
And all we can find out about
Is what goes in and what comes out.
—*Kenneth Boulding*

Kenneth Boulding—presumably somewhat tongue-in-cheek—expresses the cynic's view of systems. But this description will only be true if we fail as modelers, because the whole point of models is to provide illumination; that is, to give insight into the connections and processes of a system that otherwise seems like a big black box. So we turn this view around and say that Earth's systems may each be a black box, but a well-formulated model is the key that lets you unlock the locks and peer inside.

There are many different types of models. Some are purely conceptual, some are physical models such as in flumes and chemical experiments in the lab, some are stochastic or structure-imitating, and some are deterministic or process-imitating. The distinction also can be made between forward models, which project the final state of a system, and inverse models, which take a solution and attempt to determine the initial and boundary conditions that gave rise to it. All of the models described in this book are deterministic, forward models using variables that are continuous in time and space. One should think of the models as physical–mathematical descriptions of temporal and/or spatial changes in important geological variables, as derived from accepted laws, theories, and empirical relationships. They are "devices that mirror nature by embodying empirical knowledge in forms that permit (quantitative) inferences to be derived from them" (Dutton, 1987). The model descriptors are the conservation laws, laws of hydraulics, and first-order rate laws for material fluxes that predict future states of a system from initial conditions (ICs), boundary conditions (BCs), and a set of rules. For a given set of BCs and ICs, the model will always "determine" the same final state. Furthermore, these models are mathematical (numerical). We emphasize this type of model over other types because it represents a large proportion of extant models in the earth sciences. Dynamical models also provide a good vehicle for teaching the art of modeling. We call modeling an art because one must know what one wants out of a model and how to get it. Properly constructed, a model will rationalize the information coming to our senses, tell us what the most important data are, and tell us what data will best test our notion of how nature works as it is embodied in the model. Bad models are too complex and too uneconomical or, in other cases, too simple.

Pros and Cons of Dynamical Models

The advantage of a deterministic dynamical model is that it states formal assertions in logical terms and uses the logic of mathematics to get beyond intuition. The logic is as follows: If my premises are true, and the math is true, then the solutions must be true. Suddenly, you have gotten to a position that your intuition doesn't believe, and if upon further inspection, your intuition is taught something, then science has happened. Models also permit formulation of hypotheses for testing and help make evident complex outcomes, nonlinear couplings, and distant feedbacks. This has been one of the more significant outcomes of climate modeling, for example. If there are leads and lags in the system, it's tough for empiricists because they look for correlation in time to determine causation. But if it takes a couple of hundred years for the effect to be realized, then the empiricist is often thwarted.

Particularly relevant for geoscientists and astrophysicists, dynamical models also permit controlled experimentation by compressing geologic time. Consider the problem of understanding the collision of galaxies—how does one study that process? Astrophysicists substitute space for time by taking photographs of different galaxies at different stages of collision and then assume they can assemble these into a single sequence representing one collision. That sequence acts as a data set against which a model of collision processes can be tested where the many millions of years are compressed. The idea of a snowball Earth provides an example even closer to home, or one could ask the question: What did rivers in the earthscape look like prior to vegetation? Questions of this sort naturally lend themselves to idea-testing through dynamical models.

But dynamical models not properly constructed or interpreted can cause great trouble. Recently, Pilkey and Pilkey-Jarvis (2007) passionately argued that many environmental models are not only useless but also dangerous because they have made bad predictions that have led to bad decisions. They argue that there are many causes, including inadequate transport laws, poorly constrained coefficients ("fudge factors"), and feedbacks so complex that not even the model developers understand their behavior. Although we think the authors have painted with too broad a brush, we agree with them on one point. A simple falsifiable model that has been properly validated [even if in a more limited sense than that of Oreskes et al. (1994)] is better than an ill-conceived complex model with scores of poorly constrained proportionality constants [also see Murray (2007) for a discussion of this point]. Finally, we should never lose sight of the fact that in a model "it is not possible simultaneously to maximize generality, realism, and precision" (atmospheric scientist John Dutton, personal communication, 1982).

An Important Modeling Assumption

We assume in this book that a fruitful way to describe the earth is a series of mathematical equations. But is this mathematical abstraction an adequate description of reality? Does reality exist in our minds as mathematical formulas or is it outside of us somewhere? For example, the current understanding of the fundamental physical laws that govern the universe—string theory—is entirely a mathematical theory without experimental confirmation. To some it unites the general theory of relativity and quantum mechanics into a final unified theory. To others it is unfalsifiable and infertile (see, e.g., Smolin, 2006).

We avoid these philosophical problems by simply asserting that mathematical descriptions of the earth both past and present have proved to be a useful way of knowing. As the Nobel Laureate Eugene Wigner noted, "The miracle of the appropriateness of the language of mathematics for the formulation of the laws of physics is a wonderful gift which we neither understand nor deserve" (Wigner, 1960). An alternative view is that they are inherently quite limited in their predictive power. This view is summarized cogently by Chris Paola in a review of sedimentary models: "[A]ttempting to extract the dynamics at higher levels from comprehensive modelling of everything going on at lower levels is . . . like analyzing the creation of La Boheme as a neurochemistry problem" (Paola, 2000). Whereas we accept this point of view in the limit, we reject it for a wide range of complex systems that are amenable to reduction.

Some Examples

To set the stage for the chapters that follow, we present two problems for which modeling can provide insight. Other examples abound in the literature. Of special note for those studying Earth surface processes is the Web site of the Community Earth Surface Dynamics Modeling Initiative (CSDMS; pronounced "systems"). CSDMS (http://

csdms.colorado.edu) is a National Science Foundation (NSF)-sponsored community effort providing cyberinfrastructure aiding the development and dissemination of models that predict the flux of water, sediment, and solutes across the earth's surface. There one can find hundreds of models that incorporate the conservation and geomorphic transport laws and that can be used to solve particular problems. A companion organization, Computational Infrastructure for Geodynamics (http://www.geodynamics.org/), provides similar support for computational geophysics and related fields.

Example I: Simulation of Chicxulub Impact and Its Consequences

Probably *the* most famous event in historical geology, at least from the public's perspective, is the extraterrestrial impact event at the end of the Mesozoic Era that killed off the dinosaurs. Most schoolchildren know the standard story: A large asteroid that struck the surface of the earth in Mexico's Yucatán Peninsula created the Chicxulub Crater along with a rain of molten rock, toxic chemicals, and sun-obscuring debris that eliminated roughly three-quarters of the species living at the time. To work through the specific details of what happened and to predict the consequences of such an uncommon event is not easy because the physical and chemical processes are operating in a pressure–temperature state all but impossible to obtain experimentally. It is precisely these cases that benefit most from numerical simulation.

But is an asteroid impact computable? That is, given as many conservation equations and rate laws as there are state variables, and given initial and boundary conditions, can future states of the system be predicted with an acceptable degree of accuracy? Gisler et al. (2004) thought so. They derived a model simulating a 10-km-diameter iron asteroid plunging into 5 km of water that overlays 3 km of calcite, 7 km of basalt crust, and 6 km of mantle material. The set of equations was solved using the SAGE code from Los Alamos National Laboratory and the Science

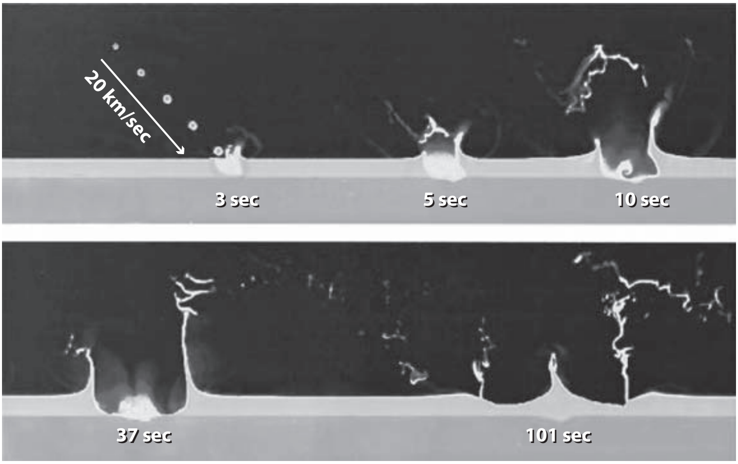

Figure 1.1. Montage of images from a three-dimensional (3-D) simulation of the impact of a 1-km-diameter iron bolide at an angle of 45 degrees into a 5-km-deep ocean. Maximum transient crater diameter of 25 km is achieved at about 35 seconds. [From Gisler, G. R., et al. (2004). Two- and three-dimensional asteroid impact simulations. *Computing in Science & Engineering* 6(3):46–55. Copyright © 2004 IEEE. Reproduced with permission.]

Applications International Corporation, which was developed under the U.S. Department of Energy's program in Accelerated Strategic Computing. Their model contained 333 million computational cells and used 1,024 processors for a total computational time of 1,000,000 CPU hours on a cluster of HP/Compaq PCs.

The results (fig. 1.1) document the dissipation of the asteroid's kinetic energy (which amounts to about 300 teratons TNT equivalent, or $\sim 4 \times 10^{21}$ J). The impact produces a tremendous explosion that melts, vaporizes, and ejects a substantial volume of calcite, granite, and water. Predictions from the model aid in understanding how, why, and where the resulting environmental changes caused the extinction.

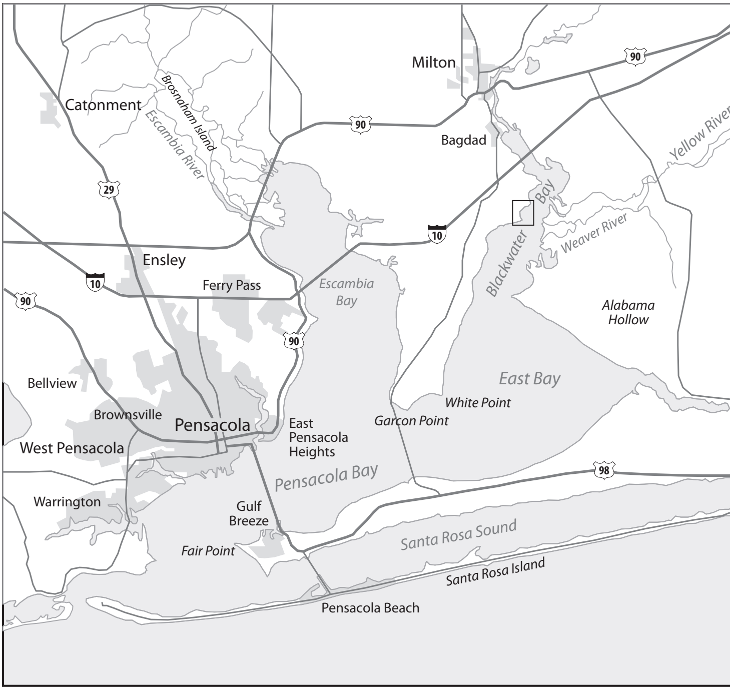

Figure 1.2. Map of Pensacola Bay and surrounding area. Hurricane Ivan passed on a trajectory due north just 20 mi to the west. The rectangle drawn in Blackwater Bay encompasses the region of interest. (Map adapted from a U.S. Geological Survey 1:250,000 topographic map.)

Example II: Storm Surge of Hurricane Ivan in Escambia Bay

On September 16, 2004, Hurricane Ivan made landfall about 35 mi (56 km) west of Pensacola, Florida (fig. 1.2). At the time of landfall, peak winds exceeded 125 mi h^{-1} (200 km h^{-1}), severely damaging many buildings in the Pensacola area. Probably equally damaging, however, was the surge of water along the coast and up Pensacola Bay. Homeowners along the bay experienced significant

Figure 1.3. The scene 3 hours after the eye passes. (Photo courtesy of Ray Slingerland.)

flooding (fig. 1.3) even though some were more than 25 mi by water from the open ocean.

Was this event an unpredictable act of God or could we have predicted the flooding? As you might suspect, the answer is that not only could it have been predicted, it was (fig. 1.4).

In chapter 10, we describe how surge models of the sort used by the U.S. Army Corps of Engineers are derived.

Steps in Model Building

So how does one construct a model of a geological phenomenon? Throughout this book, we will try to follow some logical steps in model development. First, get the physical picture clearly in mind. As an example, say one wanted to model the number of flies in a room as a function of time. The physical picture includes defining the

Figure 1.4. Observed surge high-water line (solid gray) versus those predicted (solid white) for Hurricane Ivan. Zone VE: Area subject to inundation by the 1%-annual-chance flood event with additional hazards due to storm-induced velocity wave action. Zone AE: Area subject to inundation by the 1%-annual-chance flood event determined by detailed methods. Zone X: Area of minimal flood hazard higher than the elevation of the 0.2%-annual-chance flood. See figure 1.2 for location. (From http://www.fema.gov/pdf/hazard/flood/recoverydata/ivan/maps/K33.pdf.)

dependent variable(s) (in this case the number of flies), the independent variables (time), and the size of the room. Second, one must define the physical processes to be treated and the boundaries of the model. The processes in the case of flies are flying, crawling, hatching, and dying. The boundaries of the model are those that do not pass flies such as walls, floor, and ceiling, and open boundaries such as doors and windows. Third, write down the physical laws to be used. Generally, these will be laws such as conservation of mass, Fick's law, and so on. In the case of flies, the laws are rate laws governing the flux of flies into and out of the room and laws defining the rates at which flies are created and die within the room. Fourth, put down very clearly the restrictive assumptions made. If one assumes that the flies will enter the room in proportion to the gradient in their number between inside and outside, write that assumption down. Fifth, perform a balance, first in words and then in symbols. Usually, one balances properties such as force, mass, or number. In the case of flies, we would say

> The time rate of change of flies in the room
> = the rate at which they enter through doors and windows
> – the rate at which they leave
> + the rate at which they are born
> – the rate at which they die.

We would then substitute symbols for number of flies, time, and so forth. Sixth, check units. All the terms in the balance equation must be of the same units; if they are not, we have made a mistake in our definitions, and now is the time to catch it. Seventh, write down initial and boundary conditions. By initial conditions are meant the values of the dependent variables at the start of the calculations. For example, we would specify the number of flies in the room at $t = 0$ as zero or some finite number. Boundary conditions are the values of the dependent variables at the edges of the spatial domain of interest. For example, we must specify the number of flies outside as a function of time and specific door or window. Lastly, solve the mathematical model. If you are lucky you can find an equation of similar form that has already been analytically solved. There is value in pursuing an analytic solution even if you need to reduce variable coefficients to constants or even drop terms, because the simplified equation will provide insight into your system's behavior. But often no analytic solutions will be available, and this step will require converting the equation set into a numerical form amenable for solution on a computer. Finally, you should verify and

Table 1.1. Steps in Problem Solving

1.	Get the physical picture clearly in mind.
2.	Define the physical processes to be treated and the boundaries of the model.
3.	Write down the laws and transport functions to be used.
4.	Put down very clearly the restrictive assumptions made.
5.	Perform the balance, first in words and then in symbols.
6.	Check units.
7.	Write down initial and boundary conditions.
8.	Verify, validate, and solve the mathematical model.

validate your model. According to Oberkampf and Trucano (2002), verification is the process of determining that a model implementation accurately represents your conceptual description of the model and the solution to the model. Thus, verification checks that the coding correctly implements the equations and models, whereas validation determines the degree to which a model is an accurate representation of the real world from the perspective of its intended uses. In other words, does the model agree with reality as observed in experiments and in the field. To formalize your thinking as you approach a problem, follow all of these steps in table 1.1.

Basic Definitions and Concepts

Why Models Are Often Sets of Differential Equations

We naturally find it easier to think about how an entity changes than about the entity itself. For example, my car speedometer measures my velocity, not the distance I've traveled from my garage since I started my trip. It is easier to state that the time rate of change of water in my boat equals the rate at which water enters through the open seams minus the rate at which I am bailing it out than it is to state how the volume of water actually varies with time. Changing entities of this sort are called variables, of which there are two kinds: independent (space and time) and dependent, by which we mean the state variables in question (velocity, mass of water, and so forth). The rate of change of one variable with respect to another is called a derivative, written, for example, as the ordinary derivative dV/dt if the dependent variable V is only a function of the independent variable t, or the partial derivative $\partial V/\partial t$ if V also depends upon other independent variables. Equations that express a relationship among these variables and their derivatives are differential equations.

However, often we want to know how the variables are related among themselves, not how they are related to their derivatives. So the general procedure is to derive the differential equations from first principles and then solve them for the values of the dependent variables as functions of the independent variables and other parameters.

To solve the differential equations requires more than the differential equation itself, however. The problem must be *well posed*. A well-posed problem contains as many governing equations as there are dependent variables. Also, the time and space interval over which the solution is to be obtained should be specified, and additional information concerning the dependent variables must be supplied at the start time (called initial conditions, or ICs) and the boundaries of the intervals (called boundary conditions, or BCs). This information is necessary because integration of the differential equations creates constants of integration in the case of ordinary differential equations (ODEs) and functions of integration in the case of partial differential equations (PDEs). The number of constants or functions needed is equal to the order of the differential equation. Thus, for a partial differential equation that is second order in both time and space, one must supply two functions derived from the ICs specifying the dependent variable as a function of time and two functions derived from the BCs specifying the dependent variable as a function of space. There are three possible types of BC information that can be supplied.

Dirichlet Conditions

In this type of BC, the solution itself is prescribed along the boundary, as, for example, if we were to set dependent variable $C(0,t) = P$, where P is some temporally constant value of the dependent variable.

Neumann Conditions

Alternatively, the derivatives of the solution in the normal direction to the boundary are prescribed. For any variable that obeys a first-order rate law, this is equivalent to specifying the flux across the boundary. Thus, we might know that a chemical species of concentration $C(x,t)$ diffuses across a plane in an aquifer at $x = 0$ at a flux $q = q_0$, and therefore the BC at $x = 0$ becomes

$$D\frac{\partial C}{\partial x}\bigg|_{x=0} = -q_o. \tag{1.1}$$

Mixed Conditions

This BC, sometimes called a "Robin" boundary condition, combines both of the above types. For example, if the flux through the face at $x = 0$ was not constant, but was proportional to the difference between a fixed concentration A at $x = -1$ and $C(0,t)$, the actual concentration at $x = 0$, then the appropriate BC would be

$$D\frac{\partial C}{\partial x}\bigg|_{x=0} = -k[A - C(0,t)], \tag{1.2}$$

where k is a proportionality constant with units of m s^{-1}.

Finally, for a well-posed problem, a solution must exist, be unique, and depend continuously on the auxiliary data. Most geoscience problems have solutions, and most can be made unique with proper BCs, although one should be aware that underprescription of BCs leads to nonuniqueness. The third requirement is met when small changes in BCs lead to small changes in the solution.

Nondimensionalization

Before attempting a solution, it is always useful to rewrite the well-posed problem using nondimensional variables (see table 1.2). When we nondimensionalize equations, we remove units by a suitable substitution of variables. This

Table 1.2. Steps in Nondimensionalization

1. Identify all the independent and dependent variables.
2. Define a nondimensional term for each variable by scaling each variable with a coefficient in the problem with the same units.
3. Substitute each definition into the governing equation and divide through by the coefficient of the highest-order polynomial or derivative.
4. If you have chosen well, the coefficients of many terms will become 1.

process groups together various coefficients into ensembles called parameters, thereby allowing us to predict natural system behavior more easily. We also can describe the solution in terms of a few parameters composed of the various dimensional geometric and material properties in the problem. Sometimes characteristic properties of a system emerge from these, such as a resonance frequency. Plus, one solution fits all; we don't need to define a new solution if we want to change a parameter. Finally, if we have chosen well, the solutions scale between 0 and 1, thereby allowing us to better control accuracy if the solution must be obtained by numerical techniques. The nondimensionalization process, also known as scaling, will be illustrated in detail after we have created some models.

A Brief Mathematical Review

Here we review some mathematical concepts used in the creation and solution of well-posed dynamical models. We usually seek a solution over a portion or interval of time and space. An interval is formally defined as the set of all real numbers between any two points on the number line of space or time and will be denoted as: $a < x < b$.

Definition of a Function

If to each value of an independent variable x in a specified interval there is one and only one real value of the dependent variable y, then y is a *function* of x in the interval. The concept can be extended to functions of n independent variables. For example,

$$z = f(x,y) = x + y. \quad (1.3)$$

There are two types of functions: explicit and implicit. The relationship $f(x,y) = 0$ defines y as an implicit function of x. Implicit solutions of equations often are pointless, as, for example,

$$f(x,y) = x^3 + y^3 - 3xy = 0, \quad (1.4)$$

which still does not tell us explicitly the value of y for a given x.

Ordinary Differential Equation

Let $f(x)$ define a function of x on an interval. By ordinary differential equation (ODE) we mean an equation involving x, the function $f(x)$, and its derivatives. The order is the order of the highest derivative. For any function $y = f(x)$, the geometrical meaning of the first derivative is the slope of the line tangent to a point on the function, and the second derivative is the curvature of the function at that point.

Solution of an Ordinary Differential Equation

Let $y = f(x)$ define y on an interval. $f(x)$ is an explicit solution if it satisfies the equation for *every* x on the interval, or if upon substitution, the ODE reduces to an identity.

Fundamental Theorem of Calculus

Integration is antidifferentiation. Thus, if:

$$y = x^2$$

and

$$\frac{dy}{dx} = 2x$$

then

$$\int dy = \int 2x dx = x^2 + c, \quad (1.5)$$

where c is a constant of integration.

General Solution

For a very large class of ODEs, the solution of an ODE of order n contains n arbitrary constants. Example:

$$\begin{aligned} \frac{d^2y}{dx^2} &= x \\ y &= \frac{x^3}{6} + c_1 x + c_2. \end{aligned} \tag{1.6}$$

The n-parameter family of solutions, $y = f(x, c_1 \ldots c_n)$, to an nth order ODE is called a *general solution*. Constants are called constants of integration. To find a particular solution requires additional information to uniquely specify the constant(s). This additional information comes from the initial or boundary conditions.

Systems of Ordinary Differential Equations

The pair of equations

$$\begin{aligned} \frac{dx}{dt} &= f_1(x, y, t) \\ \frac{dy}{dt} &= f_2(x, y, t) \end{aligned} \tag{1.7}$$

is called a system of two first-order ODEs. A *solution* is then a pair of functions $x(t)$, $y(t)$ on a common interval of t.

The Partial Derivative

If $z = f(x,y)$, then the partial derivative of z with respect to x at (x,y) is

$$\frac{\partial z}{\partial x} = \lim_{h \to 0} \frac{f(x+h, y) - f(x, y)}{h}, \tag{1.8}$$

and so forth. Note that a partial with respect to x is differentiated with y being regarded as a constant. The geometrical interpretation of the partial derivative is given in figure 1.5. Geologists will recognize that the solution surface at a point may be characterized by two apparent dips, one in the x direction and one in the y direction. These

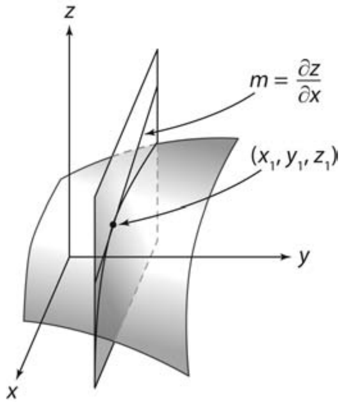

Figure 1.5. Geometrical meaning of a partial derivative. The curved surface is the value of z as a function of x and y. A line drawn tangent to the surface in the x,z plane at position y_1 has slope m equivalent to the value of the partial derivative at (x_1,y_1).

slopes are given by the partial derivatives, and therefore the apparent dip angles are given by the arctangents of the partial derivatives.

Differential of a Function of Two Independent Variables

If $z = f(x,y)$, then the differential of z is

$$dz = \frac{\partial f(x,y)\,dx}{\partial x} + \frac{\partial f(x,y)\,dy}{\partial y}. \tag{1.9}$$

Partial Differential Equations

An equation involving two or more independent variables, x_i, the function, $f(x_i)$, and its partial derivatives is called a partial differential equation (PDE). The order is the order of the highest partial derivative.

It is always helpful to classify the PDEs of your problem, because much can be learned about the behavior of the solution even without obtaining the actual solution. In fact, the method of solution often is class-dependent. A PDE can be linear or nonlinear, with the nonlinear equations being more difficult to solve. A PDE is linear if the dependent variable and all its derivatives appear in a linear fashion; that is, are not multiplied by each other, squared, and so forth. It is homogeneous if it lacks a term that is independent of the dependent variable.

Kinds of Coefficients

Coefficients may be constants, functions of the independent variables, or functions of the dependent variables. In the latter case, the equation is said to be nonlinear.

Three Basic Types of Linear Partial Differential Equations

A second-order linear equation in two variables is of the form

$$A\frac{\partial^2 u}{\partial x^2} + B\frac{\partial^2 u}{\partial x \partial y} + C\frac{\partial^2 u}{\partial y^2} + D\frac{\partial u}{\partial x} + E\frac{\partial u}{\partial y} + F = 0, \quad (1.10)$$

where A through F are constants or functions of x and y. All linear equations like equation 1.10 can be classified according to the following scheme. If:

$$B^2 - 4AC < 0 \Rightarrow \text{The PDE is elliptic:}$$
$$B^2 - 4AC = 0 \Rightarrow \text{The PDE is parabolic:}$$
$$B^2 - 4AC > 0 \Rightarrow \text{The PDE is hyperbolic:} \quad (1.11)$$

The usefulness of this classification will be shown later.

Solution of a Partial Differential Equation

A function $z = f[x,y,g_i(x,y)]$, is a solution if it satisfies the PDE upon substitution. Note that PDEs of the nth order require n *functions* of integration, $g_i(x,y)$.

Chain Rule

Suppose $z = f(x,y)$, and $x = F(t)$, and $y = G(t)$ where F and G are functions of t. What is dz/dt? Because z is a function of x and y, and x and y are functions of t:

$$\frac{dz}{dt} = \frac{\partial z}{\partial x}\frac{dx}{dt} + \frac{\partial z}{\partial y}\frac{dy}{dt}. \quad (1.12)$$

Product Rule

If $f(x) = u(x)\, v(x)$, then

$$\frac{\partial f}{\partial x} = u\frac{\partial v}{\partial x} + v\frac{\partial u}{\partial x}. \quad (1.13)$$

Taylor Series Expansion

Taylor's theorem was first derived by Brook Taylor, who was born August 18, 1685, in Edmonton, Middlesex, England. Its importance remained unrecognized until 1772 when Lagrange proclaimed it the basic principle of the differential calculus. Taylor showed that if one knows the value of a function at (x,y), then the value of the function at $(x+ dx, y)$ can be approximated as

$$f(x+dx,y) = f(x,y) + \frac{1}{1!}\frac{\partial f(x,y)}{\partial x}dx + \frac{1}{2!}\frac{\partial^2 f(x,y)}{\partial x^2}(dx)^2 + \ldots\ldots, \tag{1.14}$$

where the ellipses denote all higher-order terms in the series.

Substantial Time Derivative

Let us say we are interested in the rate at which the temperature, T, changes as we drive south in the winter from Pennsylvania to Florida. We recognize that there will be two sources of temperature change: one arising due to the change of temperature independent of any change in location (say the normal heating that occurs as night turns to day), and one arising because we are moving south through the latitudinal temperature gradient at our car speed u. Equation 1.12 captures this idea. Let $z = T$, $x =$ distance $= F(t)$, and $y = G(t) = t$. Therefore, the total time derivative of T is

$$\frac{dT}{dt} = \frac{\partial T}{\partial x}\frac{dx}{dt} + \frac{\partial T}{\partial t}\frac{dy}{dt}. \tag{1.15}$$

However, $dx/dt = u$, the car velocity, and $dy/dt = 1$; therefore,

$$\frac{dT}{dt} = u\frac{\partial T}{\partial x} + \frac{\partial T}{\partial t}. \tag{1.16}$$

The righthand side (RHS) of equation 1.16 is called the substantial time derivative (in this case in only one dimension) and often written in shorthand form as DF/Dt, where F is the dependent variable in question.

Concept of a Control Volume

A control volume is the region of space we define to perform a balance of mass, energy, and so forth. It can be either macroscopic, such as a finite volume of a river channel, or microscopic with dimensions dx, dy, dz, for example. Choosing the control volume for a problem is somewhat an art. Ideally, the boundaries should be meaningful physical surfaces through which fluxes can be easily specified without recourse to complicated geometric formulas.

The Basic Scientific Laws, Axioms, and Definitions

All of the physics and chemistry used in this book can be reduced to only 17 basic concepts. These are listed in table 1.3 for later reference.

Table 1.3. Basic Laws, Axioms, and Definitions

I. Conservation of Mass
The time rate of change of mass in a control volume equals the mass rate into the volume minus the mass rate out.

II. Newton's First Law
Any body is in a state of rest or in uniform rectilinear motion until some forces applied to it produce a change in the state of the body (motion or deformation). (NB: body = discrete entity with mass.)

III. Newton's Second Law
The rate of change of momentum of a body is proportional to the impressed force and is made in the direction of the straight line in which the force is impressed.

IV. Newton's Third Law
To every action there is always opposed and equal reaction, or the mutual actions of two bodies upon each other are always equal in magnitude and opposite in direction.

V. Corollary I
A body acted on by two forces simultaneously will move along the diagonal of a parallelogram in the same time as it would move along the sides by those forces acting separately.

VI. Conservation of Momentum
Using Newton's third law to extend Newton's second law to the total momentum of systems of particles:
The time rate of change of momentum in a control volume equals the time rate in of momentum minus the time rate out plus the sum of forces.

(*continued*)

Table 1.3. (*continued*)

VII.	The Coriolis Force Arises out of a choice to apply the laws of motion developed for an inertial reference frame to a rotating reference frame that is attached to Earth. It is quantified as twice the product of the angular velocity and the sine of the latitude.
VIII.	Quadratic Drag Law The force experienced by a large object moving through a fluid at relatively large velocity (i.e., with a Reynolds number greater than ~1,000) is proportional to the square of the velocity.
IX.	Universal Law of Gravitation Between any two particles of mass m_1 and m_2 at separation R, there exist attractive forces F_{12} and F_{21} directed from one body to the other and equal in magnitude to the product of masses and inversely proportional to square of distance between them.
X.	Equivalence of Work and Energy Work is measured by the product of an acting force and the distance traveled by a body. It is a measure of the transfer of energy from one body to another.
XI.	Conservation of Energy Energy retains a constant value in all the changes of the form of motion.
XII.	Stefan–Boltzmann Law Energy radiated from a black body is proportional to the fourth power of its temperature (Kelvin units).
XIII.	First-Order Rate Laws A substance flows down a potential or concentration gradient at a rate proportional to the magnitude of the gradient. Includes Fourier's law, Darcy's law, Newton's law of viscosity, Ohm's law, Hooke's law, and Fick's first law.
XIV.	Law of Mass Action The rate of a forward chemical reaction is proportional to the product of the reactants' concentrations (raised to the power of their stoichiometric coefficients).
XV.	Law of Radioactive Decay The rate of decay of a radioactive substance is proportional to its mass.
XVI.	Relationship Between Stress and Strain The shear stress acting on a Newtonian fluid is proportional to the rate of shear strain, with the proportionality constant being the coefficient of viscosity.
XVII.	Archimedes' Principle A body partly or wholly immersed in a fluid is buoyed up by a force acting vertically upwards through the center of mass of displaced fluid and equal to the weight of the fluid displaced.

Summary

This chapter was designed to instill in the reader a sense of the role of mathematical models in the geosciences, especially those that we focus on here—dynamical systems models. Following on some examples, we have provided a template for constructing mathematical models that we will follow religiously in this book. Many of the terms and concepts that we use in later chapters were introduced, and some necessary basic mathematics was reviewed for those needing a reminder. Now that the toolbox has been filled, we move on to the process of converting differential equations into algebraic expressions that can be solved using matrix algebra: the process of obtaining numerical solutions by finite difference.