

Chapter 2

Building a Model

2.1 the framework

The steps one must follow in building a model of a geophysical system are straightforward:

1. statement of the problem
 - What do we want to know?
 - What do we already know?
 - Why do we want to know this?
 - Identify the known and unknown quantities.
 - Identify the boundary conditions or initial conditions.
2. theory: develop a mathematical representation of the problem
 - Derive governing equations using observation and physical laws.
 - Use all appropriate simplifying assumptions.
 - Use calculus tools and boundary conditions to simplify the math if possible.
 - The mathematical representation will most likely fit one of three categories:
 - initial value problems involving single or coupled ordinary differential equations
 - boundary value problems (may be partial differential equations)
 - initial + boundary value problems (partial differential equations)
3. write a computational algorithm to solve the equation(s)
 - implementation algorithm and “pseudocode” description of computational steps
 - re-write algorithm in a programming language

- test program(s) in parts as they are written
4. analysis of model results
- Is this result reasonable?
 - If not, what should be changed?
 - If so, what have I learned?

There is no reason to assume from the outset that the result of your calculation is either correct or meaningful. Ask yourself *Does the model behave as I expected it to? If not, is the model showing me something new about the physical system being simulated or did I make a mistake (in the implementation or in the governing equations)?* Mistakes come in many varieties, from flaws in the computer program, to incorrect input, to the application of an inappropriate theory for the problem of interest. Once you've verified that the program you wrote is error-free, check the input data. Are the units correct? Discovering coding errors and errors in the input data can be a challenge. A good way to limit the number of errors and the time spent correcting them, follow the good practice of writing an implementation or pseudocode algorithm on paper first, then writing and testing your program step by step.

Errors in the theory underlying a model are not always obvious. For example, a model constructed using a simplification that is appropriate for one problem may not be appropriate for another. Such errors may be discovered by following the intuition that comes from experience or by comparing model results with observations. Indeed, models provide great tools for testing the applicability of a particular theory (or set of simplifications) to a particular problem.

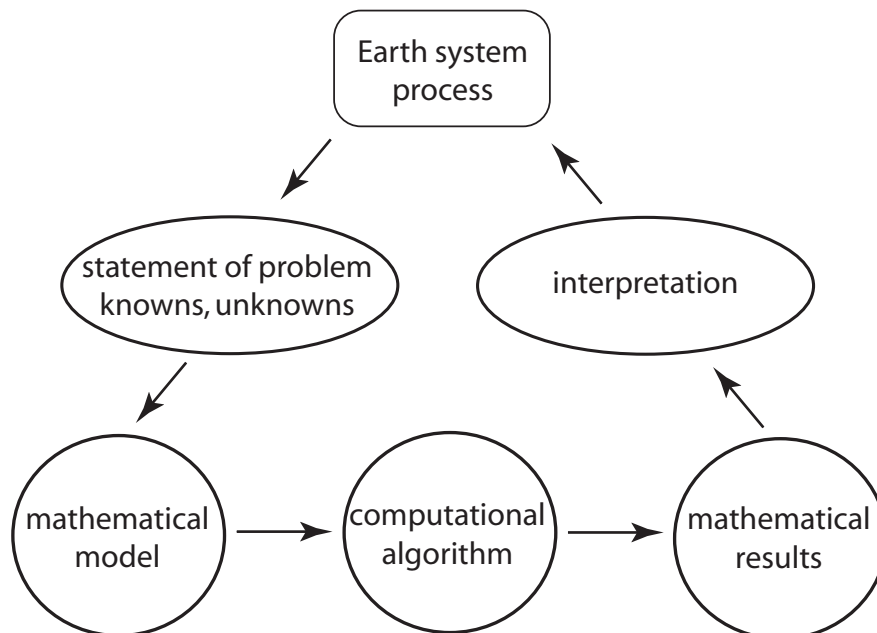


Figure 2.1: Flow chart for model life cycle.

2.2 the tools

2.2.1 pencil, paper, noggin

Your primary tools in model development should be a pencil, a piece of paper, and your brain. In many cases, your starting point will be an existing equation or set of equations. Write them down and study their parts. You must understand how the equation works before you can employ it as a problem-solving tool and must have some expectation for how the equation will behave before you can interpret model results. If you are starting from a set of observations, try drawing some pictures to help you sort out the appropriate governing equations for your problem.

2.2.2 simplifications

Once you have a set of governing equations, try to simplify them. A judicious selection of boundary conditions may allow you to find an exact analytical solution to your equation(s). If an exact analytical solution is not possible, you may still be able to find an approximate one. Can you assume some coefficients to be constant over the time or length scale of interest? Can some terms be eliminated on the basis of their magnitude or irrelevance to the problem you wish to address?

Your calculus textbook is full of useful information about integrating ordinary differential equations. Some equations are fairly simple to integrate, for example the decay equation in Section 2.3.1. More complicated equations may require techniques such as variable or trigonometric function substitutions. Before you get carried away, look your equation up in an integral table (as in the *CRC Standard Math Tables*). Chances are good that somebody has covered this ground before you.

2.2.3 computational algorithms

A wide variety of tools exist for the solution of differential equations. In this class, we will explore a very few of these tools. All numerical solutions are discrete approximations to continuous functions. The differences among computational solution methods involve primarily the manner in which the discretization is accomplished. A short list of common numerical schemes:

Quadrature methods use geometrical constructs to approximate the integration of a differential equation. Quadrature is, in essence, finding the “area under the curve” described by the differential equation. MATLAB provides several built-in quadrature functions.

Finite difference methods approximate the derivatives in a differential equation over discrete intervals (elements) of the independent variable(s) using series approximation.

Finite element schemes approximate *global* functions as sums of *local* “shape functions” defined for a set of discrete *elements*. The solution is approximated locally by interpolation within each model element. The individual elements are linked together and the equations are solved simultaneously with the requirement that errors be minimized. In a finite difference scheme,

the governing equations are required to be true at specific points within the model domain. In a finite element scheme, the equations are required to be true in an integral sense.

Finite volume methods are hybrids between finite differences and finite elements. The model domain is treated as discrete volumes that exchange fluxes at their boundaries and use volume-averages of properties within the *volume elements*.

2.2.4 development environment

Pick a programming language and platform that work for you and your problem. If you have a choice in computers to use, pick one that is fast enough to implement your program in a timely manner. It is often the case that you will spend more time developing the problem and its solution (that is, your model) than running the programs written to use it.

2.3 examples

2.3.1 decay equations

The simplest models are single ordinary differential equations and their associated coefficients and boundary conditions. With a wise choice for those conditions, these expressions may be solved exactly. The decay of a radioactive element falls into this category. The observation that the change in concentration δc of a radiogenic nuclide over an interval of time δt is proportional to its concentration c is expressed:

$$\frac{\delta c}{\delta t} \propto c(t)$$

where δ indicates a small change in a quantity. Further, we know that as time proceeds, the concentration of the nuclide decreases (this is the meaning of decay) and that different radiogenic elements decay at different rates. Thus, the proportionality may be written as an equality with the addition of a material property, the decay constant λ of the nuclide:

$$\frac{\delta c}{\delta t} = -\lambda c(t) \tag{2.1}$$

The negative sign indicates decay. The decay constant λ is an empirically-derived quantity. Taking the limit as δ goes to zero, equation (2.1) is written as an ordinary differential equation:

$$\frac{dc}{dt} = -\lambda c(t) \tag{2.2}$$

This equation may be integrated with an appropriate boundary condition, the concentration at $t = 0$, and then solved exactly.

2.3.2 buoyancy, a classic example

The buoyant rise (or descent) of an object in a fluid is a classic example that will give us experience with building useful models. It has some interesting applications in Earth science.

The mathematical description of buoyant rise begins with a physical principle, Newton's Second Law of Motion

$$\mathbf{F} = \frac{d}{dt}(m\mathbf{v}) \quad (2.3)$$

“The alteration of motion is ever proportional to the motive force impress'd; and is made in the direction of the right line in which that force is impress'd” (Motte's 1729 translation from Newton's Latin *Mathematical Principles of Natural Philosophy*). In more modern language we might write that the net force \mathbf{F} on an object of fixed mass m is, in an inertial reference frame, equal to the time rate of change in its linear momentum $m\mathbf{v}$. Bold face indicates a vector-valued term. You may be more familiar with the the form:

$$\sum \mathbf{F} = m \mathbf{a} \quad (2.4)$$

in which the time derivative of the velocity \mathbf{v} is written as the acceleration \mathbf{a} represents its acceleration. This law states that if the sum of all forces acting on an object is not zero, the object accelerates. When the forces acting on an object are in *equilibrium*, they sum to zero and a must equal zero. Force balance is a fundamental concept in many Earth science problems.

Next, the forces acting on the mass must be identified and described mathematically. Here, we limit the derivation to one space dimension, the direction of \mathbf{g} , the acceleration due to gravity. We will define our one dimensional axis to be positive in the positive g direction (that is, toward the center of the mass responsible for g).

The three forces we must consider for a freely-floating object are due to

1. gravity (that is, the weight of the object):

$$W = m g \quad (2.5)$$

2. buoyancy (recall Archimedes' Principle):

$$F_B = m g \frac{\rho_f}{\rho_s} \quad (2.6)$$

where ρ_f and ρ_s represent densities of the fluid and object, respectively, and

3. the drag between the object and the fluid. The third force depends on the geometry and speed of the moving object. For a sphere, the drag force is:

$$F_D = C_D \left(\frac{1}{2} \rho_f w^2 \right) A \quad (2.7)$$

where C_D is a drag coefficient, w represents the speed of the sphere, and A represents its cross-sectional area. The drag coefficient depends, in a complicated way, on the shape and speed of the sphere and the properties of the fluid:

$$C_D \propto \left(\frac{\rho_f w}{\mu_f} \right)$$

where μ_f is the viscosity of the fluid. The complete force balance equation is written by substituting equations (2.5), (2.6), and (2.7) into (2.4) and recognizing that the acceleration of the sphere is the time-derivative of its speed,

$$\frac{dw}{dt} = g \left(1 - \frac{\rho_f}{\rho_s} \right) - \frac{C_D \rho_f A}{2 m} w^2 \quad (2.8)$$

This is a first-order differential equation. Unfortunately, equation (2.8) is not as simple as it appears because the drag coefficient depends on the speed of the sphere, w . However, simplifications may still be made that allow us to model particular situations. For example, we may assume that C_D is constant over some limited range of $w\rho_f/\mu_f$.

A dimensionless number, the Reynolds number, is used to provide a quantitative measure of the relationship among fluid density, fluid viscosity, the geometry, and the speed of the sphere:

$$\text{Re} = \left| \frac{\rho_f D w}{\mu_f} \right| \quad (2.9)$$

where D represents the diameter of the sphere. The drag force for a sphere and small Reynolds number (< 1), was derived by George Gabriel Stokes (part of the work leading to his seminal paper on hydrodynamics in 1851):

$$F_D = 3 \pi D \mu_f w \quad (2.10)$$

Using equation (2.10), a more readily solvable equation can be written:

$$\frac{dw}{dt} = g \left(1 - \frac{\rho_f}{\rho_s} \right) - \frac{3 \pi D \mu_f}{m} w \quad (2.11)$$

This is often referred to as *Stokes' Law* or *Stokes flow*. The equation can also be written:

$$m \frac{dw}{dt} = (\rho_s - \rho_f) \frac{g\pi D^3}{6} - 3 \pi D \mu_f w \quad (2.12)$$

a formulation that emphasizes the difference in density between the sphere and the fluid through which it moves.

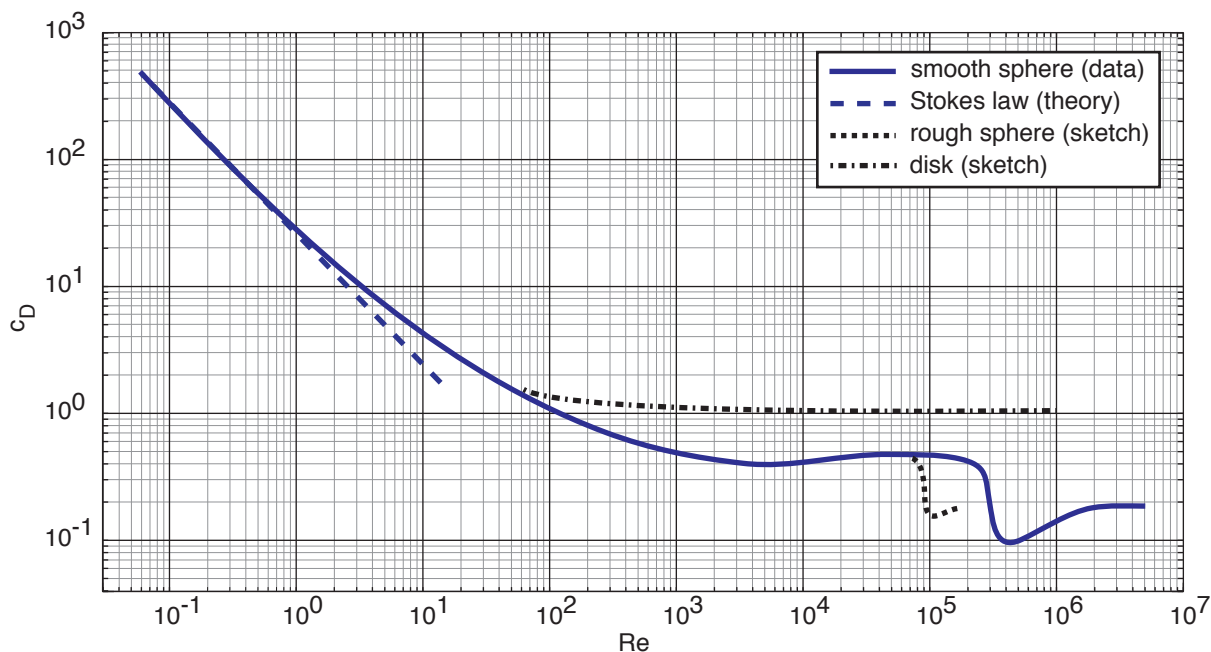


Figure 2.2: Empirical relationship between Reynolds number and drag coefficient, using data from engineering reference tables.

2.3.3 escape from (or to) Earth

Hominids have been hopping, skipping, and jumping close to Earth's surface for perhaps the last 7 million years (although just where *Sahelanthropus tchadensis* sits on the family tree is open to discussion) but it wasn't until the latter half of the 20th century that we started ejecting ourselves from the planet entirely. Asteroids have been doing a similar job for a much longer time via collisions and as a result we had samples of the moon and Mars right here on Earth, long before we developed the technology to go collect them for ourselves. Those missions were, of course, the best way to verify the sample source localities.

Years before Apollo 11 landed on the moon, Eugene Shoemaker (Shoemaker et al., 1963) proposed:

The occurrence of secondary craters in the rays extending as much as 500 km from some large craters on the moon shows that fragments of considerable size are ejected at speeds nearly half the escape velocity from the moon (2.4 km/sec). At least a small amount of material from the lunar surface and perhaps as much or more than the impacting mass is probably ejected at speeds exceeding the escape velocity by impacting objects moving in asteroidal orbits. Some small part of this material may follow direct trajectories to the earth, some will go into orbit around the earth, and the rest will go into independent orbit around the sun. Much of it is probably ultimately swept up by earth.

This hypothesis was supported observationally in 1983 by Ursula Marvin when she published a

remarkable discovery:

Antarctic meteorite ALHA81005, discovered in the Allan Hills region of Victoria Land, is a polymict anorthositic breccia which differs from other meteorites in mineralogical and chemical composition but is strikingly similar to lunar highlands soil breccias.

Following Marvin's report, H. Jay Melosh reasoned that the golf-ball sized ALHA81005 could only have been ejected from the moon by the impact of a much larger meteorite. The meteorite did not appear to have experienced very large shock pressures, giving Melosh additional information with which he developed a model (Melosh, 1985) to explore the relationship between impact speed, fragment size, and ejection speed. He concluded that faster impact by larger meteorites increased opportunity for meteoroids ejection but also led to smaller fragments. More recent analyses support the idea that moderate-size impacts are the most likely to produce the meteorites found on Earth (c.f. Basilevsky, et al., 2010).

So what does it take to send samples of the moon to Earth, or vice versa, without a machine? The challenge in escaping from a large mass is to acquire enough kinetic energy to overcome the potential energy due to the gravitational attraction between that mass and the escaping object. Put another way, the escaping mass must have a momentum that allows it to overcome the force due to gravity. Complications arise if the planet (or moon) has an atmosphere.

There is more than one way to consider this problem, here Newton's laws of motion and gravitation are used. Our goal is to build a mathematical model of the speed of an object with mass m moving away from a second object with mass M , in opposition to the gravitational attraction between them. There are at least three forces we must consider

1. the force associated with the motion of the escaping object, that is its momentum
2. the force due to gravity
3. a drag force arising from the fluid through which the object is escaping.

If the particles are very small, radiation pressure, solar wind pressure and the Lorentz force yield additional terms.

Sir Isaac Newton both stated and discussed the implications of a universal law of gravitation in his treatise, *Philosophiæ Naturalis Principia Mathematica*, first published in July of 1687. The law states that there is a force \mathbf{F} acting between objects due to their masses M and m and its strength goes as the inverse of the square of the distance \mathbf{r} between them

$$\mathbf{F} = -G \frac{Mm}{\|\mathbf{r}\|^2} \hat{\mathbf{r}} \quad (2.13)$$

in which the universal gravitational constant G is a constant of proportionality. As before, bold face indicates a vector quantity and \mathbf{r} is the unit vector

$$\frac{\mathbf{r}}{\|\mathbf{r}\|}$$

where $\|\mathbf{r}\|$ is the L2 norm of \mathbf{r} . The unit vector retains the correct orientation in an external reference frame.

The problem may be simplified by assuming the object is ejected at a right angle to the surface of the planet and by neglecting the drag force. The balance of forces, following equation 2.3 and assuming $\frac{dm}{dt} = 0$, is thus

$$m \frac{dv}{dt} = -G \frac{Mm}{z^2} \quad (2.14)$$

in which $m \frac{dv}{dt}$ is the linear momentum of the object moving away from the surface of the planet and z represents the distance between the centers of the planet and the escaping object. R will be used to represent the radius of the planet with mass M . Equation 2.14 can be simplified by canceling m . *Interesting.*

It is important at this point to underline the fact that Newton's laws of motion are for non-accelerating *inertial* frames of reference. He wrote the first law of motion, which is not so much a law as a statement, in order to make this clear (Newton, 1687):

Lex I: Corpus omne perseverare in statu suo quiescendi vel movendi uniformiter in directum, nisi quatenus a viribus impressis cogitur statum illum mutare.

Law I: Every body persists in its state of being at rest or of moving uniformly straight forward, except insofar as it is compelled to change its state by force impressed.

To be more complete, our statement of conservation should include angular velocity of the rotating frame. This is important in many fluid dynamics (including astrophysics) applications.

Equation 2.14 must be integrated if we wish to solve for v . In this case, we can integrate by hand to find an exact solution. The derivative $\frac{dv}{dt}$ is rewritten using the chain rule

$$\frac{dv}{dt} = \frac{dv}{dz} \frac{dz}{dt}$$

and the definition of speed

$$v = \frac{dz}{dt}$$

so that v

$$v \frac{dv}{dz} = -G \frac{M}{z^2} \quad (2.15)$$

is a function of z only. Separation of variables yields

$$\int v dv = -GM \int \frac{1}{z^2} dz \quad (2.16)$$

an indefinite integral with the solution

$$\frac{1}{2} v^2 = \frac{GM}{z} + C \quad (2.17)$$

in which the constant of integration C is evaluated using the initial value $v = v_0$ at $z = R$. Our mathematical model of the speed of the ejected object is thus

$$v^2 = v_0^2 + 2GM \left(\frac{1}{z} - \frac{1}{R} \right) \quad (2.18)$$

This model will allow us to answer the question: what minimum initial speed v_0 at $z = R$ is required for the speed $v(z)$ of the object to remain positive for any value of z (that is, away from the planet)? We must keep in mind the simplification made at the start, that the planet has no atmosphere and thus the drag force is zero. As we saw in the case of buoyancy problems, the drag force adds considerable complications to our model (we are unlikely to end up in the low Re range here).

Escape from the gravity well of the parent body is only the first step in the delivery of a meteoroid (or spacecraft) to another solar system object. If the *ejection* speed v_{ej} , the speed at which material moves away from the surface of a planet due to the impact of another object, is close to the *escape* speed v_{esc} , the meteoroid will be trapped in a heliocentric orbit near its parent. This velocity v_∞ is defined

$$v_\infty = \left(v_{ej}^2 - v_{esc}^2 \right)^{1/2} \quad (2.19)$$

2.4 references

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	mean radius (km)	mass ($\times 10^{24}$ kg)	mean surface or tropopause temperature (K)
Earth	6371	5.9736	218
Earth's moon	1737	0.0735	250
Mars	3389	0.6418	213
Mercury	2440	0.3302	442
Z	6052	4.8685	300
X	25,360	86.832	49

Table 2.1: Some useful quantities.

2.5 exercises

The following problems can be solved without writing any programs. However, one of the benefits of a computational algorithm is that once written, it can be used repeatedly with very little additional work. Use the data provided in table 2.1 wherever appropriate. Be sure to explain how you arrived at each answer.

- Use the model developed in section 2.3.3 to compute the escape speed v_0 at $z = R$ from an object with mass M . Use $G = 6.67 \times 10^{-11} \text{ m}^3 \text{ kg}^{-1} \text{ s}^{-2}$.
 - Begin by arranging equation 2.18 so that it is in the correct form to answer this question.
 - Next, write a Matlab function to solve the resulting equation for any variable values. As always, you should begin by writing an implementation algorithm.
 - Use your model to make a prediction: should there be more marian meteorites on Earth or more terran meteorites on Mars?
- Using Shoemaker's (1977) calculation of 22 km s^{-1} as the most probable speed for asteroid impacts on the moon, use your model to test the hypothesis that Antarctic meteorite ALHA81005 originated on the moon.
- Of the 50,000 or so meteorites that have been found (and recognized as such) on Earth, fewer than 100 have been identified as martian, according to the *Meteoritical Bulletin* meteorite database. Use your model to make a prediction: might some of the remaining stony meteorites of unknown origin come from Mercury?
- Consider planet Z in table 2.1.
 - Predict whether or not planet Z should produce meteoroids.
 - As it turns out, there are no known meteoroids from planet Z. Why might that be the case?
- The average kinetic energy of gas molecules

$$\frac{1}{2}m\bar{v}^2$$

in which the overbar indicates an average property, is proportional to the absolute temperature. Making use of the ideal gas law and kinetic theory, that relationship may be expressed

$$\frac{1}{2}m\bar{v}^2 = \frac{3}{2}k_B T \quad (2.20)$$

in which k_B represents the Boltzmann constant (the gas constant divided by the Avogadro number) and T represents the absolute temperature. The value of k_B in SI units is 1.38×10^{-23} J K⁻¹. Use your escape speed model to explain why Earth's atmosphere contains more nitrogen than helium.

6. Does planet X in table 2.1 have an atmosphere?