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Chapter 1

The Modelling Process

1.1 Perspectives of the Modelling Process

Here we give an overview of the modelling process and describe a general procedural framework for the mathematical modelling of physical processes or situations that may be of interest. The key steps in this framework are usually best illustrated and understood in reference to model problems.

The modelling process begins with a physical problem or situation of interest. There will usually be a motivating reason for carrying out modelling in that we either wish for a better understanding of the problem or there are some issues or questions that require answers in the form of quantitative feedback. This gives an idea of what features of the process we are actually interested in. We intend to describe in a quantitative manner the important features of the system that we wish to study. Often, a relevant simulation of a process is also an efficient way, in both time and cost, to study the consequences of changing the process conditions.

Firstly, the key physical features of the problem are represented mathematically. This mathematical model is then analysed to obtain mathematical results, which can then be interpreted in the context of the original model. By initially setting out key objectives for the modelling, it is possible to determine whether these objectives are met. We can identify deficiencies, rectify them and then, if required, we can refine the model. This general modelling loop is illustrated in figure 1.1.

We begin by reducing the physical problem to the key ideas and then establishing a simple mathematical model incorporating these processes. The model ought to be a recognisable imitation of the real problem and it should be parsimonious i.e. we wish to minimise the initial number of variables/parameters without making the model too simplistic and comprising key features. Assumptions

are made and certain second order effects are neglected in order to make the model initially focus on key features. These effects may become significant in certain circumstances and can subsequently be included for a more sophisticated and realistic model if the initial analysis shows that this is required.

This process involves specification of objectives, choice of appropriate variables, identification of key parameters and then nondimensionalisation. The aims and objectives are very important as they are the criteria by which we judge results and they provide a direction in which to analyse the problem. Indeed, the subsequent model and analysis may highlight further effects or questions that require consideration. Obtaining an analytical or a numerical solution is not always necessary in determining a relevant answer to the original question.

In general we can carry out a combination of numerical and analytical techniques (such as perturbation and asymptotic analysis) on the mathematical model equations. We have to make judgements on which method to use and sometimes it is appropriate to try a combination of several techniques as the different methods often complement one another. Asymptotics give limiting behaviour of a set of equations whilst numerical analysis may encounter difficulties at these limits. On the other hand, numerical analysis is valid for regions where asymptotics would be of limited use. This is illustrated in figure 1.2.

There are many different physical processes that have the same underlying mathematical structure. Some areas have been investigated to a greater degree than others and their results can be used in the less developed application areas. The results need to be physically reinterpreted in specific areas of interest. This may be referred to as technology transfer (see figure 1.3).

Mathematical modelling is to some extent an open ended process where the results obtained can be analysed and the feedback used to check the validity of the conceptual model and thereby refine it. Often it is necessary to refine the model to give more realistic results, since the preliminary analysis that are performed are usually only partially successful in answering some or all of the initial objectives posed.

MODELLING PROCESS: OVERVIEW

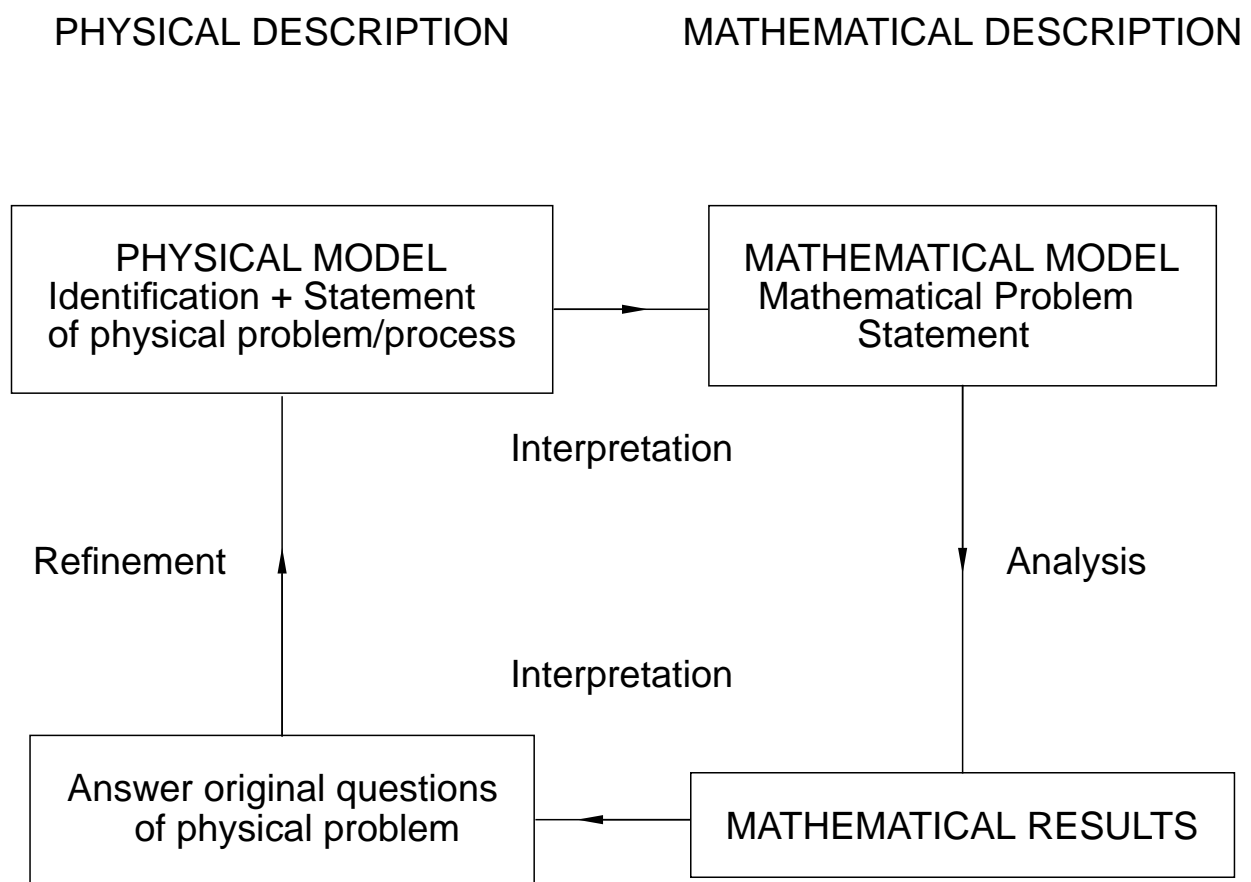


Figure 1.1: Modelling Process: Overview.

MODELLING PROCESS: ANALYSIS

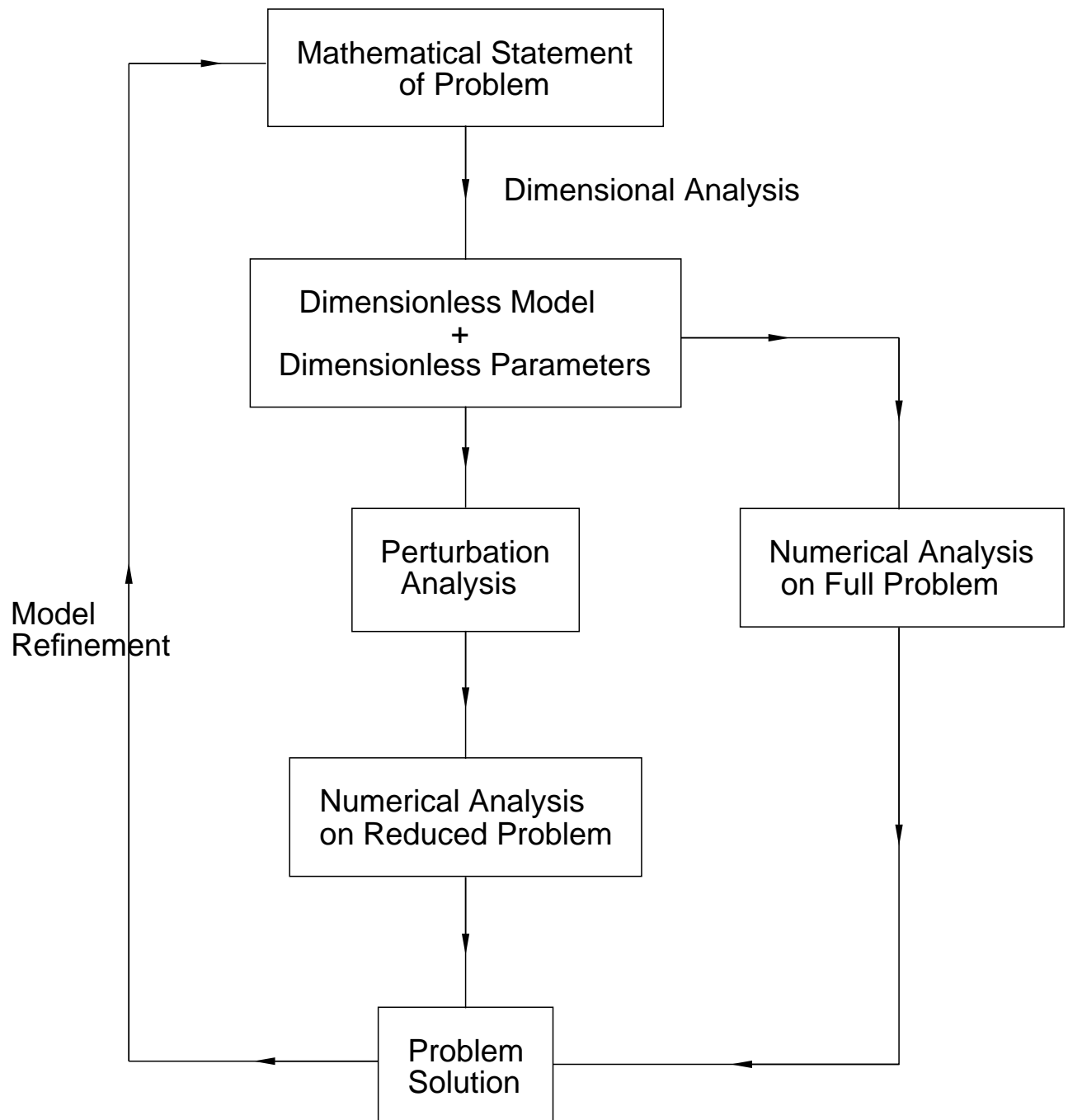
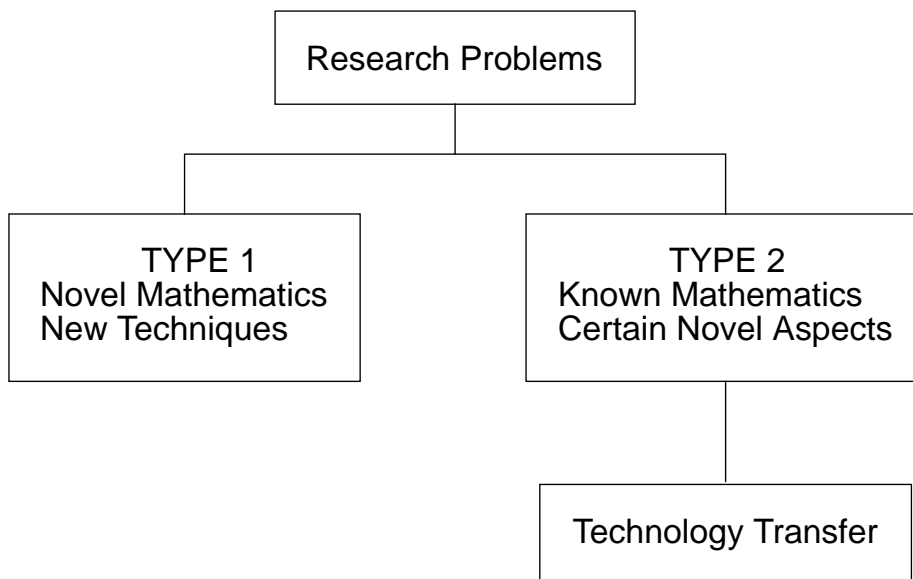


Figure 1.2: Modelling Process: Analysis.

RESEARCH PROBLEMS CLASSIFICATION



TECHNOLOGY TRANSFER

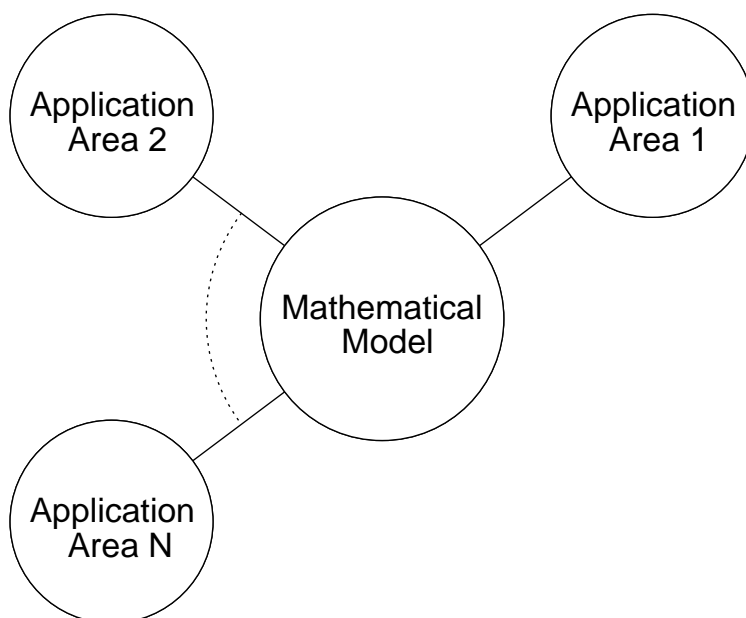


Figure 1.3: Research problems classification and technology transfer.

1.2 Mathematical Modelling in applied mechanics and the sciences

Applied mechanics is mathematics applied to problems which arise from continuum considerations.

A microscopic rather than an atomic or quantum view of the phenomena is adopted.

Attention is directed to those areas in which observations or experiments are reproducible and measured data are available in some form.

The objective is to construct a mathematical simulation or model of a given phenomenon that agrees with existing measurements to within a specified accuracy and can be used with confidence to predict future observations and behaviour.

Stemming from this continuous viewpoint the mathematical models will naturally involve relationships between continuous functions (variables) of space and time which describe the application of fundamental principles of homogeneity, isotropy and conservation to a given problem area.

To pursue mathematical modelling successfully, two contrasting but complementary skills are needed:

1. The ability to formulate a given problem in appropriate mathematical terms
2. Sufficient knowledge to obtain useful information from that mathematical model

The skill in formulation lies in finding a model which is simple enough to give useful information easily, but which is diverse enough to give all the information required with sufficient accuracy. A bottom-up approach is usually advocated rather than a top-down.

A model might be appropriate in one set of circumstances but of no value in others because it is either over-complicated or too simple.

The use of analogy between well-established models and new problems is a valuable aid.

1.3 The model building and formulation process

1. We start with a phenomenon of interest that we wish to describe or explain.
2. Observations of the phenomenon can lead to a hypothetical mechanism that can explain the phenomenon.
3. The purpose of a model is then to formulate a description of the mechanism in quantitative terms.
4. Analysis of the resulting model leads to results that can be tested against observations.
5. Ideally, the model also leads to predictions which if verified lend authenticity to the model.

Importantly, all model are idealisations and limited in applicability.

Sometimes we aim to over-simplify, the idea being that if the model is basically correct then it can subsequently be made more complicated and its analysis facilitated by considering the simpler version first.

Thus initially we consider the simplest situation and formulation of the problem that captures the essential features of the system.

In constructing a model, judgement is required about which features to include and which to neglect.

If an important feature is omitted then the model will not describe the observed phenomenon accurately enough or the model may not be self-consistent.

If unnecessary features are included then the model will be more difficult to solve due to its increased complexity.

The advice is to adopt a simple approach with a minimum of features included at first and then additional features added if necessary later i.e. a bottom-up approach.

1.4 Structure for a written report

1. Problem Background and Description/Introduction.

- Describe the essential features of the physical process.
- Identify objectives - key questions requiring answers.

2. Problem formulation.

- Identify key physical processes.
- Interpret these mathematically.
- Establish a mathematical model - governing equations and suitable initial conditions and boundary conditions.
- State clearly the assumptions.

3. Analysis.

- Non-dimensionalise
- Analogies with other related problems
- Use analytical and numerical methods to obtain solutions/results.

4. Results/Conclusions/Discussion.

- Interpret results with respect to the original physical process and objectives.
- Identify limitations and extensions

Chapter 2

Continuum Models

In formulating continuous models, there are 3 main ways of prescribing governing equations:

1. The classical procedure is to formulate exact conservation laws e.g. the laws of mass, momentum and energy in fluid mechanics.
2. Empirical conservation laws e.g. Darcy's law for fluid flow in a porous medium

$$\mathbf{v} = -\frac{k}{\mu}(\nabla p - \rho\mathbf{g})$$

where k is permeability, μ viscosity, p pressure, \mathbf{g} gravity and ρ the fluid density. Such laws may not be uniquely determined and may depend on the precise physical constitution of the fluid.

3. Hypothetical conservation laws. These are based on qualitative reasoning in absence of precise rules and usually involve phenomenological assumptions e.g. predator - prey models in mathematical biology. Usually such relationships have no quantitative basis.

When formulating new problems in mathematical terms it is valuable to have experience of successful models. Moreover many new problems are extensions or variations of the classical models.

2.1 Heat and mass transfer

Consider a material occupying a volume V with temperature $T = T(\mathbf{x}, t)$ with \mathbf{x} space, t time. Heat conservation gives

$$\frac{d}{dt} \int_V \rho c T dV = - \int_{\partial V} \mathbf{H} \cdot \mathbf{n} dS$$

where ρ is the density, c is the specific heat, \mathbf{n} is outward normal to V on its surface ∂V , \mathbf{H} is the heat flux vector. If applicable, a heat source term per unit volume is usually included as a additional term.

Assuming \mathbf{H} is continuously differentiable we have by the divergence theorem that

$$\int_V \left\{ \frac{\partial}{\partial t} (\rho c T) + \nabla \cdot \mathbf{H} \right\} dV = 0.$$

If the integrand is continuous and V is arbitrary then

$$\frac{\partial}{\partial t} (\rho c T) + \nabla \cdot \mathbf{H} = 0.$$

Fourier's Law gives $\mathbf{H} = -\mathbf{k} \nabla T$, where k is the thermal conductivity which is a constitutive law that is empirical or experimentally based (k can be measured for many materials). Hence

$$\frac{\partial}{\partial t} (\rho c T) = \nabla \cdot (k \nabla T).$$

If ρ, c and k are constant then we obtain the linear heat or diffusion equation

$$\frac{\partial T}{\partial t} = \kappa \nabla^2 T$$

where $\kappa = \frac{k}{\rho c}$ is the thermal diffusivity. If $k = k(T)$, but ρ, c are constant then we obtain the nonlinear heat equation

$$\rho c \frac{\partial T}{\partial t} = \nabla \cdot (k(T) \nabla T).$$

In a closed domain D the diffusion equation usually requires an initial condition and a boundary condition applied on the surface of the domain ∂D . The main types of boundary conditions are:

1. Dirichlet conditions: $T = f(\mathbf{x}, t)$ on ∂D which apply to a conducting surface.

2. Neumann boundary conditions: $-k \frac{\partial T}{\partial n} = q(\mathbf{x}, t)$ on ∂D

where $\frac{\partial T}{\partial n} = \mathbf{n} \cdot \nabla T$ and \mathbf{n} is the unit outward normal from D on ∂D .

3. Mixed or Robin boundary conditions:

$$-k \frac{\partial T}{\partial n} = h(T - T_u) \quad \text{on} \quad \partial D$$

where h is the heat transfer coefficient, T_0 is the temperature of the surroundings.

An analogous set of equations arise in mass transfer problems particular the diffusion of a solute in a liquid. The flux is determined by Fick's law

$$\mathbf{H} = -D\nabla c$$

where c is the concentration of the solute and gives

$$\frac{\partial c}{\partial t} = \nabla \cdot (D \nabla c).$$

The Stefan problem

Differential equations subject to conditions on the boundary of a known domain are termed boundary-value problems. In certain problems the domain is not known in advance but has to be determined as part of the solution. The term free boundary problem is used when the boundary is stationary (and a steady-state problem exists). be determined as a function of time and space. The term moving boundary problem is used when the boundary has to be determined as a function of time and space.

A simple version of the Stefan problem is the melting of a semi-infinite sheet of ice initially at the melting temperature of zero. At time $t = 0$ the surface of the ice at $x = 0$ is raised to a temperature $T_0 > 0$ and maintained. An interface on which melting occurs moves into the ice and separates a region of water (a liquid phase) from one of ice (a solid phase) at zero temperature. Denoting the position of the water/ice interface at time t by $S(t)$ then the problem formulation for the temperature $T(x, t)$ is

$$\text{in } 0 < x < s(t), \quad t > 0 \quad \rho c \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial x^2}, \quad (2.1)$$

$$\text{at } x = 0 \quad T = T_0, \quad (2.2)$$

$$\text{at } x = s(t) \quad T = 0, \quad -k \frac{\partial T}{\partial x} = L\rho \frac{ds}{dt}, \quad (2.3)$$

$$\text{at } t = 0 \quad s = 0, \quad (2.4)$$

where L is the latent heat per unit mass required to melt the ice, ρ, c, k are the density, specific heat and conductivity of the water phase. The second condition in (2.3) is termed the Stefan condition and expresses heat balance on the interface. It is needed to determine the position of the interface $s(t)$. We have to solve for both $T(x, t)$ and $s(t)$.

This is a one-phase problem since the temperature variation in the ice is unimportant. If the temperature of the ice initially was below melting temperature then heat flow will occur in the ice and a two-phase problem results.

2.2 Fluid mechanics

To describe the motion of a fluid (liquid or gas) the continuum hypothesis is that the locally averaged velocity vector field \mathbf{v} is a twice continuously differentiable function of \mathbf{x} and t .

Conservation of mass gives the continuity equation

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{v} = 0$$

where ρ is the fluid density and

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla$$

is the material derivative.

Conservation of linear momentum gives

$$\rho \frac{Dv_i}{Dt} = \frac{\partial \sigma_{ij}}{\partial x_j} + \rho F_i \quad i = 1, 2, 3,$$

where \mathbf{F} is the body force per unit mass, σ_{ij} is the stress tensor (second order).

Conservation of angular momentum gives that the stress tensor is symmetric i.e. $\sigma_{ij} = \sigma_{ji}$. For a conducting fluid with temperature T , conservation of energy gives

$$\rho \frac{D(cT)}{Dt} = \nabla \cdot (k \nabla T) + \Phi$$

where c is the specific heat capacity and

$$\Phi = \sigma_{ij} \frac{\partial v_i}{\partial x_j}$$

is usually a source term.

An equation of state usually relates ρ to pressure p and temperature T e.g. for gases $p = \rho RT$, where R ideal gas constant, whilst for liquids $\frac{D\rho}{Dt} = 0$ is taken i.e. that they are incompressible.

The constitutive equation relates stress to the rate of strain:

- For an inviscid fluid $\sigma_{ij} = -p\delta_{ij}$ where p is the pressure .
- For a Newtonian fluid $\sigma_{ij} = -p\delta_{ij} + T_{ij}$ where T_{ij} is the deviatoric stress tensor given by

$$T_{ij} = \lambda \frac{\partial v_k}{\partial x_k} \delta_{ij} + \mu \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) = \lambda \nabla \cdot \mathbf{v} \delta_{ij} + 2\mu \epsilon_{ij}$$

where μ is the dynamic shear viscosity, λ is the bulk viscosity and ϵ_{ij} is the rate of strain tensor.

- For a viscoelastic fluid, the Upper Convected Maxwell model is

$$T_{ij} + \lambda_1 \left\{ \frac{D}{Dt} T_{ij} - T_{ik} \frac{\partial v_k}{\partial x_j} - \frac{\partial v_k}{\partial x_i} T_{kj} \right\} = 2\mu \epsilon_{ij}$$

where λ_1 is the relaxation time.

For an incompressible Newtonian fluid we have the Navier-Stokes equations

$$\nabla \cdot \mathbf{v} = 0, \quad \rho \frac{D\mathbf{v}}{Dt} = -\nabla p + \mu \nabla^2 \mathbf{v} + \rho \mathbf{F}.$$

If $\mu = 0$, we obtain the Euler equations for inviscid flow.

In the energy equation we have $\Phi = 2\mu(\epsilon_{ij})^2$ representing viscous dissipation.

On a stationary solid boundary we can impose no-slip and solid wall condition i.e. $\mathbf{v} = \mathbf{0}$.

The traction vector \mathbf{t} has components $t_i = \sigma_{ij} n_j$ and represents the force per unit area exerted by a fluid on a surface with unit normal \mathbf{n} into the fluid.

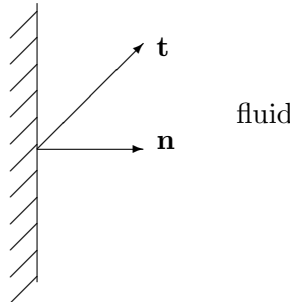


Figure 2.1: Stress \mathbf{t} exerted by the fluid on the boundary with normal \mathbf{n} .

At a free surface e.g. air-water interface we usually prescribe continuity of velocity and stress. If surface tension is taken into account then balancing the stresses gives

$$\sigma_{ij}^{(1)} n_j - \sigma_{ij}^{(2)} n_j = -\gamma \kappa n_i \quad i = 1, 2, 3$$

where $t_i^{(1)} = \sigma_{ij}^{(1)} n_j$, $t_i^{(2)} = \sigma_{ij}^{(2)} n_j$ are the i th component of the stresses, \mathbf{n} is a unit normal from fluid (2) into fluid (1), γ is the surface tension coefficient and κ is the curvature. The surface tension acts in the direction of the normal to the interface.

If fluid (1) is air which exerts a constant pressure p_a only then $t_i^{(1)} = \sigma_{ij}^{(1)} n_j = -p_a n_i$.

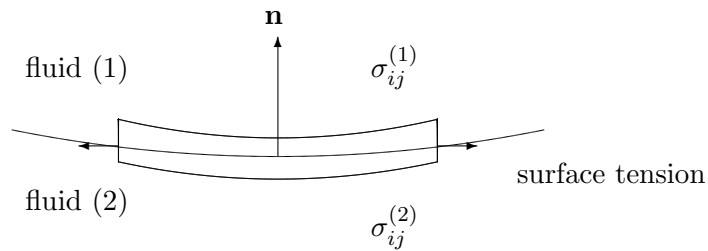


Figure 2.2: Stress exerted on an interface between two fluids with surface tension effects included.

For a plane curve $y = \eta(x, t)$ the curvature is

$$\kappa = \frac{\eta_{xx}}{(1 + \eta_x^2)^{3/2}}$$

and in general $\kappa = \frac{1}{R_1} + \frac{1}{R_2}$ where R_1, R_2 are the radii of curvature of the interface in any two orthogonal directions.

In addition at a free surface, the kinematic boundary condition is usually imposed. This is simply that fluid elements in the surface remain there. Denoting the surface by $f(\mathbf{x}, t) = 0$ then

$$\text{On } f(\mathbf{x}, t) = 0 \quad \frac{D}{Dt}f(\mathbf{x}, t) = 0 \implies \frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f = 0.$$

Since the surface can move, its determination is part of the problem and this is the extra condition necessary to specify the problem analogous to the Stefan condition in the melting ice problem.

2.3 Mathematical Finance: Option pricing

Options are some of the commonest examples of derivative securities (also termed financial derivatives or simply derivatives).

A European call option is a contract with the following conditions:

- At a prescribed time in the future known as the expiry date
- the holder of the option may purchase a prescribed asset known as the underlying asset or simply the underlying
- for a prescribed amount known as the exercise or strike price.

The holder of the option (i.e. the buyer of the option) has the right but not the obligation to purchase the underlying at the exercise price at expiry.

The writer of the option (i.e. the seller of the option) must sell the underlying at the exercise price if the holder chooses to buy it.

A European put option is a contract that allows the holder of the option to sell the underlying asset at the exercise price at expiry date. The writer of the put option must buy the underlying asset at the exercise price at expiry if the holder chooses to sell.

American call and put options are similar to European call and put options except that they may be exercised at any time prior to and including expiry.

A simple model for asset prices

Let S be the asset price at time t . Then a simple stochastic differential equation for S is

$$\frac{dS}{S} = \mu dt + \sigma dX \quad (2.5)$$

where μ is the drift (a constant)

σ is the volatility (a constant)

$dX \sim N(0, dt)$ i.e. a normal r.v. with mean 0, variance dt

dS is change in asset price in time interval dt (a Wiener process)

This is consistent with the efficient market hypothesis:

- Past history is fully reflected in the current price and does not hold any further information.
- Markets respond immediately to new information on an asset.

Thus changes in the asset price are a Markov process. Note that (2.5) does not refer to past history of asset price and next asset price $S + dS$ depends only on today's price (Markov property).

$$E[ds] = \mu S dt, \quad var[ds] = \sigma^2 S^2 dt$$

i.e. S undergoes a log normal random walk.

Itô's Lemma

Let $dS = \mu S dt + \sigma S dX$ and consider $f = f(S, t)$. Then

$$\begin{aligned} df &= f(S + dS, t + dt) - f(S, t) \\ &= dS \frac{\partial f}{\partial S} + dt \frac{\partial f}{\partial t} + \frac{1}{2} dS^2 \frac{\partial^2 f}{\partial S^2} + \frac{1}{2} dt^2 \frac{\partial^2 f}{\partial t^2} + dS dt \frac{\partial^2 f}{\partial S \partial t} + O(dS^3, dt dS^2, dt^2 dS, dt^3) \\ &= (\sigma S dX + \mu S dt) \frac{\partial f}{\partial S} + dt \frac{\partial f}{\partial t} + \frac{1}{2} \sigma^2 S^2 dt \frac{\partial^2 f}{\partial S^2} + O(dX dt) \end{aligned}$$

(since $dX^2 \rightarrow dt$ with probability 1 and hence $dS^2 \rightarrow \sigma^2 S^2 dt$). Thus

$$df = \sigma \frac{\partial f}{\partial S} dX + \left(\frac{\partial f}{\partial t} + \mu S \frac{\partial f}{\partial S} + \frac{1}{2} \sigma^2 S^2 \frac{\partial^2 f}{\partial S^2} \right) dt \quad \text{as } dt \rightarrow 0.$$

Black-Scholes analysis

Let $V(S, t)$ denote the value of an option that depends only on the underlying asset price S and time t .

Consider a portfolio consisting of one option and a number $(-\Delta)$ of the underlying asset. Let the value of this portfolio be Π where

$$\Pi = V - \Delta S.$$

Then the change in the value of this portfolio in a small time step dt is

$$d\Pi = dV - \Delta dS$$

where Δ is held fixed during the small time step dt .

By *Itô's lemma*, the random walk followed by V is

$$dV = \sigma S \frac{\partial V}{\partial S} dX + \left(\mu S \frac{\partial V}{\partial S} + \frac{1}{2} \sigma^2 S^2 \frac{\partial^2 V}{\partial S^2} + \frac{\partial V}{\partial t} \right) dt$$

and hence Π follows the random walk

$$d\Pi = \sigma S \left(\frac{\partial V}{\partial S} - \Delta \right) dX + \left(\mu S \frac{\partial V}{\partial S} + \frac{1}{2} \sigma^2 S^2 \frac{\partial^2 V}{\partial S^2} + \frac{\partial V}{\partial t} - \mu \Delta S \right) dt.$$

Choosing $\Delta = \frac{\partial V}{\partial S}$ (the value at the start of the short-time step dt) then

$$d\Pi = \left(\frac{\partial V}{\partial t} + \frac{1}{2} \sigma^2 S^2 \frac{\partial^2 V}{\partial S^2} \right) dt$$

which is wholly deterministic.

Assuming no arbitrage (and no transaction costs) then the return on the portfolio Π must be that at the risk free interest rate r . Thus $d\Pi = r\Pi dt$ which gives the Black-Scholes (B-S) pde

$$\frac{\partial V}{\partial t} + \frac{1}{2} \sigma^2 S^2 \frac{\partial^2 V}{\partial S^2} + rS \frac{\partial V}{\partial S} - rV = 0.$$

Remarks:

- $\Delta = \frac{\partial V}{\partial S}$ is termed the delta of the option
- the drift μ is absent in the B-S equation
- B-S equations is a backwards diffusion equation

Required assumptions:

1. The underlying asset price follows a lognormal random walk.
2. The risk-free interest rate r and the asset volatility σ are known functions of time over the life of the option.
3. There are no transaction costs associated with hedging a portfolio.
4. The underlying asset pays no dividends during the life of the option.
5. No arbitrage possibilities.
6. Trading of the underlying asset can take place continuously.
7. Short selling is permitted and the assets are divisible.

A European call option $C(S, t)$

Let $C(S, t)$ denote the value of an European call option

E be the exercise price

T be the expiry time.

Then C satisfies

$$\frac{\partial C}{\partial t} + \frac{1}{2}\sigma^2 S^2 \frac{\partial^2 C}{\partial S^2} + rS \frac{\partial C}{\partial S} - rC = 0 \quad 0 < t < T, 0 < S < \infty.$$

As boundary conditions we take

$$\text{at } S = 0 \quad C = 0,$$

i.e. if S is ever zero then it remains zero and

$$\text{as } S \rightarrow \infty \quad C \sim S.$$

As a final condition we take

$$\text{at } t = T \quad C = \begin{cases} 0 & \text{if } S < E, \\ S - E & \text{if } S \geq E, \end{cases}$$

i.e. $C(S, T) = \max(S - E, 0)$ which is termed the pay off function.

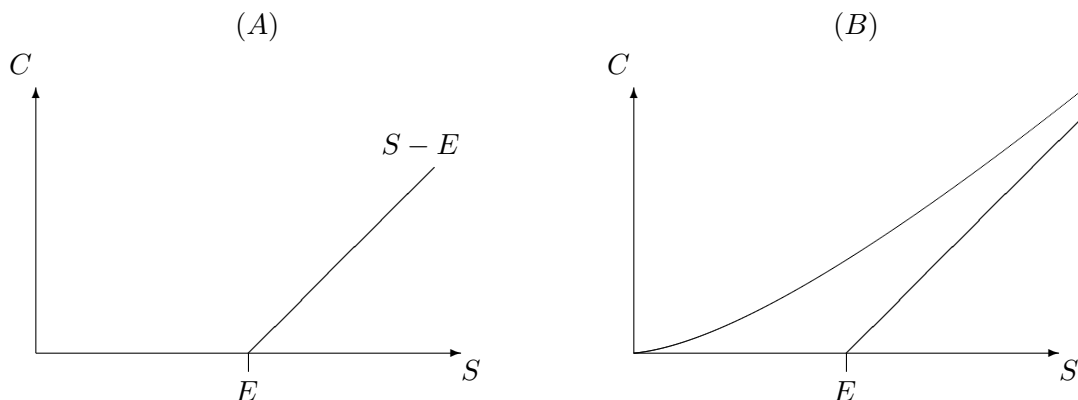


Figure 2.3: (A) illustrates the pay-off function or intrinsic value i.e. $C(S, T)$. (B) shows schematically the solution $C(S, t)$ at time t earlier than expiry T .

A European put option $P(S, t)$.

$$\begin{array}{ll}
 \text{in } 0 < S < \infty, \quad 0 < t < T & \frac{\partial P}{\partial t} + \frac{1}{2}\sigma^2 S^2 \frac{\partial^2 P}{\partial S^2} + rS \frac{\partial P}{\partial S} - rP = 0, \\
 \text{at } S = 0 & P = Ee^{-r(T-t)}, \\
 \text{as } S \rightarrow \infty & P \rightarrow 0, \\
 \text{at } t = T & P(S, T) = \max(E - S, 0).
 \end{array}$$

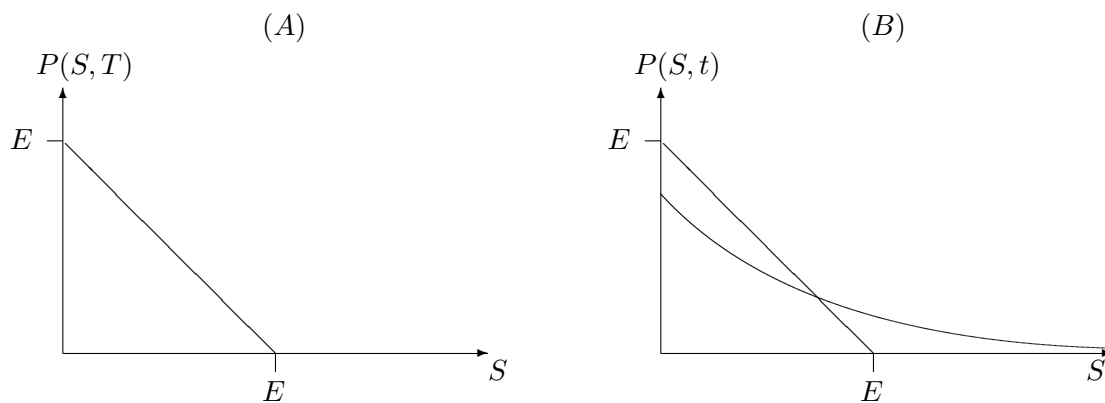


Figure 2.4: (A) illustrates the pay-off function or intrinsic value i.e. $P(S, T)$. (B) shows schematically the solution $P(S, t)$ at time t earlier than expiry T .

The American Put option $P(S, t)$

Early exercise of the option is possible leading naturally to a moving boundary $S_f(t)$ where the option is exercised if $S \leq S_f(t)$ and held if $S > S_f(t)$.

Suppose $P(S, t) < \max(E - S, 0)$ the intrinsic value or pay-off function then there exists an immediate arbitrage opportunity:

- buy the asset for S
- buy the put for P
- immediately exercise the put for E

to give $E - S - P > 0$ as a risk-free profit.

Thus when early exercise is possible then $P(S, t) \geq \max(E - S, 0)$.

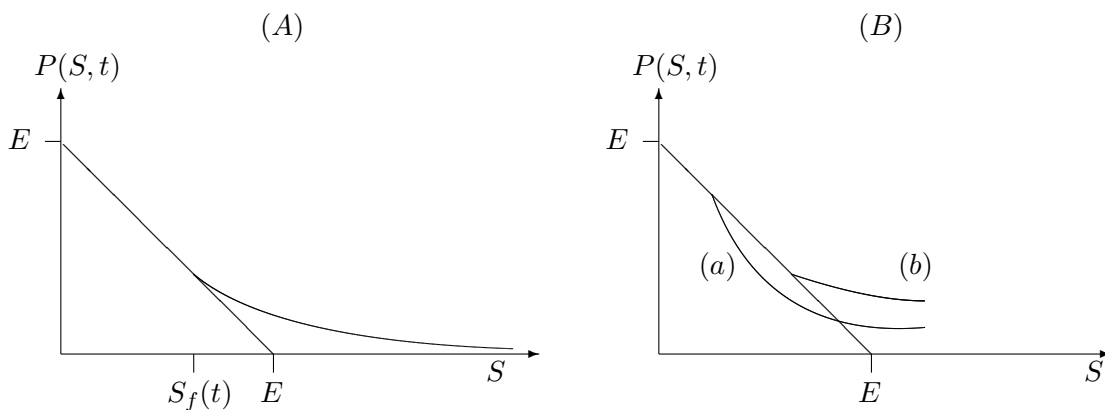


Figure 2.5: (A) illustrates schematically the solution American put solution $P(S, t)$ at time $t < T$. (B) illustrates two alternative situations in which the solution may meet the pay-off function; in (a) $\frac{\partial P}{\partial S} < -1$ and in (b) $\frac{\partial P}{\partial S} > -1$.

in $0 < S < S_f(t)$	$P = E - S,$
in $S_f(t) < S < \infty$	$\frac{\partial P}{\partial t} + \frac{1}{2}\sigma^2 S^2 \frac{\partial^2 P}{\partial S^2} + rS \frac{\partial P}{\partial S} - rP = 0,$
at $S = S_f(t)$	$P = \max(E - S_f(t), 0), \quad \frac{\partial P}{\partial S} = -1,$
as $S \rightarrow \infty$	$P \rightarrow 0,$
at $t = T$	$P = \max(E - S, 0), \quad S_f(T) = E.$

Chapter 3

Nondimensionalisation

The first and arguably the most important step in the analysis of a system of differential equations.

It involves scaling each variable (dependent and independent) by a typical or reference value, leaving a nondimensional variable whose typical scale is $O(1)$.

Nondimensionalisation or problem normalisation has several important uses:

1. It identifies the dimensionless groups (ratios of dimensional parameters) which control the solution behaviour.
2. Terms in the equations are now dimensionless and so allows comparison of their sizes.

This allows the identification of the important (i.e. dominant) terms in the equations and their interaction in different regimes, giving insight into the structure of solutions and the dominant physical mechanisms at work.

In particular, negligible terms can be identified leading to simplification in many circumstances.

3. It allows estimates of the effects of additional features to the original model through the new dimensional group(s) associated with the additional term(s). This allows measurement of the effect of the physical feature(s) in the model.
4. Finally, it can reduce the number of parameters occurring in the problem by forming the nondimensional parameters or dimensionless groups.

3.1 Scaling

If an equation has a variable u , say, then we nondimensionalise that variable by writing, for example,

$$u = [u]\bar{u}$$

where $[u]$ is the chosen scale (with the same dimensions as u) and \bar{u} is the corresponding dimensionless variable. If a system of equations describes a real process then it is dimensionally homogeneous i.e. consistent. The process of nondimensionalisation will necessarily give a set of equations, each of whose terms is dimensionless, after division through by the dimensions of the equations. It is then possible to compare terms in a meaningful way.

The art of nondimensionalisation lies in the choice of scales. There is no right or wrong way to do it (other than to only partially nondimensionalise the equations) and in more complicated problems, the choice of scales can be the difficult part of the analysis. The basic principle is that the scales must ultimately be chosen self-consistently by balancing terms in the equations. Because the purpose is to obtain ‘properly scaled’ equations in which the largest dimensionless terms are numerically of $O(1)$, the simplest choices arise when the scales can be chosen so that all the dimensionless parameters are $O(1)$.

This provides our rationale. Given no other information, one assumes a priori that dimensionless variables and their derivatives are $O(1)$, until we are forced to assume otherwise. It is only when inconsistencies arise that the process of rescaling becomes necessary. The generic situation in which this happens is where singular perturbation theory is appropriate. In general, not all dimensionless parameters can be chosen to be $O(1)$, in which case they are first assumed to be $O(1)$ and then the limit in which they become large is taken.

3.2 Examples

3.2.1 Example 1

The number of atoms $N(t)$ at time t of a radioactive substance is governed by the differential equation

$$\frac{dN}{dt} = -\lambda N$$

with an initial condition $N = N_0$ at $t = 0$. Here λ is a decay constant with units of $[\text{time}]^{-1}$.

We nondimensionalise as follows

$$N = N_0 \bar{N}, \quad t = \frac{\bar{t}}{\lambda},$$

where N_0 is taken as the reference value for N and $1/\lambda$ for the time scale. This gives the dimensionless problem

$$\frac{d\bar{N}}{d\bar{t}} = -\bar{N} \quad \text{with } \bar{N} = 1 \text{ at } \bar{t} = 0,$$

for $\bar{N}(\bar{t})$.

3.2.2 Example 2

The motion of a linearly damped pendulum is governed by the equation

$$\ell \frac{d^2\theta}{dt^2} + k \frac{d\theta}{dt} + g \sin \theta = 0, \quad (3.1)$$

with the initial conditions

$$\text{at } t=0 \quad \theta = \theta_0 \quad \text{and} \quad \frac{d\theta}{dt} = \omega_0. \quad (3.2)$$

Here $\theta(t)$ represents the angle that the pendulum makes to the vertical at time t , the initial angle being θ_0 and initial angular speed ω_0 . The dimensional parameters are the length ℓ of the pendulum, the coefficient of resistance k and acceleration due to gravity g .

We nondimensionalise as follows

$$\theta = \theta_0 \bar{\theta}, \quad t = \frac{\theta_0}{\omega_0} \bar{t},$$

using the initial values to give characteristic scales for the dependent variable θ and independent variable t . Thus we obtain the dimensionless problem

$$\frac{d^2\bar{\theta}}{d\bar{t}^2} + K \frac{d\bar{\theta}}{d\bar{t}} + G \sin(\theta_0 \bar{\theta}) = 0, \quad (3.3)$$

subject to

$$\text{at } \bar{t} = 0 \quad \bar{\theta} = 1 \quad \text{and} \quad \frac{d\bar{\theta}}{d\bar{t}} = 1, \quad (3.4)$$

where we have introduced the dimensionless parameters

$$K = \frac{k\theta_0}{\omega_0\ell}, \quad G = \frac{g\theta_0}{\omega_0^2\ell},$$

in addition to θ_0 .

The dimensional problem has 5 parameters, the four dimensional parameters ℓ, k, g, ω_0 and the dimensionless parameter θ_0 . The dimensionless problem has three dimensionless parameters K, G, θ_0 .

If observational values are available for the parameters $\ell, k, g, \omega_0, \theta_0$ then these may be used to infer the sizes of the dimensionless groups K, G, θ_0 . The sizes of these dimensionless parameters determine whether they are to be taken as $O(1)$ or a suitable limit needs to be considered in which their values are small or large. The latter cases lead to either a regular or singular perturbation problem.

As an example, suppose we have the situation in which $\theta_0 = \pi/4$ radians, $\omega_0 = 1$ radian per second, $\ell = 1$ m, $k = 0.1$ m/s and $g = 10$ m/s². Then $K \approx 0.079, G \approx 7.9, \theta_0 \approx 0.79$. Thus we are interested in analyzing the dimensionless problem in the limit $K \rightarrow 0$ with $G = O(1), \theta_0 = O(1)$ which should be regular.

If in contrast $k = 100$ m/s then we would have $K \approx 79, G \approx 7.9, \theta_0 \approx 0.79$. Thus we are now interested in analyzing the dimensionless problem in the limit $K \rightarrow \infty$ with $G = O(1), \theta_0 = O(1)$ which is singular.

3.2.3 Example 3

Consider the following boundary-value problem (BVP) for one-dimensional heat flow in a bar,

$$\text{in } 0 < x < \ell, \quad t > 0 \quad \rho c \frac{\partial u}{\partial t} = k \frac{\partial^2 u}{\partial x^2} + q, \quad (3.5)$$

$$\text{at } x = 0 \quad u = u_0, \quad (3.6)$$

$$\text{at } x = \ell \quad -k \frac{\partial u}{\partial x} = h(u - u_i), \quad (3.7)$$

$$\text{at } t = 0 \quad u = u_i, \quad (3.8)$$

where u_i is the initial temperature (which is also the external surrounding temperature), u_0 is the temperature at the end of the bar which is raised above u_i , h denotes the heat transfer coefficient, ρ, c, k denote the density, specific heat and conductivity of the bar respectively. The length of the bar is ℓ and q represents a constant heat source term. All variables are assumed dimensional, this being the statement of the dimensional problem.

We nondimensionalise as follows

$$x = \ell \bar{x}, \quad t = \frac{\ell^2}{\kappa} \bar{t}, \quad u = u_i + (u_0 - u_i) \bar{u},$$

with $\kappa = k/\rho c$ and introduce the two dimensionless parameters

$$Q = \frac{q \ell^2}{k(u_0 - u_i)}, \quad H = \frac{h \ell}{k},$$

to obtain

$$\text{in } 0 < \bar{x} < 1, \bar{t} > 0 \quad \frac{\partial \bar{u}}{\partial \bar{t}} = \frac{\partial^2 \bar{u}}{\partial \bar{x}^2} + Q, \quad (3.9)$$

$$\text{at } \bar{x} = 0 \quad \bar{u} = 1, \quad (3.10)$$

$$\text{at } \bar{x} = 1 \quad -\frac{\partial \bar{u}}{\partial \bar{x}} = H\bar{u}, \quad (3.11)$$

$$\text{at } \bar{t} = 0 \quad \bar{u} = 0. \quad (3.12)$$

It is assumed that H, Q are $O(1)$ quantities. If they are not, then the appropriate limit needs to be taken which will lead to either a regular or singular perturbation problem.

3.2.4 Example 4

Consider the Navier-Stokes equations of an incompressible Newtonian viscous fluid

$$\begin{aligned} \nabla \cdot \mathbf{v} &= 0, \\ \rho \left(\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} \right) &= -\nabla p + \mu \nabla^2 \mathbf{v} + \rho \mathbf{F}, \\ \rho c \left(\frac{\partial T}{\partial t} + (\mathbf{v} \cdot \nabla) T \right) &= k \nabla^2 T + \Phi, \end{aligned}$$

where \mathbf{v} is the velocity, p is the pressure, T is the temperature and are functions of spatial coordinates \mathbf{x} and time t . Also,

$$\Phi = \frac{1}{2} \mu \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right)^2$$

is the viscous dissipation term. The dimensional parameters of density ρ , specific heat c , conductivity k and viscosity μ are assumed constant.

The body force per unit mass \mathbf{F} is assumed to be gravity so that $\mathbf{F} = \mathbf{g} = g\bar{\mathbf{g}}$ with $g = |\mathbf{g}|$.

These equations arise from the application of the physical laws of conservation of mass, momentum and energy.

In the momentum equation, the physical effects modelled are: inertia, viscous forces, gravity respectively.

In the heat equation, the physical effects modelled are: heat convection (or advection), heat conduction, viscous dissipation respectively.

The problem is completed by specification of suitable boundary conditions to give a well-posed BVP.

Consequently typical scales or reference values for the variables will be given.

Let U be a typical velocity scale

L be a typical length

$T_1 - T_0$ be a typical temperature deviation (T_0 is an ambient or equilibrium temperature)

then we may nondimensionalise as follows

$$\mathbf{x} = L\bar{\mathbf{x}}, \quad \mathbf{v} = U\bar{\mathbf{v}}, \quad t = \frac{L}{U}\bar{t}, \quad p = P\bar{p}, \quad T = T_0 + (T_1 - T_0)\bar{T},$$

where P is to be determined, which gives

$$\begin{aligned} \bar{\nabla} \cdot \bar{\mathbf{v}} &= 0, \\ \left(\frac{\partial \bar{\mathbf{v}}}{\partial \bar{t}} + (\bar{\mathbf{v}} \cdot \bar{\nabla}) \bar{\mathbf{v}} \right) &= -\frac{P}{\rho U^2} \bar{\nabla} \bar{p} + \frac{\mu}{\rho U L} \bar{\nabla}^2 \bar{\mathbf{v}} + \frac{Lg}{U^2} \bar{\mathbf{g}}, \\ \left(\frac{\partial \bar{T}}{\partial \bar{t}} + (\bar{\mathbf{v}} \cdot \bar{\nabla}) \bar{T} \right) &= \frac{k}{\rho c U L} \bar{\nabla}^2 \bar{T} + \frac{\mu U}{\rho c L (T_1 - T_0)} \bar{\Phi}, \end{aligned}$$

where

$$\bar{\Phi} = \frac{1}{2} \left(\frac{\partial \bar{v}_i}{\partial \bar{x}_j} + \frac{\partial \bar{v}_j}{\partial \bar{x}_i} \right)^2, \quad \bar{\nabla} = \left(\frac{\partial}{\partial \bar{x}_1}, \frac{\partial}{\partial \bar{x}_2}, \frac{\partial}{\partial \bar{x}_3} \right).$$

Introduce the dimensionless parameters

Reynolds number $Re = \frac{\rho U L}{\mu}$ compares effects of inertia and viscous forces

Froude number $Fr = \frac{U^2}{Lg}$ compares inertia and gravity

Peclet number $Pe = \frac{\rho c U L}{k} = \frac{UL}{\mu U^{\frac{k}{\rho c}}}$ compares convection to conduction

Brinkman number $Br = \frac{\mu U^2}{k(T_1 - T_0)}$ compares viscous dissipation with heat conduction

Prandtl number $Pr = \frac{\mu c}{k} = \frac{Pe}{Re}$ compares viscous terms to those of heat conduction

Hence we have

$$\begin{aligned} \bar{\nabla} \cdot \bar{\mathbf{v}} &= 0, \\ \left(\frac{\partial \bar{\mathbf{v}}}{\partial \bar{t}} + (\bar{\mathbf{v}} \cdot \bar{\nabla}) \bar{\mathbf{v}} \right) &= -\bar{\nabla} \bar{p} + \frac{1}{Re} \bar{\nabla}^2 \bar{\mathbf{v}} + \frac{1}{Fr} \bar{\mathbf{g}}, \\ \left(\frac{\partial \bar{T}}{\partial \bar{t}} + (\bar{\mathbf{v}} \cdot \bar{\nabla}) \bar{T} \right) &= \frac{1}{Pe} \bar{\nabla}^2 \bar{T} + \frac{Br}{Pe} \bar{\Phi}, \end{aligned}$$

where we have chosen $P = \rho U^2$ i.e. the pressure scale is based on inertial forces.

The choice of pressure scale is not unique and could have been based on viscous forces so that

$$P = \frac{\mu U}{L} = \frac{\rho U^2}{Re}.$$

The appropriate scalings are dictated by the problem and the numerical values of the dimensionless parameters.

The identification of dimensionless parameters allows model similitude i.e. a model will represent (dynamically similar to) a practical situation if the values of the dimensionless parameters are the same for both.

The limits of large and small Reynolds number Re are of particular interest.

Simplification of the equations by neglecting a term multiplied by a small dimensionless parameter is the first step in a systematic procedure for obtaining an asymptotic expansion for the full solution in terms of the small parameter.

If we consider the above model with $1/Pr = Br = 0$ and no temperature variation then

$$\bar{\mathbf{v}} = \bar{\mathbf{v}}(\bar{\mathbf{x}}, \bar{t}, Re) \quad \text{and} \quad \bar{p} = \bar{p}(\bar{\mathbf{x}}, \bar{t}, Re).$$

If $Re \ll 1$ then we may expand in regular powers of Re to obtain the asymptotic expansions

$$\bar{p} = \bar{p}_0(\bar{\mathbf{x}}, \bar{t}) + Re \bar{p}_1(\bar{\mathbf{x}}, \bar{t}) + \dots, \quad \bar{\mathbf{v}} = \bar{\mathbf{v}}_0(\bar{\mathbf{x}}, \bar{t}) + Re \bar{\mathbf{v}}_1(\bar{\mathbf{x}}, \bar{t}, Re) + \dots,$$

where \bar{p}_0 and $\bar{\mathbf{v}}_0$ are the solutions to the simplified model with $Re = 0$.

This is a regular perturbation procedure and may be used if $\bar{p}(\bar{\mathbf{x}}, \bar{t}, Re)$ and $\bar{\mathbf{v}}(\bar{\mathbf{x}}, \bar{t}, Re)$ are regular functions of Re near $Re = 0$.

In some circumstances the expansion is invalid and a singular perturbation procedure must be used. In these cases the solution of the problem with $Re = 0$ and the solution for $Re \neq 0$ but $Re \ll 1$ are very different.

An example is the high Reynolds number flow $Re \gg 1$. A regular expansion in powers of $1/Re$ gives the inviscid flow equations at leading order. In this case the highest derivative term $\bar{\nabla}^2 \bar{\mathbf{v}}$ is neglected and consequently not all boundary conditions can be satisfied (usually the no slip condition). Thus thin regions develop where this term must be brought back, which are termed boundary layers.

3.2.5 Example 5

The one-phase Stefan problem for the temperature $T(x, t)$ in the water phase for a melting ice problem can be written as

$$\text{in } 0 < x < s(t), \quad t > 0 \quad \rho c \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial x^2}, \quad (3.13)$$

$$\text{at } x = 0 \quad T = T_0, \quad (3.14)$$

$$\text{at } x = s(t) \quad T = 0, \quad -k \frac{\partial T}{\partial x} = L\rho \frac{ds}{dt}, \quad (3.15)$$

$$\text{at } t = 0 \quad s = 0, \quad (3.16)$$

where $s(t)$ denotes the moving ice/water interface, L is the latent heat per unit mass, ρ, c, k are the density, specific heat and conductivity of the water. The water (liquid phase) occupies the region $0 < x < s(t)$ and the ice (solid phase) $x > s(t)$. Initially there is no water present i.e. $s(0)=0$. $T_0 (> 0)$ is the temperature of the water at the fixed boundary $x = 0$.

We nondimensionalise as follows

$$x = \ell \bar{x}, \quad s = \ell \bar{s}, \quad t = \beta \bar{t}, \quad T = T_0 \bar{T},$$

where the scales ℓ and β have to be found. The system (3.13)–(3.16) becomes

$$\text{in } 0 < \bar{x} < \bar{s}(\bar{t}), \quad \bar{t} > 0 \quad \frac{\partial \bar{T}}{\partial \bar{t}} = \frac{k}{\rho c} \frac{\beta}{\ell^2} \frac{\partial^2 \bar{T}}{\partial \bar{x}^2}, \quad (3.17)$$

$$\text{at } \bar{x} = 0 \quad \bar{T} = 1, \quad (3.18)$$

$$\text{at } \bar{x} = \bar{s}(\bar{t}) \quad \bar{T} = 0, \quad -\frac{\partial \bar{T}}{\partial \bar{x}} = \frac{L\rho}{kT_0} \frac{\ell^2}{\beta} \frac{d\bar{s}}{d\bar{t}}, \quad (3.19)$$

$$\text{at } \bar{t} = 0 \quad \bar{s} = 0, \quad (3.20)$$

The governing equation (3.17) suggests

$$\beta = \frac{\rho c}{k} \ell^2,$$

and the Stefan condition on the moving interface then suggests introducing the dimensionless parameter λ where

$$\lambda = \frac{L\rho}{kT_0} \frac{\ell^2}{\beta} = \frac{L}{cT_0},$$

which is commonly termed the Stefan number. The dimensionless problem is thus

$$\text{in } 0 < \bar{x} < \bar{s}(\bar{t}), \quad \bar{t} > 0 \quad \frac{\partial \bar{T}}{\partial \bar{t}} = \frac{\partial^2 \bar{T}}{\partial \bar{x}^2}, \quad (3.21)$$

$$\text{at } \bar{x} = 0 \quad \bar{T} = 1, \quad (3.22)$$

$$\text{at } \bar{x} = \bar{s}(\bar{t}) \quad \bar{T} = 0, \quad -\frac{\partial \bar{T}}{\partial \bar{x}} = \lambda \frac{d\bar{s}}{d\bar{t}}, \quad (3.23)$$

$$\text{at } \bar{t} = 0 \quad \bar{s} = 0, \quad (3.24)$$

where the length scaling ℓ remains arbitrary; this is not unexpected given that the original problem had no inherent spatial length scale. The fact that ℓ is not fixed leads to the existence of a similarity solution of this problem termed the Neumann solution (one of the few explicit solutions that exist for moving boundary problems).

3.3 Dimensional analysis

The topic of dimensional analysis formalises the procedure of nondimensionalisation. An important theorem in which is the Buckingham Pi theorem:

If n quantities Q_1, Q_2, \dots, Q_n (dependent, independent variables and parameters) involving r separate fundamental dimensional components (usually $r = 3$, these being mass, length, time, i.e. M,L,T, but see the table below) are related by a unique dimensionally consistent function $f(Q_1, \dots, Q_n) = 0$, then we can find $n - r$ dimensionless combinations of Q_i , say $\Pi_j(Q_1, \dots, Q_n)$, $j = 1, \dots, n - r$, such that the solution can be expressed as $F(\Pi_1, \dots, \Pi_{n-r}) = 0$.

As a first illustration of this theorem, consider Example 2. Let $f(\theta, t, \ell, k, g, \theta_0, \omega_0) = 0$ be the solution of the IVP (3.1)–(3.2). There are two dimensionless quantities (θ, θ_0) and $n = 5$ dimensional quantities involving $r = 2$ fundamental dimensions (L,T). Thus the solution can be expressed in terms of θ, θ_0 and $n - r = 3$ dimensionless quantities namely $F(\theta, \theta_0, \bar{t}, K, G) = 0$ as shown by (3.3)–(3.4).

As a second illustration of this theorem, consider Example 3. Let $f(u - u_i, x, t, \rho c, k, q, h, \ell, u_0 - u_i) = 0$ be the solution of the BVP (3.5)–(3.8). There are $n = 9$ dimensional quantities involving $r = 4$ fundamental dimensions (M,L,T, Θ). Thus the solution can be expressed in terms of $n - r = 5$ dimensionless quantities namely $F(\bar{u}, \bar{x}, \bar{t}, Q, H) = 0$ as shown by (3.9)–(3.12).

As a third illustration, we consider Example 4. Let $f(\mathbf{v}, p, T - T_0, \mathbf{x}, t, \rho, \mu, c, k, T_1 - T_0, g, L, U) = 0$ be the solution of the dimensionless governing equations. There are $n = 17$ dimensional quantities involving $r = 4$ fundamental dimensions (M,L,T, Θ). Thus the solution can be expressed in terms of $n - r = 13$ dimensionless quantities namely $F(\bar{\mathbf{v}}, \bar{p}, \bar{T}, \bar{\mathbf{x}}, \bar{t}, Re, Fr, Pe, Br) = 0$ as shown by the dimensionless equations.

As a fourth illustration, we consider Example 5. Let $f(T, s, x, t, \rho, c, k, L, T_0) = 0$ be the solution of the moving boundary problem (3.13)–(3.16). There are $n = 9$ dimensional quantities involving $r = 4$ fundamental dimensions (M,L,T, Θ). Thus the solution can be expressed in terms of $n - r = 5$ dimensionless quantities namely $F(\bar{T}, \bar{s}, \bar{x}, \bar{t}, \lambda) = 0$ as shown by (3.21)–(3.24).

Note 1. The function f may be a solution of a PDE, a BVP or IVP.

Note 2. If a PDE involves fewer fundamental dimensions than dimensional quantities, it must admit a simplified solution in accordance with the Buckingham Pi Theorem.

The International System (SI) of fundamental units are:

Fundamental Dimension	Base Unit
Length (L)	metre, m
Mass (M)	kilogram, kg
Time (T)	second, s
Electric current (A)	ampere, A
Thermodynamic temperature (Θ)	kelvin, K
Amount of substance (X)	mole, mol
Luminous intensity (I)	candela, cd

Chapter 4

Similarity Methods

Chapter 5

Asymptotic Methods

Chapter 6

Model Problems