PART I

INTRODUCTION AND FOUNDATIONS

CHAPTER 1

DIFFERENTIAL EQUATIONS

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The main requirement for this book is the basic knowledge of calculus and statistics as covered by most undergraduate courses in engineering and science subjects. However, we will provide a brief review of mathematical foundations in the first few chapters so as to help readers to refresh some of the most important concepts.

Most mathematical models in physics, chemistry, biology and many other applications are formulated in terms of differential equations. If the variables or quantities (such as velocity, temperature, pressure) change with other independent variables such as spatial coordinates and time, their relationship can in general be written as a differential equation or even a set of differential equations.

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1.1 ORDINARY DIFFERENTIAL EQUATIONS

An ordinary differential equation (ODE) is a relationship between a function $y(x)$ of an independent variable x and its derivatives y', y'', ..., $y^{(n)}$. It can be written in a generic form

$$\Psi(x, y, y', y'', ..., y^{(n)}) = 0, \tag{1.1}$$

where Ψ is a function of $x, y, ...,$ and $y^{(n)}$. The solution of the equation is a function $y = f(x)$, satisfying the equation for all x in a given domain Ω. The order of the differential equation is equal to the order n of the highest derivative in the equation. Thus, the so-called Riccati equation

$$y' + a(x)y^2 + b(x)y = c(x), \tag{1.2}$$

is a first-order ODE, and the following equation of Euler-type

$$x^2y'' + a_1xy' + a_0y = 0, \tag{1.3}$$

is a second order. The degree of an equation is defined as the power to which the highest derivative occurs. Therefore, both the Riccati equation and the Euler equation are of the first degree.

An equation is called linear if it can be arranged into the form

$$a_n(x)y^{(n)} + ... + a_1(x)y' + a_0(x)y = \phi(x), \tag{1.4}$$

where all the coefficients depend on x only, not on y or any of its derivatives. If any of the coefficients is a function of y or any of its derivatives, then the equation is nonlinear. If the right-hand side is zero or $\phi(x) = 0$, the equation is homogeneous. It is called nonhomogeneous if $\phi(x) \neq 0$.

To find a solution of an ordinary differential equation is not always easy, and it is usually very complicated for nonlinear equations. Even for linear equations, solutions can be found in a straightforward way for only a few simple cases. The solution of a differential equation generally falls into three types: closed form, series form and integral form. A closed form solution is the type of solution that can be expressed in terms of elementary functions and some arbitrary constants. Series solutions are the ones that can be expressed in terms of a series when a closed form is not possible for certain types of equations. The integral form of solutions or quadrature is sometimes the only form of solution that is possible. If all these forms are not possible, the alternatives are to use approximate and numerical solutions.

1.1.1 First-Order ODEs

1.1.1.1 Linear ODEs A first-order linear differential equation can generally be written as

$$y' + a(x)y = b(x), \tag{1.5}$$

where $a(x)$ and $b(x)$ are the known functions of x. Multiplying both sides of the equation by $\exp[\int a(x)dx]$, called the integrating factor, we have

$$y'e^{\int a(x)dx} + a(x)ye^{\int a(x)dx} = b(x)e^{\int a(x)dx}, \tag{1.6}$$

which can be written as

$$[ye^{\int a(x)dx}]' = b(x)e^{\int a(x)dx}. \tag{1.7}$$

By simple integration, we have

$$ye^{\int a(x)dx} = \int b(x)e^{\int a(x)dx}dx + C. \tag{1.8}$$

So its solution becomes

$$y(x) = e^{-\int a(x)dx} \int b(x)e^{\int a(x)dx}dx + Ce^{-\int a(x)dx}, \tag{1.9}$$

where C is an integration constant.

■ **EXAMPLE 1.1**

For example, from $y'(x) - y(x) = e^{-x}$, we have $a(x) = -1$ and $b = e^{-x}$, so the solution is

$$y(x) = e^{-\int(-1)dx} \int e^{-x}e^{\int(-1)dx} + Ce^{-\int(-1)dx}$$

$$= e^x \int e^{-2x}dx + Ce^x = -\frac{1}{2}e^{-x} + Ce^x. \tag{1.10}$$

1.1.1.2 Nonlinear ODEs For some nonlinear first-order ordinary differential equations, sometimes a transform or change of variables can convert it into the standard first-order linear equation (1.5). This is better demonstrated by an example.

The Bernoulli's equation can be written in the generic form

$$y' + p(x)y = q(x)y^n, \qquad n \neq 1. \tag{1.11}$$

In the case of $n = 1$, it reduces to a standard first-order linear ordinary differential equation. By dividing both sides by y^n and using the change of variables

$$u(x) = \frac{1}{y^{n-1}}, \qquad u' = \frac{(1-n)y'}{y^n}, \tag{1.12}$$

we have

$$u' + (1-n)p(x)u = (1-n)q(x), \tag{1.13}$$

which is a standard first-order linear differential equation whose general solution is given earlier in (1.9).

■ EXAMPLE 1.2

In the simpler case when $p(x) = 2x$, $q(x) = -1$ and $n = 2$, we have

$$u' - 2xu = 1, \qquad u(x) = \frac{1}{y(x)}.$$

For the initial condition $y(0) = 1$, we have $u(0) = 1$. Using solution (1.9), we have

$$u(x) = \frac{\sqrt{\pi}}{2} e^{x^2} \mathrm{erf}(x) + Ae^{x^2},$$

where A is the integration constant to be determined.

If we further set $u(0) = 1$ as an initial condition, we have $A = 1$. Thus, the solution for $y(x)$ becomes

$$y(x) = \frac{2e^{-x^2}}{(\sqrt{\pi}\,\mathrm{erf}(x) + 2)}.$$

In general, such transformations are not always possible.

1.1.2 Higher-Order ODEs

Higher-order ODEs are more complicated to solve even for the linear equations. For the special case of higher-order ODEs where all the coefficients $a_n, ..., a_1, a_0$ are constants,

$$a_n y^{(n)} + \cdots + a_1 y' + a_0 y = f(x), \tag{1.14}$$

its general solution $y(x)$ consists of two parts: a complementary function $y_c(x)$ and a particular integral or particular solution $y_p^*(x)$. We have

$$y(x) = y_c(x) + y_p^*(x). \tag{1.15}$$

The complementary function which is the solution of the linear homogeneous equation with constant coefficients can be written in a generic form

$$a_n y_c^{(n)} + a_{n-1} y_c^{(n-1)} + \cdots + a_1 y_c' + a_0 = 0. \tag{1.16}$$

Assuming $y = Ae^{\lambda x}$ where A is a constant, we get the characteristic equation as a polynomial

$$a_n\lambda^n + a_{n-1}\lambda^{(n-1)} + \cdots + a_1\lambda + a_0 = 0, \tag{1.17}$$

which has n roots in the general case. Then, the solution can be expressed as the summation of various terms $y_c(x) = \sum_{k=1}^{n} c_k e^{\lambda_k x}$ if the polynomial has n distinct zeros $\lambda_1, ...\lambda_n$. For complex roots, and complex roots always occur in pairs $\lambda = r \pm i\omega$, the corresponding linearly independent terms can then be replaced by $e^{rx}[A\cos(\omega x) + B\sin(\omega x)]$.

The particular solution $y_p^*(x)$ is any $y(x)$ that satisfies the original inhomogeneous equation (1.14). Depending on the form of the function $f(x)$, the particular solutions can take various forms. For most of the combinations of basic functions such as $\sin x, \cos x$, e^{kx}, and x^n, the method of the undetermined coefficients is widely used. For $f(x) = \sin(\alpha x)$ or $\cos(\alpha x)$, then we can try $y_p^* = A\sin\alpha x + B\sin\alpha x$. We then substitute it into the original equation (1.14) so that the coefficients A and B can be determined. For a polynomial $f(x) = x^n$ where $n = 0, 1, 2, ..., N$, we then try $y_p^* = A + Bx + ... + Qx^n$ (polynomial). For $f(x) = e^{kx}x^n$, we can try $y_p^* = (A + Bx + ...Qx^n)e^{kx}$. Similarly, for $f(x) = e^{kx}\sin\alpha x$ or $f(x) = e^{kx}\cos\alpha x$, we can use $y_p^* = e^{kx}(A\sin\alpha x + B\cos\alpha x)$. More general cases and their particular solutions can be found in various textbooks.

A very useful technique is to use the method of differential operator D. A differential operator D is defined as

$$D \equiv \frac{d}{dx}. \tag{1.18}$$

Since we know that $De^{\lambda x} = \lambda e^{\lambda x}$ and $D^n e^{\lambda x} = \lambda^n e^{\lambda x}$, so they are equivalent to $D \mapsto \lambda$, and $D^n \mapsto \lambda^n$. Thus, any polynomial $P(D)$ will map to a corresponding $P(\lambda)$. On the other hand, integral operator $D^{-1} = \int dx$ is just the inverse of differentiation. The beauty of the differential operator form is that one can factorize it in the same as for a polynomial, then solve each factor separately. The differential operator is very useful in finding out both the complementary functions and particular integral. This method also works for $\sin x, \cos x, \sinh x$ and others, and this is because they are related to $e^{\lambda x}$ via $\sin\theta = \frac{1}{2i}(e^{i\theta} - e^{-i\theta})$ and $\cosh x = (e^x + e^{-x})/2$.

Higher-order differential equations can conveniently be written as a system of differential equations. In fact, an nth-order linear equation can always be written as a linear system of n first-order differential equations. A linear system of ODEs is more suitable for mathematical analysis and numerical integration.

1.1.3 Linear System

For an nth order linear equation (1.16), it can always be written as a linear system

$$\frac{dy}{dx} = y_1, \ \frac{dy_1}{dx} = y_2, \ ..., \ \frac{dy_{n-1}}{dx} = y_{n-1},$$

$$-a_n(x)y'_{n-1} = a_{n-1}(x)y_{n-1} + ... + a_1(x)y_1 + a_0(x)y + \phi(x), \tag{1.19}$$

which is a system for $u = [y \ y_1 \ y_2 \ ... \ y_{n-1}]^T$. If the independent variable x does not appear explicitly in y_i, then the system is said to be autonomous with important properties. For simplicity and in keeping with the convention, we use $t = x$ and $\dot{u} = du/dt$ in our following discussion. A general linear system of nth order can be written as

$$\begin{pmatrix} \dot{u}_1 \\ \dot{u}_2 \\ \vdots \\ \dot{u}_n \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & ... & a_{1n} \\ a_{21} & a_{22} & ... & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & ... & a_{nn} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{pmatrix}, \tag{1.20}$$

or

$$\dot{\mathbf{u}} = \mathbf{A}\mathbf{u}. \tag{1.21}$$

If we $\mathbf{u} = \mathbf{v}\exp(\lambda t)$, then this becomes an eigenvalue problem,

$$(\mathbf{A} - \lambda\mathbf{I})\mathbf{v} = \mathbf{0}, \tag{1.22}$$

which will have non-null solution only if

$$\det(\mathbf{A} - \lambda\mathbf{I}) = 0. \tag{1.23}$$

1.1.4 Sturm-Liouville Equation

One of the commonly used second-order ordinary differential equations is the Sturm-Liouville equation in the interval $x \in [a, b]$

$$\frac{d}{dx}\Big[p(x)\frac{dy}{dx}\Big] + q(x)y + \lambda r(x)y = 0, \tag{1.24}$$

with the boundary conditions

$$y(a) + \alpha y'(a) = 0, \qquad y(b) + \beta y'(b) = 0, \tag{1.25}$$

where the known function $p(x)$ is differentiable, and the known functions $q(x), r(x)$ are continuous. The parameter λ to be determined can only take certain values λ_n, called the eigenvalues, if the problem has solutions. For the obvious reason, this problem is called Sturm-Liouville eigenvalue problem.

Sometimes, it is possible to transform a nonlinear equation into a standard Sturm-Liouville equation, and this is better demonstrated by an example.

■ **EXAMPLE 1.3**

The Riccati equation can be written in the generic form

$$y' = p(x) + q(x)y + r(x)y^2, \qquad r(x) \neq 0.$$

If $r(x) = 0$, then it reduces to a first-order linear ODE. By using the transform

$$y(x) = -\frac{u'(x)}{r(x)u(x)},$$

or

$$u(x) = e^{-\int r(x)y(x)dx},$$

we have

$$u'' - P(x)u' + Q(x)u = 0,$$

where $P(x) = -r'(x)/r(x) + q(x)$ and $Q(x) = r(x)p(x)$.

For each eigenvalue λ_n, there is a corresponding solution ψ_{λ_n}, called an eigenfunction. The Sturm-Liouville theory states that for two different eigenvalues $\lambda_m \neq \lambda_n$, their eigenfunctions are orthogonal. That is

$$\int_a^b \psi_{\lambda_m}(x)\psi_{\lambda_n}(x)r(x)dx = 0, \quad \text{or} \quad \int_a^b \psi_{\lambda_m}(x)\psi_{\lambda_n}(x)r(x)dx = \delta_{mn},$$

where $\delta_{mn} = 1$ if $m = n$, otherwise $\delta_{mn} = 0$ if $m \neq n$. It is possible to arrange the eigenvalues in an increasing order

$$\lambda_1 < \lambda_2 < ... < \lambda_n < ... \to \infty.$$

Now let us study a real-world problem using differential equations. Many fluid flow problems are related to flow through a pipe, including the water flow through a pipe, oil in an oil pipeline. Let us look at the Poiseuille flow in a cylindrical pipe.

■ **EXAMPLE 1.4**

The laminar flow of a viscous fluid through a pipe with a radius $r = a$ is under a constant pressure gradient (see Fig. 1.1)

$$\nabla p = \Delta P/L = (P_o - P_i)/L,$$

where P_i and P_o ($< P_i$) are the pressures at inlet and outlet, respectively. L is the length of the pipe. The drag force is balanced by pressure change, and this leads to the following second-order ordinary differential

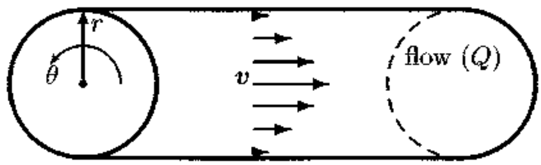

Figure 1.1 Flow through a pipe under pressure gradient.

equation

$$\frac{\Delta P}{L} = \eta \frac{1}{r}\frac{d}{dr}\Big[r\frac{dv(r)}{dr}\Big],$$

where η is the viscosity of the fluid. This equation implies that the flow velocity v is not uniform, it varies with r. Integrating the above equation twice, we have

$$v(r) = \frac{\Delta P}{4\eta L}r^2 + A\ln r + B,$$

where A and B are integrating constants. The velocity must be finite at $r = 0$, which means that $A = 0$. The no-slip boundary $v = 0$ at $r = a$ requires that

$$\frac{\Delta P}{4\eta L}a^2 + B = 0.$$

Thus, the velocity profile is

$$v(r) = -\frac{\Delta P}{4\eta L}(a^2 - r^2).$$

Now the total flow rate Q down the pipe is given by integrating the flow over the whole cross section. We have

$$Q = \int_0^a 2\pi r v(r) dr = -\frac{\pi \Delta P}{2\eta L}\int_0^a (a^2 r - r^3)dr = -\frac{\pi\Delta P}{8\eta L}a^4. \qquad (1.26)$$

Here the negative sign means the flow down the pressure gradient.

We can see that the flow rate is proportional to the pressure gradient, inversely proportional to the viscosity. Double the radius of the pipe, and the flow rate will increase to 16 times.

1.2 PARTIAL DIFFERENTIAL EQUATIONS

Partial differential equations are much more complicated compared with ordinary differential equations. There is no universal solution technique for nonlinear equations, even numerical simulations are usually not straightforward. Thus, we will mainly focus on the linear partial differential equations and equations of special interest.

A partial differential equation (PDE) is a relationship containing at least one partial derivative. Similar to the ordinary differential equation, the highest nth partial derivative is referred to as the order n of the partial differential equation. The general form of a partial differential equation can be written as

$$\psi\Big(u, x, y, ..., \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}, \frac{\partial^2 u}{\partial x^2}, \frac{\partial^2 u}{\partial y^2}, \frac{\partial^2 u}{\partial x \partial y}, ...\Big) = 0. \tag{1.27}$$

where u is the dependent variable, and $x, y, ...$ are the independent variables.

A simple example of partial differential equations is the linear first-order partial differential equation, which can be written as

$$a(x,y)\frac{\partial u}{\partial x} + b(x,y)\frac{\partial u}{\partial y} = f(x,y). \tag{1.28}$$

for two independent variables and one dependent variable u. If the right-hand side is zero or simply $f(x, y) = 0$, then the equation is said to be homogeneous. The equation is said to be linear if a, b and f are functions of x, y only, not u itself.

For simplicity in notation in the studies of PDEs, compact subscript forms are often used in the literature. They are

$$u_x \equiv \partial_x u \equiv \frac{\partial u}{\partial x}, \;\; u_y \equiv \partial_y u \equiv \frac{\partial u}{\partial y}, \;\; u_{xx} \equiv \frac{\partial^2 u}{\partial x^2}, \;\; u_{xy} \equiv \frac{\partial^2 u}{\partial x \partial y}, \;\; ... \tag{1.29}$$

and thus we can write (1.28) as

$$au_x + bu_y = f. \tag{1.30}$$

1.2.1 First-Order PDEs

A first-order linear partial differential equation can be written as

$$a(x,y)u_x + b(x,y)u_y = f(x,y), \tag{1.31}$$

which can be solved using the method of characteristics in terms of a parameter s

$$\frac{dx}{ds} = a, \;\; \frac{dy}{ds} = b, \;\; \frac{du}{ds} = f, \tag{1.32}$$

which essentially forms a system of first-order ordinary differential equations. The simplest example of first-order linear partial differential equations is the first-order hyperbolic equation

$$u_t + cu_x = 0, \tag{1.33}$$

where c is a constant. It has a general solution

$$u = \psi(x - ct), \tag{1.34}$$

which is a travelling wave along the x-axis with a constant speed c. If the initial shape is $u(x, 0) = \psi(x)$, then $u(x, t) = \psi(x - ct)$ at time t, therefore the shape of the wave does not change with time though its position is constantly changing.

1.2.2 Classification of Second-Order PDEs

A linear second-order partial differential equation can be written in the generic form in terms of two independent variables x and y,

$$au_{xx} + bu_{xy} + cu_{yy} + gu_x + hu_y + ku = f, \tag{1.35}$$

where a, b, c, g, h, k and f are functions of x and y only. If $f(x, y, u)$ is also a function of u, then we say that this equation is quasi-linear.

If $\Delta = b^2 - 4ac < 0$, the equation is elliptic. One famous example is the Laplace equation $u_{xx} + u_{yy} = 0$.

If $\Delta > 0$, it is hyperbolic. A good example is the wave equation $u_{tt} = c^2 u_{xx}$.

If $\Delta = 0$, it is parabolic. Diffusion and heat conduction are of the parabolic type $u_t = \kappa u_{xx}$.

1.3 CLASSIC MATHEMATICAL MODELS

Three types of classic partial differential equations are widely used and they occur in a vast range of applications. In fact, almost all books or studies on partial differential equations will have to deal with these three types of basic partial differential equations.

Laplace's and Poisson's Equation: In heat transfer problems, the steady state of heat conduction with a source is governed by the Poisson equation

$$k\nabla^2 u = f(x, y, t), \qquad (x, y) \in \Omega, \tag{1.36}$$

or

$$u_{xx} + u_{yy} = q(x, y, t), \tag{1.37}$$

for two independent variables x and y. Here k is thermal diffusivity and $f(x, y, t)$ is the heat source. Ω is the domain of interest, usually a physical region. If there is no heat source ($q = f/\kappa = 0$), it becomes the Laplace equation. The solution of a function is said to be harmonic if it satisfies Laplace's equation.

In order to determine the temperature u completely, the appropriate boundary conditions are needed. A simple boundary condition is to specify the temperature $u = u_0$ on the boundary $\partial\Omega$. This type of problem is the Dirichlet problem.

On the other hand, if the temperature is not known, but the gradient $\partial u/\partial \boldsymbol{n}$ is known on the boundary where $\boldsymbol{n}$ is the outward-pointing unit normal, this forms the Neumann problem. Furthermore, some problems may have a mixed type of boundary conditions in the combination of

$$\alpha u + \beta \frac{\partial u}{\partial \boldsymbol{n}} = \gamma,$$

which naturally occurs as a radiation or cooling boundary condition.

Parabolic Equation: Time-dependent problems, such as diffusion and transient heat conduction, are governed by the parabolic equation

$$u_t = k u_{xx}. \tag{1.38}$$

Written in the n-dimensional case $x_1 = x, x_2 = y, x_3 = z, ...,$ it can be extended to the reaction-diffusion equation

$$u_t = k\nabla^2 u + f(u, x_1, .., x_n, t). \tag{1.39}$$

Wave Equation: The vibration of strings and travelling seismic waves are governed by the hyperbolic wave equation.

The 1D wave equation in its simplest form is

$$u_{tt} = c^2 u_{xx}, \tag{1.40}$$

where c is the velocity of the wave. Using a transformation of the pair of independent variables

$$\xi = x + ct, \tag{1.41}$$

and

$$\eta = x - ct, \tag{1.42}$$

for $t > 0$ and $-\infty < x < \infty$, the wave equation can be written as

$$u_{\xi\eta} = 0. \tag{1.43}$$

Integrating twice and substituting back in terms of x and t, we have

$$u(x,t) = f(x + ct) + g(x - ct), \tag{1.44}$$

where f and g are functions of $x + ct$ and $x - ct$, respectively. We can see that the solution is composed of two independent waves. One wave moves to the right and one travels to the left at the same constant speed c.

1.4 OTHER MATHEMATICAL MODELS

We have shown examples of the three major equations of second-order linear partial differential equations. There are other equations that occur frequently in engineering and science. We will give a brief description of some of these equations.

Elastic Wave Equation: A wave in an elastic isotropic homogeneous solid is governed by the following equation in terms of displacement $\mathbf{u}$,

$$\rho \frac{\partial^2 \mathbf{u}}{\partial t^2} = \mu \nabla^2 \mathbf{u} + (\lambda + \mu) \nabla (\nabla \cdot \mathbf{u}) + \mathbf{f}, \tag{1.45}$$

where ρ is density, λ and μ are Lamé constants, and $\mathbf{f}$ is body force. Such an equation can describe two types of wave: transverse wave (S wave) and longitudinal or dilatational wave (P wave). The speed of the longitudinal wave is

$$v_p = \sqrt{(\lambda + 2\mu)/\rho}, \tag{1.46}$$

and the transverse wave has the speed

$$v_s = \sqrt{\mu/\rho}. \tag{1.47}$$

Reaction-Diffusion Equation: The reaction-diffusion equation is an extension of heat conduction with a source f

$$u_t = D\nabla^2 u + f(x, y, z, u), \tag{1.48}$$

where D is the diffusion coefficient and f is the reaction rate. One example is the combustion equation

$$u_t = Du_{xx} + Que^{-\lambda/u}, \tag{1.49}$$

where Q and λ are constants.

Navier-Stokes Equations: The Navier-Stokes equations for incompressible flow in the absence of body forces can be written, in terms of the velocity $\mathbf{u}$ and the pressure p, as

$$\nabla \cdot \mathbf{u} = 0, \qquad \rho[\mathbf{u}_t + (\mathbf{u} \cdot \nabla)\mathbf{u}] = \mu \nabla^2 \mathbf{u} - \nabla p, \tag{1.50}$$

where ρ and μ are the density of the fluid and its viscosity, respectively. In computational fluid dynamics, most simulations are mainly related to these equations. We can define the Reynolds number as $\mathrm{Re} = \rho UL/\mu$ where U is the typical velocity and L is the length scale.

In the limit of $\mathrm{Re} \ll 1$, we have the Stokes flow governed by

$$\mu \nabla^2 \mathbf{u} = \nabla p. \tag{1.51}$$

In the other limit of Re $\gg 1$, we have the inviscous flow

$$\nabla \cdot \mathbf{u} = 0, \qquad \rho[\mathbf{u}_t + (\mathbf{u} \cdot \nabla)\mathbf{u}] = -\nabla p, \tag{1.52}$$

where there is still a nonlinear term $(\mathbf{u} \cdot \nabla)\mathbf{u}$.

Groundwater Flow: The general equation for three-dimensional groundwater flow is

$$S_\sigma \frac{\partial p}{\partial t} = \frac{k}{\mu} \nabla^2 p - S_\sigma B \frac{\partial \sigma}{\partial t} + Q, \tag{1.53}$$

where $\sigma = \sigma_{kk}/3$ is the mean stress, p is the pore water pressure, and Q is source or sink term. S_σ is the specific storage coefficient and B is the Skempton constant. k is the permeability of the porous medium and μ is the viscosity of water. This can be considered as the inhomogeneous diffusion equation for pore pressure.

1.5 SOLUTION TECHNIQUES

Each type of equation usually requires different solution techniques. However, there are some methods that work for most of the linearly partial differential equations with appropriate boundary conditions on a regular domain. These methods include separation of variables, method of series expansion and transform methods such as the Laplace and Fourier transforms.

1.5.1 Separation of Variables

The separation of variables attempts a solution of the form

$$u = X(x)Y(y)Z(z)T(t), \tag{1.54}$$

where $X(x), Y(y), Z(z), T(t)$ are functions of x, y, z, t, respectively. By determining these functions that satisfy the partial differential equation and the required boundary conditions in terms of eigenvalue problems, the solution of the original problem is then obtained.

As a classic example, we now try to solve the 1D heat conduction equation in the domain $x \in [0, L]$ and $t \geq 0$

$$u_t = k u_{xx}, \tag{1.55}$$

with the initial value and boundary conditions

$$u(0,t) = 0, \qquad \frac{\partial u(x,t)}{\partial x}\Big|_{x=L} = 0, \qquad u(x,0) = \psi(x). \tag{1.56}$$

Letting $u(x,t) = X(x)T(t)$, we have

$$\frac{X''(x)}{X} = \frac{T'(t)}{kT}. \tag{1.57}$$

As the left-hand side depends only on x and the right-hand side only depends on t, therefore, both sides must be equal to the same constant, and the constant can be assumed to be $-\lambda^2$. The negative sign is just for convenience because we will see below that the finiteness of the solution $T(t)$ requires that eigenvalues $\lambda^2 > 0$ or λ are real. Hence, we now get two ordinary differential equations

$$X''(x) + \lambda^2 X(x) = 0, \qquad T'(t) + k\lambda^2 T(t) = 0, \tag{1.58}$$

where λ is the eigenvalue. The solution for $T(t)$ is

$$T = A_n e^{-\lambda^2 kt}. \tag{1.59}$$

The basic solution for $X(x)$ is simply

$$X(x) = \alpha \cos \lambda x + \beta \sin \lambda x. \tag{1.60}$$

So the fundamental solution for u is

$$u(x,t) = (\alpha \cos \lambda x + \beta \sin \lambda x) e^{-\lambda^2 kt}, \tag{1.61}$$

where we have absorbed the coefficient A_n into α and β because they are the undetermined coefficients anyway. As the value of λ varies with the boundary conditions, it forms an eigenvalue problem. The general solution for u should be derived by superposing solutions of (1.61), and we now have

$$u = \sum_{n=1}^{\infty} X_n T_n = \sum_{n=1}^{\infty} (\alpha_n \cos \lambda_n x + \beta_n \sin \lambda_n x) e^{-\lambda_n^2 kt}. \tag{1.62}$$

From the boundary condition $u(0,t) = 0$ at $x = 0$, we have

$$0 = \sum_{n=1}^{\infty} \alpha_n e^{-\lambda_n^2 kt}, \tag{1.63}$$

which leads to $\alpha_n = 0$ since $\exp(-\lambda^2 kt) > 0$.

From $\frac{\partial u}{\partial x}\Big|_{x=L} = 0$, we have

$$\lambda_n \cos \lambda_n L = 0, \tag{1.64}$$

which requires

$$\lambda_n L = \frac{(2n-1)\pi}{2}, \qquad (n = 1, 2, ...). \tag{1.65}$$

Therefore, λ cannot be continuous, and it only takes an infinite number of discrete values, called eigenvalues.

Each eigenvalue $\lambda = \lambda_n = \frac{(2n-1)\pi}{2L}$, $(n = 1, 2, ...)$ has a corresponding eigenfunction $X_n = \sin(\lambda_n x)$. Substituting into the solution for $T(t)$, we have

$$T_n(t) = A_n e^{-\frac{[(2n-1)\pi]^2}{4L^2}kt}. \tag{1.66}$$

By expanding the initial condition into a Fourier series so as to determine the coefficients, we have

$$u(x,t) = \sum_{n=1}^{\infty} \beta_n \sin\Big(\frac{(2n-1)\pi x}{2L}\Big) e^{-[\frac{(2n-1)\pi}{2L}]^2 kt},$$

$$\beta_n = \frac{2}{L}\int_0^L \psi(x) \sin\Big[\frac{(2n-1)\pi x}{2L}\Big] dx. \tag{1.67}$$

■ EXAMPLE 1.5

In the special case when initial condition $u(x, t = 0) = \psi = u_0$ is constant, the requirement for $u = u_0$ at $t = 0$ becomes

$$u_0 = \sum_{n=1}^{\infty} \beta_n \sin\frac{(2n-1)\pi x}{2L}. \tag{1.68}$$

Using the orthogonal relationships

$$\int_0^L \sin\frac{m\pi x}{L} \sin\frac{n\pi x}{L} dx = 0, \qquad m \neq n,$$

and

$$\int_0^L (\sin\frac{n\pi x}{L})^2 dx = \frac{L}{2}, \qquad (n = 1, 2, ...),$$

and multiplying both sides of Eq.(1.68) by $\sin[(2n-1)\pi x/2L]$, we have the integration

$$\beta_n \frac{L}{2} = \int_0^L \sin\frac{(2n-1)\pi x}{2L} u_0 dx = \frac{2u_0 L}{(2n-1)\pi}, \quad (n = 1, 2, ...),$$

which leads to

$$\beta_n = \frac{4u_0}{(2n-1)\pi}, \qquad n = 1, 2, ...,$$

and thus the solution becomes

$$u = \frac{4u_0}{\pi} \sum_{n=1}^{\infty} \frac{1}{(2n-1)} e^{-\frac{(2n-1)^2\pi^2 kt}{4L^2}} \sin \frac{(2n-1)\pi x}{2L}. \quad (1.69)$$

This solution is essentially the same as the classical heat conduction problem discussed by Carslaw and Jaeger in 1959. This same solution can also be obtained using the Fourier series of u_0 in $0 < x < L$.

1.5.2 Laplace Transform

The integral transform can reduce the number of the independent variables. For the 1D time-dependent case, it transforms a partial differential equation into an ordinary differential equation. By solving the ordinary differential equation and inverting it back, we can obtain the solution for the original partial differential equation. As an example, we now solve the heat conduction problem over a semi-infinite interval $[0, \infty)$,

$$u_t = k u_{xx}, \qquad u(x,0) = 0, \quad u(0,t) = T_0. \quad (1.70)$$

■ **EXAMPLE 1.6**

Let $\bar{u}(x,s) = \int_0^\infty u(x,t)e^{-st}dt$ be the Laplace transform of $u(x,t)$, then Eq.(1.70) becomes

$$s\bar{u} = k\frac{d^2\bar{u}}{dx^2}, \qquad \bar{u}_{x=0} = \frac{T_0}{s},$$

which is an ordinary differential equation whose general solution can be written as

$$\bar{u} = Ae^{-\sqrt{\frac{s}{k}}x} + Be^{\sqrt{\frac{s}{k}}x}.$$

The finiteness of the solution as $x \to \infty$ requires that $B = 0$, and the boundary condition at $x = 0$ leads to

$$\bar{u} = \frac{T_0}{s} e^{-\sqrt{\frac{s}{k}}x}.$$

By using the inverse Laplace transform, we have

$$u = T_0 \text{erfc}\Big(\frac{x}{2\sqrt{kt}}\Big),$$

where $\text{erfc}(x)$ is the complementary error function.

The Fourier transform works in a similar manner to the Laplace transform.

1.5.3 Similarity Solution

Sometimes, the diffusion equation

$$u_t = \kappa u_{xx}, \tag{1.71}$$

can be solved by using the so-called similarity method by defining a similar variable

$$\eta = \frac{x}{\sqrt{\kappa t}}, \quad \text{or} \quad \zeta = \frac{x^2}{\kappa t}. \tag{1.72}$$

One can assume that the solution to the equation has the form

$$u = (\kappa t)^{\alpha} f\Big[\frac{x^2}{(\kappa t)^{\beta}}\Big]. \tag{1.73}$$

By substituting it into the diffusion equation, the coefficients α and β can be determined. For most applications, one can assume $\alpha = 0$ so that $u = f(\zeta)$. In this case, we have

$$4\zeta u'' + 2u' + \zeta\beta(\kappa t)^{\beta-1}u' = 0, \tag{1.74}$$

where $u' = du/d\zeta$. In deriving this equation, we have used the chain rules of differentiations

$$\frac{\partial}{\partial x} = \frac{\partial}{\partial \zeta}\frac{\partial \zeta}{\partial x}, \quad \frac{\partial}{\partial t} = \frac{\partial}{\partial \zeta}\frac{\partial \zeta}{\partial t}. \tag{1.75}$$

Since the original equation does not have time-dependent terms explicitly, this means that all the exponents for any t-terms must be zero. Therefore, we have

$$\beta = 1. \tag{1.76}$$

Now, the diffusion equation becomes

$$\zeta f''(\zeta) = -\Big(\frac{1}{2} + \frac{\zeta}{4}\Big)f'. \tag{1.77}$$

Using $(\ln f')' = f''/f'$ and integrating the above equation once, we get

$$f' = \frac{K e^{-\zeta/4}}{\sqrt{\zeta}}. \tag{1.78}$$

Integrating it again and using the substitution $\zeta = 4\xi^2$, we obtain

$$u = A\int_0^{\xi} e^{-\xi^2} d\xi = C\mathrm{erf}\Big(\frac{x}{\sqrt{4\kappa t}}\Big) + D, \tag{1.79}$$

where C and D are constants that can be determined from appropriate boundary conditions.

For the same problem as (1.70), the boundary condition as $x \to \infty$ implies that $C + D = 0$, while $u(0,t) = T_0$ means that $D = -C = T_0$. Therefore, we finally have

$$u = T_0\Big[1 - \mathrm{erf}\Big(\frac{x}{\sqrt{4\kappa t}}\Big)\Big] = T_0 \mathrm{erfc}\Big(\frac{x}{\sqrt{4\kappa t}}\Big).$$

1.5.4 Change of Variables

In some cases, the partial differential equation cannot be written in any standard form; however, it can be converted into a known standard equation by a change of variables. For example, the following simple reaction-diffusion equation

$$\frac{\partial u}{\partial t} = k\frac{\partial^2 u}{\partial x^2} - \alpha u, \tag{1.80}$$

describes the heat conduction along a wire with a heat loss term $-\alpha u$. Carslaw and Jaeger show that it can be transformed into a standard equation of heat conduction using the following change of variables

$$u = ve^{-\alpha t}, \tag{1.81}$$

where v is the new variable. By simple differentiations, we have

$$\frac{\partial u}{\partial t} = \frac{\partial v}{\partial t}e^{-\alpha t} - \alpha v e^{-\alpha t} = \frac{\partial v}{\partial t}e^{-\alpha t} - \alpha u, \qquad \frac{\partial^2 u}{\partial x^2} = \frac{\partial^2 v}{\partial x^2}e^{-\alpha t}, \tag{1.82}$$

we have

$$\frac{\partial u}{\partial t} = \underbrace{\frac{\partial v}{\partial t}e^{-\alpha t}} - \alpha u = k\frac{\partial^2 u}{\partial x^2} - \alpha u = k\underbrace{\frac{\partial^2 v}{\partial x^2}e^{-\alpha t}} - \alpha u, \tag{1.83}$$

which becomes

$$\frac{\partial v}{\partial t}e^{-\alpha t} = k\frac{\partial^2 v}{\partial x^2}e^{-\alpha t}. \tag{1.84}$$

After dividing both sides by $e^{-\alpha t} > 0$, we have

$$\frac{\partial v}{\partial t} = k\frac{\partial^2 v}{\partial x^2}, \tag{1.85}$$

which is the standard heat conduction equation for v.

For given initial (usually constant) and boundary conditions (usually zero), we can use all the techniques for solving the standard equation to get solutions. However, for some boundary conditions such as $u = u_0$, a more elaborate form of change of variables is needed. Crank introduced Danckwerts's method by using the following transform

$$u = \alpha \int_0^t ve^{-\alpha\tau} d\tau + ve^{-\alpha t}. \tag{1.86}$$

Noting that $\frac{\partial u}{\partial t} = \alpha v e^{-\alpha t} - \alpha v e^{-\alpha t} + \frac{\partial v}{\partial t} e^{-\alpha t}$, it is straightforward to show

$$\frac{\partial u}{\partial t} + \alpha u = k \frac{\partial^2 u}{\partial x^2}. \tag{1.87}$$

For the boundary condition $u = u_0$, we have $v = v_0 = u_0$, and this is because

$$u = u_0 = \alpha v_0 \int_0^t e^{-\alpha \tau} d\tau + v_0 e^{-\alpha t} = v_0 - v_0 e^{-\alpha t} + v_0 e^{-\alpha t} = v_0, \tag{1.88}$$

which is the same boundary condition as that for u.

There are other important methods for solving partial differential equations. These include Green's function, series methods, asymptotic methods, approximate methods, perturbation methods and naturally the numerical methods.

EXERCISES

1.1 The so-called Coriolis force or effect exists in a rotational system, which makes the falling object lands slightly to the east (without considering air resistance). Assume the falling height is h, estimate the distance deviation to the east due to this Coriolis acceleration $a = 2\omega v$ where ω is the angular velocity of the Earth's rotation and v is its falling velocity.

1.2 Find the general solution $x^2 y'' - y = 0$ for $x > 0$.

1.3 The governing equation for the damped simple harmonic motion can be written as a general second-order ordinary differential equation

$$\ddot{u} + 2\eta\omega_0 \dot{u} + \omega_0^2 u = 0,$$

where ω_0 is the so-called undamped frequency, and η is called damping coefficient. Show that $\eta > 1$ and $\eta < 1$ will lead to different characteristics in the system.

1.4 The Laplace equation is often written as $\Delta u = 0$ or $\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$ in 2D case. Define a polar coordinate system (r, θ) so that $x = r\cos\theta$ and $y = r\sin\theta$, and then write the Laplace equation in the polar coordinates.

1.5 The FitzHugh-Nagumo equation occurs in many applications such as biology, genetics and heat transfers. In the 1D case, it can be written as

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + u(u-1)(\lambda - u),$$

where λ is a constant. Show that this equation supports a traveling wave solution

$$u(x,t) = \frac{A\exp(\eta_1) + \lambda B \exp(\eta_2)}{A\exp(\eta_1) + B\exp(\eta_2) + K},$$

where

$$\eta_1 = \Big(\frac{1}{2} - \lambda\Big)t \pm \frac{x}{\sqrt{2}}, \quad \eta_2 = \lambda\Big(\frac{\lambda}{2} - 1\Big)t \pm \frac{\lambda x}{\sqrt{2}},$$

and A, B and K are arbitrary constants.

1.6 The Klein-Gordon equation $\frac{\partial^2 u}{\partial t^2} = a^2 \frac{\partial^2 u}{\partial x^2} - bu$ occurs in quantum field theory and other applications. Verify that $u(x,t) = \sin(\lambda x)[A\cos(\omega t) + B\sin(\omega t)]$ is a solution if $b = -a^2\lambda^2 + \omega^2$. If $u(x,t) = \exp(\pm\lambda x)[A\cos(\omega t) + B\sin(\omega t)]$ is also a solution, what is the relationship between a, b, λ and ω.

1.7 In many applications, partial differential equations can be rewritten in other forms so that they can be linked with other well-known equations. For example, the so-called telegraph equation

$$\frac{\partial^2 u}{\partial t^2} + v\frac{\partial u}{\partial t} = a^2\frac{\partial^2 u}{\partial x^2} + bu, \quad v > 0, b < 0,$$

can be transformed into the Klein-Gordon equation by a transform $u(x,t) = \exp(-\frac{1}{2}vt)w(x,t)$. Show that this is true.

1.8 The Burgers equation in one-dimensional case is often written as

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + u\frac{\partial u}{\partial x}.$$

Show that it can be transformed into the standard linear diffusion equation by the so-called Hopf-Cole transformation $u(x,t) = \frac{2}{\phi}\frac{\partial \phi}{\partial x}$.

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