Contents

1 Mathematical Modeling: Introductory Remarks. 1
  1.1 Examples ................................................................. 1

2 Dimensional Analysis and Scaling Laws 3
  2.1 The yield of a nuclear explosion by G.I. Taylor ................. 4
  2.2 The Nonlinear Pendulum ............................................. 5
  2.3 Scaling ................................................................. 5
  2.4 The Navier Stokes equations and the Reynolds number ....... 6
  2.5 The drag problem revisited ........................................ 7
1 Mathematical Modeling: Introductory Remarks.

Applied mathematics deals with problems arising in the sciences, engineering and social sciences. Starting with a \textit{word} problem, the goal is to give it a mathematical structure, mostly in terms of equations, analyze these equations, set them in a computational framework, and come up with quantitative results on the original problem. A \textit{validation process} should be put in place to evaluate whether the results obtained accurately reflect the original problem.

The task of the applied mathematician may be summarized as follows:

- Consider problems emerging from science, engineering, medicine, social sciences, and, in general from \textit{real life}.

- Give them a mathematical structure as appropriate, for instance, using the laws of physics (such as balance laws, mass, linear momentum, energy, ...), or make reasonable assumptions motivated by the experiments in question, or by whatever information is available on the problem. Once the model is built, it is very important to examine how it can be \textit{transported} to problems that have emerged from very different situations.

- Apply methods of analysis to study the mathematical model at hand. These methods may relate to differential equations (ordinary, partial, stochastic,...), linear algebra, statistics,... In many occasions, new mathematics have emerged from the process of solving a real life problems. For instance, calculus emerged from the the study of gravity and planetary motion; the Maxwell equations and their analysis resulted from the study of electromagnetic phenomena and its applications.

- Cast the mathematical models in a computer amenable form. In problems formulated as systems of differential equations, this process typically involves discretization of space and time. Such discrete models are then analyzed by numerical methods, that are subsequently processes in a computer.

- Validation and revision of the computer generated data in terms of the original problem, for instance, comparing the results to experimental measurements.

1.1 Examples

The equation of the \textbf{harmonic oscillator} shown in figure 1 is

\[ m \frac{d^2x}{dt^2} + kx = 0. \tag{1} \]

The general solution is

\[ x(t) = A \cos \sqrt{\frac{k}{m}} t + B \sin \sqrt{\frac{k}{m}} t, \tag{2} \]

where \(A\) and \(B\) are constants that depend on the prescribed initial data.

The equation for the harmonic oscillator can be generalized to include friction \((c > 0\) denotes the friction coefficient), and also the presence of an external force \(F = F(t)\):

\[ m \frac{d^2x}{dt^2} + c \frac{dx}{dt} + kx = F(t). \tag{3} \]
Figure 1: A mass $m$ attached to a spring of constant $k$ oscillates about the equilibrium location $x = 0$. Graphs by Doug Davis, EIU, 2002.

**Heat equation.** Let $D$ be a bounded domain in $\mathbb{R}^3$, with smooth boundary $\partial D$. The equation giving the distribution of temperature $u = u(x, t)$ in $D$ is

$$
\rho c \frac{\partial T}{\partial t} = k \nabla^2 T,
$$

(4)

$\rho$ denotes the density of the material, $c$ the specific heat capacity, $k$ the conductivity. The independent variables are space $x \in D$, and time $t \geq 0$. The unknown function $T = T(x, t)$ denotes temperature.

To solve this equation, initial and boundary conditions need to be specified. The latter could be isothermal conditions, that is, the temperature is prescribed on the boundary, or flux conditions when the amount of heat going through the boundary is given.

Both, the linear oscillator equation and the heat equation are linear.

Topics on ordinary differential equations that we will study:

- Initial value problems for nonlinear, second order, and also special higher order equations. Analyze the evolution of the solution with time and its meaning. In the former case, we will study energy methods and the phase plane. One of the models that we will analyze is the nonlinear pendulum equation. We will also study some equations of third order, such as the Lorenz system, and population models such as the evolution of HIV.

- In many applications, the equations governing phenomena of interest contain one or more parameters. Consequently, solutions will also depend on such parameters. When there is a scale separation among parameters, perturbation methods are called for. We will study regular and singular perturbation methods. Here is a simple example of an ordinary differential equation that can be explicitly solved (rare!!):

$$
\frac{dy}{dx} = 1 + y^2, \quad y(0) = 0.
$$

(5)

We can see that the solution of this initial value problem is

$$
y = \tan x.
$$

(6)
Can we use this information to solve the modified equations

\[ \frac{dy}{dx} = 1 + (1 + \epsilon)y^2, \quad |\epsilon| << 1. \tag{7} \]

Again, this latter problem has also an exact solution. How does the solution depend on the parameter \( \epsilon \)? How do we solve problems for which there is no exact solution? The answer is provided by *perturbation methods*.

- Perturbation methods and stability, such as the normal mode analysis, and eigenvalue problems.
- Boundary value problems and bifurcation.

The heat equation is a statement of *balance of energy*. Balance equations are very important in physics. We will present a derivation of the heat equation in terms of balance of energy.

The heat equation is also associated with *diffusive* processes (e.g., as when salt is dissolved in water). From this point of view, the equation is associated with *stochastic* phenomenon. We will also study the heat equation in such a context.

Prior to developing mathematical methods to solve certain problems, we will explore information that can be obtained on a problem from purely common sense.

## 2 Dimensional Analysis and Scaling Laws

Let us discuss the following example\(^1\) When we ride a bike, we notice that the *force of air resistance* is positively related to the *speed* and to the *cross-sectional area* (skinny versus broad rider). The force exerted upon a moving object opposing its motion is known as *drag force*. The understanding of such a force is essential in the design of airplanes, cars, bicycles, boats, and any moving objects, aiming to the reduction of drag.

We want to find an equation that relates the force \( F \) with the velocity \( v \) and the area \( A \). We could write a prototype equation such as \( F = f(A, v) \). However, since the force involves *mass*, the equation cannot depend on \( v \) and \( A \) only. So, let us start with the equation

\[ F = f(\rho, A, v) \]

where \( \rho \) denotes air *density*, and with \( f \) the relation to be determined. So, let us start with an equation of the form

\[ F = K\rho^x A^y v^z, \tag{8} \]

where \( K \) is a constant without units (i.e., a dimensionless constant). We use the symbols \( M \), \( L \) and \( T \) to denote *mass*, *length* and *time*, respectively.

Let us set up the *dimensional equation* associated with (8):

\[ MTL^{-2} = (ML^{-3})^x(L^2)^y(LT^{-1})^z. \tag{9} \]

\(^1\)Sam Howison
Equating the exponents of the three above quantities, we arrive at

\[ x = 1, \quad y = 1, \quad z = 2. \]

So, the force equation becomes

\[ F = k \rho A v^2. \]

**Remark.** Understanding scaling can help us to build small scale models of large phenomenon, such as wind tunnels to model airplanes.

We will revisit the previous problem at the end of the section. In particular, notice that we have omitted a very important ingredient in the derivation: the viscosity of the air.

### 2.1 The yield of a nuclear explosion by G.I. Taylor

G.I.Taylor (1940’s, Cambridge University) computed the energy yield of the first atomic explosion (New Mexico, 1945) after viewing the photographs of the spread of the fireball. He assume that there exists a physical law of the form

\[ g(t, r, \rho, E) = 0. \]

Here

- \( r \) denotes the radius of the front at time \( t \),
- \( \rho \) is the initial air density,
- \( E \) is the energy realised by the explosion.

We first ask how many dimensionless groups we can form with the quantities \( \{t, r, \rho, E\} \)? We find that

\[ \frac{r^5 \rho}{t^2 E} \]

is dimensionless and that there are no other independent dimensionless quantities that we can form with \( \{t, r, \rho, E\} \).

By the Pi-Theorem (any physical law has a dimensionless form), we rewrite the original equation as

\[ f\left(\frac{r^5 \rho}{t^2 E}\right) = 0, \]

that is, \( f \) is a function of a single variable. Note that the solution corresponds to a root \( C \) (constant) of the previous equation. So,

\[ \frac{r^5 \rho}{t^2 E} = C, \]

which implies that

\[ r = \left(\frac{CEt^2}{\rho}\right)^{\frac{1}{5}}. \]

---

\(^2\)Sam Howison

This last relation is known as a scaling law and it states how the radius of the fireball grows with time.

\[ r \approx t^{2.5}. \]

It is confirmed by experiments and photographs.

### 2.2 The Nonlinear Pendulum

Sam Howison, page 32.

### 2.3 Scaling

Scaling is a procedure that reduces the original model, expressed in terms of dimensional variables, to one formulated in terms of the dimensionless variables. Scaling unveils the relative size of the parameters, reducing their number.

Let us consider the population model stating that the rate of growth of the number of individuals \( p \), at time \( t \), is proportional to the current population

\[
\frac{dp}{dt} = rp(t), \quad p(0) = p_0, \tag{10}
\]

where \( p_0 \) is the population at the beginning of the count; \( r > 0 \) is the growth rate, a quantity that has dimensions of \( t^{-1} \), where \( t > 0 \) denotes time. This model, known as the classical Malthus model (Thomas Malthus, who lived during the period 1766-1843, was an English essayist and one of the first individuals to study demographics and food supply).

This model predicts an exponential growth of the population, \( p(t) = p_0e^{rt} \), which it is obviously not realistic at all. The model neglects the competition effects among individuals of a population group and also the limitations to growth. A modification of Malthus model, known as the logistics model, incorporates competition by accounting for the number of encounters, \( p^2 \), and also for the limitations of the environment to support unlimited growth:

\[
\frac{dp}{dt} = rp\left(1 - \frac{p}{K}\right), \quad p(0) = p_0. \tag{11}
\]

Here \( K > 0 \) denotes the carrying capacity, which is the maximum number of individuals that the ecosystem can sustain.

Note that the problem has three parameters: \( K, p_0, r \). Let us rewrite the model in terms of dimensionless variables, time and population. Let

\[ \tau = tr, \quad P = \frac{p}{K}. \]

(We could also scale \( p \) with \( p_0 \)). The equation becomes

\[
\frac{dP}{d\tau} = P(P - 1), \quad P(0) = \alpha, \tag{11}
\]

where \( \alpha = p_0/K \). The problem can be solved by separation of variables, giving

\[
P(\tau) = \frac{\alpha}{\alpha + (1 - \alpha)e^{-\tau}}.
\]

5
Note that 
\[ \lim_{\tau \to \infty} P(\tau) = 1. \]
The population grows up to reaching the carrying capacity.

Note that the scaled equation only contains one parameter, \( \alpha \), down from the 3 constants of the original problem.

### 2.4 The Navier Stokes equations and the Reynolds number

The flow of an *incompressible viscous fluid* is governed by the *Navier-Stokes* equations for the velocity field \( \mathbf{v} \) and the pressure \( p \) of the fluid,

\[
\rho \left( \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{v} \right) = -\nabla p + \mu \nabla^2 \mathbf{v}, \quad \nabla \cdot \mathbf{v} = 0,
\]

where \( \mu > 0 \) is the *viscosity* of the fluid, and \( \rho > 0 \) is the *density*; both such quantities are constant. The pressure \( p \) is the Lagrange multiplier associated with the incompressibility constraint.

Let us introduce the scaled (dimensionless) variables

\[
\bar{t} = \frac{t}{T}, \quad \bar{x} = \frac{x}{L}, \quad \bar{v} = \frac{v}{U},
\]

where \( L, T, U = \frac{L}{T} \) and \( P \) denote typical length, time, velocity and pressure scales, respectively.

Obviously, out of the three quantities \( L, T, U \) only two are independent. Likewise, \( P \) cannot be chosen independently from other parameters of the problem. We will determine \( P \) in terms of other parameters of the model with the goal of obtaining the simplest possible coefficients. Recall that \([P] = \frac{\text{force}}{\text{area}} \).

Now, let us write (12) in terms of the dimensionless variables (after dividing through by \( \rho \)) denoted with an upper bar) to obtain

\[
\frac{\partial \bar{v}}{\partial \bar{t}} + \frac{UT \rho}{L \rho} (\bar{v} \cdot \bar{\nabla}) \bar{v} = -\bar{\nabla} \bar{p} + \frac{\mu T}{L^2 \rho} (\bar{\nabla} \bar{\nabla} \bar{v}).
\]

(13)

Let us choose \( P \) so that

\[
\frac{PT}{LU \rho} = 1.
\]

This gives

\[
\frac{\partial \bar{v}}{\partial \bar{t}} + (\bar{v} \cdot \bar{\nabla}) \bar{v} = -\bar{\nabla} \bar{p} + \frac{\mu T}{L^2 \rho} (\bar{\nabla} \bar{v}).
\]

(14)

We define the *Reynolds number* as

\[
\text{Re} = \frac{L^2 \rho}{\mu T} = \frac{\rho U L}{\mu}.
\]

(15)

So, we finally write

\[
\frac{\partial \bar{v}}{\partial \bar{t}} + (\bar{v} \cdot \bar{\nabla}) \bar{v} = -\bar{\nabla} \bar{p} + \frac{1}{\text{Re}} (\bar{\nabla} \bar{v}).
\]

(16)
Note that, although the original equation involved several parameters, the scaled nondimensional version depends only on one parameter, $Re$.

This allows us to simplify the equation at the limits of small and large Reynolds number. In particular, the case of $Re$ large, corresponds to small viscosity $\mu$ (large compared with $UL$), in which case, we can replace (16) with

$$\frac{\partial v}{\partial t} + (v \cdot \nabla)v = -\nabla p,$$

$$\nabla \cdot v = 0. \tag{17}$$

These are known as Euler equations of inviscid fluid. (We dropped the 'bar' notation.)

**What about the limit $Re$ small?**

We get the Stokes problem

$$0 = -\nabla p + \frac{1}{Re}(\triangle v), \quad \nabla \cdot v = 0. \tag{19}$$

### 2.5 The drag problem revisited

Let us return to the problem of determining the drag force on the bike rider. Pioneering studies of this problem go back to Stokes (19th century, Ireland and the UK), who studied the motion of an oscillating surface on water. Let us consider the simpler problem of a sphere moving in a fluid (air, water, ...). As in the case of the bicycle, we postulate that the drag force

$$F = f(R,v,\rho,\mu), \tag{20}$$

where $R$ denotes the radius of the sphere, $v$ its velocity, and $\rho$ and $\mu$ the density and viscosity of the fluid, respectively. A dimensional analysis of the previous equation allows us to write

$$[F] = [R^a v^b \rho^c \mu^d], \tag{21}$$

that is

$$MLT^{-2} = L^{a+b-3c-d}T^{-b-d}M^{c+d}. \tag{22}$$

Equating both sides of the equation gives

$$a + b - 3c - d = 1, \tag{23}$$

$$-b - d = -2, \tag{24}$$

$$c + d = 1. \tag{25}$$

We find that

$$a = 2 - d = b, \quad c = 1 - d.$$  

Hence, a possible expression of $F$ is

$$F = \alpha \rho R^2 v^2 \left( \frac{\mu}{\rho v R} \right) = \alpha \rho R^2 v^2 (Re)^{-d}, \tag{26}$$

4M.H. Holmes, section 1.2
where $\alpha$ as well as $d$ are arbitrary constants. The fact that $\alpha$ and $d$ are arbitrary allows us to obtain more (general) solutions to the problem:

$$F = \rho R^2 v^2 \left[ \alpha_1 (\text{Re})^{-d_1} + \alpha_2 (\text{Re})^{-d_2} + \ldots \right].$$  \hspace{1cm} (27)

In general, we can state

$$F = \rho R^2 v^2 G(\text{Re}^{-1}).$$  \hspace{1cm} (28)

The function $G$ has been experimentally obtained for different fluids.

### 3 Models Derived from Balance Laws

We mentioned that some mathematical models, especially those coming from mechanics, can be formulated in terms of balance laws. The next example presents a statement of balance of energy leading to the heat equation.

#### 3.1 Equation of Balance of Energy

We derive an equation governing the flow of heat in a homogeneous, isotropic and continuous solid.

This picture represents a bounded domain $\mathcal{D} \subset \mathbb{R}^3$, with smooth boundary, $\partial \mathcal{D}$. The vector $\mathbf{n}$ denotes the unit outward normal to the boundary, and $\mathbf{q}$ represents the heat flux vector. In addition to $\mathbf{q}$, we introduce the energy density $E(x, t)$ (energy per unit volume at a point $x$ and at time $t$). This energy is associated with random molecular motion. Recall that $\mathbf{q} \cdot \mathbf{n}$ represents the amount of energy (heat) going out of the domain across the boundary per unit area and per unit time. (So, $-\mathbf{q} \cdot \mathbf{n}$ is the influx).

The following equation is the statement of balance of energy in the body $\mathcal{D}$:

$$\frac{d}{dt} \int_{\mathcal{D}} E(x, t) \, dx = - \int_{\partial \mathcal{D}} \mathbf{q} \cdot \mathbf{n} \, ds. \hspace{1cm} (29)$$

Applying the divergence theorem to the surface integral gives

$$\frac{d}{dt} \int_{\mathcal{D}} E(x, t) \, dx + \int_{\mathcal{D}} \nabla \cdot \mathbf{q} \, dx = 0 \hspace{1cm} (30)$$
Note that this statement of balance of energy can be applied to any part of the body $\mathcal{D}$. It, then, follows that the integrand is identically zero. (Here we assume that the integrand is continuous, in which case, the localization theorem applies). Hence,

$$\frac{\partial}{\partial t}E(x, t) + \nabla \cdot \mathbf{q} = 0. \tag{31}$$

We observe that this equation has more unknowns than variables. So, we need to specify constitutive equations, that is, relations between $E$ and $\mathbf{q}$ so as to get a single unknown field. Constitutive equations also specify the type of material under consideration. In this case, we assume that

$$E(x, t) = \rho cT(x, t), \tag{32}$$
$$\mathbf{q}(x, t) = -k\nabla T(x, t). \tag{33}$$

The first equation gives the energy of the body as function of the absolute temperature. This is consistent with temperature as measure of random molecular motion. The second equation is Fourier Law of heat conduction expressing the fact that heat flows from hot to cold. Here,

- $\rho > 0$ denotes the material mass density, and $c > 0$ the specific heat capacity (the amount of heat required to raise the temperature of unit of mass of the material, at temperature $T$, by one degree,
- $k > 0$ represents the heat conductivity.

So, substituting the previous constitutive relations into the equation of balance of energy (local form), we get the heat equation:

$$\frac{\partial T}{\partial t} = \nabla \cdot (\kappa \nabla T), \quad \kappa = \frac{K}{\rho c}, \tag{34}$$

where $\kappa$ is the thermal diffusivity of the material. Examples of thermal conductivity values in $m^2/sec$ units (square meters per second):

- water: $1.4 \times 10^{-7}$,
- air : $2.2 \times 10^{-5}$,
- gold $1.27 \times 10^{-4}$ (best heat conductor).

3.2 A priori estimates on the heat equation: Uniqueness of solution

After having derived the heat equation, we give an example on how to use properties of the equation to obtain information on solutions. Let us consider the following initial boundary value problem. $\mathcal{D} \subset \mathbb{R}^n$, $n = 1, 2$ is an open, bounded set with smooth boundary $\partial \mathcal{D}$, and $\partial \mathcal{D}_i \subset \partial \mathcal{D}$, satisfying $\partial \mathcal{D}_1 \cup \partial \mathcal{D}_2 = \partial \mathcal{D}$, $\partial \mathcal{D}_1 \cap \partial \mathcal{D}_2 = \emptyset$. are as

$$\frac{\partial u}{\partial t} - \kappa \Delta u = 0, \quad \text{in } \mathcal{D} \tag{35}$$
$$u = 0, \quad \text{on } \partial \mathcal{D}_1, \tag{36}$$
$$\frac{\partial u}{\partial \mathbf{n}} = 0, \quad \text{on } \partial \mathcal{D}_2. \tag{37}$$

$\mathbf{n}$ denotes the outward unit normal vector to the boundary.
Theorem 3.1. Suppose that \( u : \mathcal{D} \rightarrow \mathbb{R} \) is a solution of the initial boundary value problem (38)-(41). Then it satisfies the following energy relation:

\[
\frac{1}{2} \frac{d}{dt} \int_{\mathcal{D}} u^2 \, dx = -\kappa \int_{\mathcal{D}} |\nabla u|^2 \, dx. \tag{38}
\]

Consequently,

\[
\int_{\mathcal{D}} u^2(x, t) \, dx \leq \int_{\mathcal{D}} u^2(x, 0) \, dx, \quad t \geq 0 \tag{39}
\]

holds.

Proof. We first multiply (38) by \( u(x, t) \) and integrate over \( \mathcal{D} \). Next, we apply the following vector identity to the term containing \( \Delta u \):

\[
u \Delta u = \nabla \cdot (u \nabla u) - |\nabla u|^2. \tag{40}\]

These yield the equation

\[
\frac{1}{2} \frac{d}{dt} \int_{\mathcal{D}} u^2 \, dx + \kappa \int_{\mathcal{D}} |\nabla u|^2 \, dx - \int_{\partial \mathcal{D}} u \frac{\partial u}{\partial n} \, dS = 0. \tag{41}
\]

Note that we have applied the divergence theorem to the volume integral of the term \( \nabla \cdot (u \nabla u) \), resulting in the surface integral in (38). The result follows by applying the boundary conditions (42) and (43) on this surface integral term. \( \square \)

From this energy identity, uniqueness of solution of the inhomogeneous, linear heat equation follows. Specifically, consider the problem

\[
\begin{align*}
\frac{\partial u}{\partial t} - \kappa \Delta u &= f, \quad \text{in } \mathcal{D} \tag{42} \\
u &= \bar{u}, \quad \text{on } \partial \mathcal{D}_1, \tag{43} \\
\frac{\partial u}{\partial n} &= g, \quad \text{on } \partial \mathcal{D}_2, \tag{44}
\end{align*}
\]

where \( f, \bar{u} \) and \( g \) are prescribed, smooth fields.

Corollary Let \( u \) be a solution of the initial boundary value problem (38)-(41). Then it is unique. The proof follows by contradiction, that is, assuming that there are two distinct solutions \( u_1 \) and \( u_2 \) to the the problem (38)-(41).