Differential Equations

At the heart of practically all of the problems that we wish to solve lies a differential equation. Indeed, one of the first equations that was encountered when we started to study physics is an example of a differential equation. Recall that Newton's second law of motion states that the sum of the external forces acting upon an object is proportional to the acceleration experienced by that object, where the constant of proportionality is the mass of the object. Mathematically we can write this as

$$\sum F_{ext}(x,t) = m\frac{d^2x}{dt^2}.$$

When one or more of the forces depends upon the position, $\mathbf{x}$, of the object, then we have an equation in which the derivatives of the variable that we are trying to solve for, in this case $\mathbf{x}(t)$, depends on the selfsame, unknown function $\mathbf{x}$.

There are a number of techniques that can be employed to solve differential equations. Practically all of these techniques depend upon the fact that the relationship between the derivatives and the function is either linear, or can be approximated to be linear for most of the region of interest. This limits the number of equations for which we can find closed solutions. The beauty of computational methods is that it frees us from the necessity of dealing only with analytic solutions, and thus expands the range over which we can solve problems.

In this lecture we consider three major types of practical numerical methods for solving initial value problems and boundary problems for ordinary differential equations.

- Runge-Kutta methods: Runge-Kutta methods propagate a solution over an interval by combining the information from several Euler-style

steps (each involving one evaluation of the right-hand I's), and then using the information obtained to match a Taylor series expansion up to some higher order.

- Richardson extrapolation and its particular implementation as the Bulirsch-Stoer method: Richardson extrapolation uses the powerful idea of extrapolating a computed result to the value that would have been obtained if the step size had been very much smaller than it actually was. In particular, extrapolation to zero step size is the desired goal. The first practical ODE integrator that implemented this idea was developed by Bulirsch and Stoer, and so extrapolation methods are often called Bulirsch-Stoer methods.

- Predictor-corrector methods: Predictor-corrector methods store the solution along the way, and use those results to extrapolate the solution

one step advanced; they then correct the extrapolation using derivative information at the new point. These are best for very smooth functions.

20 Basic Concepts

Before beginning to discuss numerical solutions to differential equations, let's review some basic concepts. We define the order of a differential equation to be the degree of the highest derivative in the equation. For example,

$$\frac{dx}{dt} - f(x,t) = 0$$

is a first order differential equation, while

$$\frac{d^2x}{dt^2} - f(\frac{dx}{dt}, x, t) = 0$$

is a second order equation. In general, we can write

$$\sum_{i=0}^{N} a_i(x,t)\frac{d^i x}{dt^i} = 0$$

as the basic equation of an N^{th} order differential equation.

Notice that in all of the equations, the time t is the independent variable and the position x is the dependent variable. In other words, while we are free to vary the time at the solution is to be found, we cannot vary the value of the position at that time. Another way of looking at this is that the time acts as a parameter that specifies the particular solution to the equation, while the position x is the function into which the parameter goes. Since

a function acts like a black box that takes independent variables in one end and passes a result out the other end, obviously we cannot change the function without affecting the result!

We can cast the difference between independent and dependent variables into a form that has more relevance in a computational setting. We again consider the independent variables as parameters that are used to specify a particular solution, and think of each the dependent variable as a specific function that returns a result. This description sounds very familiar; it is the same description used to describe a function in a programming language! The independent variables are the parameters passed to the function in the calling line, while the code that carries out the calculation represents the effects of the dependent variable. So once again we see that, while the independent variables can be freely adjusted, we cannot change the dependent variable.

In addition to the order of the equation, it is important to understand the linearity of the equation. A linear equation is one in which the function and its derivatives appear only to first order. Thus, the equation

$$\frac{d^2x}{dt^2} - \frac{g}{l}x = 0$$

is linear. Equations that are not linear are classified as nonlinear equations. Examples of nonlinear equations are

$$\frac{d^2x}{dt^2} - \frac{g}{l}\sin x = 0$$

and

$$\frac{d^2x}{dt^2} = \lambda x - \lambda^2 x^2$$

Traditionally, we are limited in our ability to study nonlinear equations if we want to express the results in a closed form. While techniques exist

to find solutions, practically all of them involve either taking roots (if the nonlinear portion is in the highest order derivative) or expanding the dependent variable as a power series and keeping only the linear term.

One of the reasons that linear equations have traditionally been considered important (other than the fact that they are the only ones that can be solved analytically) is that they obey the law of linear superposition. This tells us that if we find more than one solution of a linear equation, then the sum of these solutions is also a solution.

20.1 Example:

What is the most general solution to the differential equation

$$\frac{d^2x}{dt^2} + \frac{g}{l}x = 0?$$

One of the nicer aspects of solving differential equations is the uniqueness theorem, which tells us that if we can find a solution to the differential equation by any means then this is the only solution. Thus, if we can guess at a solution and find that it satisfies the equation, then we know that it is the solution.

In this case, since the differential equation is of second order, we know that there must be two independent solutions to the equation. Let's try

$$x_1(t) = A \sin\left[(g/l)^{1/2}t + \delta\right]$$

and

$$x_2(t) = B \cos\left[(g/l)^{1/2}t + \delta\right]$$

Taking the second derivative of each and substituting back into the differential equation, we find that our equation is indeed satisfied. The general solution is then

$$\begin{aligned} x(t) &= \alpha x_1(t) + \beta x_2(t) \\ &= \alpha A \sin\left[(g/l)^{1/2}t + \delta\right] + \beta B \cos\left[(g/l)^{1/2}t + \delta\right] \end{aligned}$$

$$x(t) = A' \sin\left[(g/l)^{1/2}t + \delta'\right]$$

The coefficients will be determined by the initial condition or boundary condition.

20.2 Example

Nonlinear equations do not necessarily follow the law of linear superposition, as can been seen in the following example.

A solution of the differential equation

$$\frac{dx}{dt} = \lambda x - \lambda^2 x^2$$

is

$$x = \frac{a}{a\lambda + be^{-\lambda t}}$$

This can be verified through substitution. However, if we formed a superposition of this solution we would get

$$\begin{aligned} x' &= x_1 + x_2 \\ &= \frac{a_1}{a_1\lambda + b_1 e^{-\lambda t}} + \frac{a_2}{a_2\lambda + b_2 e^{-\lambda t}} \end{aligned}$$

The derivative of this is

$$\frac{dx'}{dt} = \lambda x_1 - \lambda^2 x_1^2 + \lambda x_2 - \lambda^2 x_2^2$$

Thus, solutions to this nonlinear differential equation cannot be superpositioned with each other.

20.3 Dynamical Forms

The last concept that we need to remember is that any solution of an N^{th} order differential equation will contain N unknown constants. The values of these constants are fixed by specifying the initial conditions associated with the problem. This fact remains true regardless of whether we are

solving the problem analytically or numerically. If we do not know all of the initial conditions for a particular problem, we cannot solve it exactly.

One of the most useful methods of solving ordinary differential equations is to cast them into their dynamical form. The dynamical form of an ordinary differential equation is that form in which the left hand side of the equation consists of a first order differential while the right hand side of the equation contains a function that depends only on the values of the various parameters and dynamic variables. This immediately implies that if we have a differential equation of order 2 or more, then we will be forced to develop additional equations expressing intermediate results. Indeed, the dynamical form of an N^{th} order ordinary differential equation consists of a set of N first order linked differential equations that must be solved simultaneously.

Example: Write the differential equation for the driven damped harmonic oscillator in dynamical form.

The equation of motion for a driven damped harmonic oscillator is

$$m\frac{d^2x}{dt^2} + \gamma\frac{dx}{dt} + m\omega_0^2 x - F_{ext} = 0$$

where $F_{ext}(t)$ is the driving force, γ is the damping constant, and ω_0 is the natural frequency of the oscillator. In order to eliminate the second order derivative term, use the definition of velocity, $v = dx/dt$, to rewrite the equation as

$$m\frac{dv}{dt} + \gamma v + m\omega_0^2 x - F_{ext} = 0$$

Thus, the dynamical form of equation is the set

$$\begin{cases} \frac{dx}{dt} = v \\ m\frac{dv}{dt} = F_{ext} - \gamma v - m\omega_0^2 x \end{cases}$$

21 Types of differential equations

A differential equation expresses the relation between a function, its derivative and the independent variables. The order of the equation is determined by the highest order derivative involved.

21.1 Several differential equations

Several common differential equations in physics are listed here.

(1). The equation for the harmonic motion.

$$\mu \frac{d^2\phi}{dt^2} = -k\phi.$$

This is a second-order linear differential equation: "second order" means the highest derivative is $\frac{d^2\phi}{dt^2}$, and "linear" means that ϕ and its derivatives appear in the first order and there are no products between them.

(2). The equation of motion for a vibrating string.

$$\frac{d^2\phi}{dx^2} - \frac{1}{v^2}\frac{d^2\phi}{dt^2} = 0.$$

If ϕ has more than a single independent variable, partial derivatives enter into the equation, for example, in the case of a vibrating string .

(3). Two-dimensional Poisson equation

$$\frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} = -\rho(x, y).$$

It describes the field $\phi(x)$ of a charge distribution $\rho(x, y)$ in two dimensions.

(4). The diffusion equation

$$\frac{\partial \phi}{\partial t} = -\frac{\partial}{\partial x}\left(D\frac{\partial \phi}{\partial x}\right).$$

ϕ may be the concentration of a certain kind of particle and D is its diffusion coefficient.

21.2 Initial and boundary value problems

Differential equations can be classified into initial value and boundary value problems. For numerical solutions, the differences between these two categories can often be more important than some of the considerations above. This comes from the fact that an initial value problem propagates the solution forward from the values given at the starting point. In contrast, a

boundary value problem has constraints that must be satisfied at both the start and the end of the interval. The distinction between temporal and spatial variables is mainly in their physical significance. As far as numerical solutions are concerned, there are very few differences between them except, perhaps, in the manner they appear in the equation under certain circumstances. Our primary concern in the differences between initial value and boundary value problems is in the way the constraints are placed on the solution. If all the conditions that must be satisfied by the solution are given at one end of the interval, we have an initial value problem. On the other hand, if the constraints on the solution are applied to both ends of the interval, we have a boundary value problem. For partial differential equations, it may also happen that the conditions for some independent variables are given in the form of initial values and others as boundary conditions. If this happens, we have an initial value boundary problem, a mixture of both types in one.

21.3 Euler's method for initial value problems

The general philosophy behind the numerical solutions to differential equation can be illustrated using Euler's method to solve the simple harmonic motion. The algorithm is simple and straightforward.

$$\frac{d^2\phi}{dt^2} + \omega_0^2\phi = 0$$

by expressing the spring constant k and mass μ in terms of the angular frequency for simple harmonic motion $\omega_0 = (k/\mu)^{1/2}$. Similar to what we did in numerical integration, the first step is to discrete the interval of interest into a grid or mesh consisting of finite of points in the interval $t = [t_0, t_N]$. For the numerical solution we can find the values of ϕ at a discrete numbers of points $t = t_1, t_2, \cdots, t_{N-1}$. The distance between two consecutive points, or step size, is

$$h = t_{i+1} - t_i.$$

On this discrete space, the second-order derivative at t_i is written as

$$\left.\frac{d^2\phi}{dt^2}\right|_{t=t_i} \rightarrow \frac{1}{h^2}\left\{\phi(t_{i+1}) - 2\phi(t_i) + \phi(t_{i-1})\right\}$$

The equation is reduced to a discrete form

$$\phi(t_{i+1}) - 2\phi(t_i) + \phi(t_{i-1}) + h^2\omega_0^2\phi(t_i) = 0$$

$$\phi(t_{i+1}) + \left(h^2\omega_0^2 - 2\right)\phi(t_i) + \phi(t_{i-1}) = 0$$

This is called the finite difference equation (FDE). As an initial value problem, we need two independent pieces of input on ϕ at the starting time. Physically, these initial conditions may be supplied in terms of the location and velocity of the mass at $t = t_0$. For example,

$$\begin{aligned} \phi(t_0) &= 0 \\ \left.\frac{d\phi}{dt}\right|_{t=t_0} &= 0 \end{aligned}$$

Using finite difference, the second condition can be expressed as

$$\phi(t_0) = \phi(t_1).$$

These two conditions provide a possibility to evaluate the value of ϕ at $t = t_2$.

$$\phi(t_2) = \left(2 - h^2\omega_0^2\right)\phi(t_1) - \phi(t_0)$$

Once $\phi(t_2)$ is found, we can evaluate $\phi(t_3)$. These process continue until $i = N - 1$,

$$\phi(t_{i+1}) = \left(2 - h^2\omega_0^2\right)\phi(t_i) - \phi(t_{i-1}).$$

In this way, the solution for ϕ is propagated forward one step at a time and all the ϕ are found one after another.

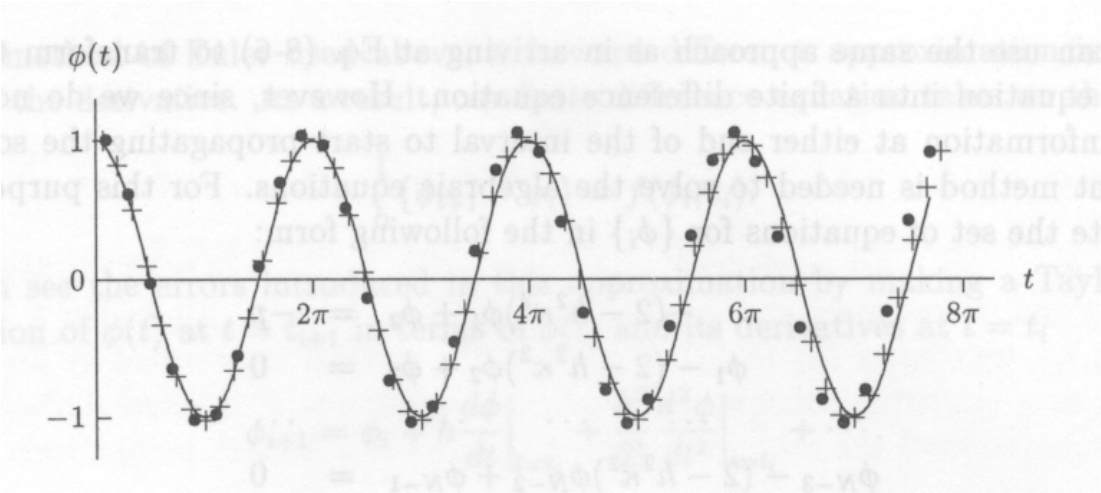

Figure 1: Solutions for the simple harmonic oscillation: dots for h=0.63; plus for h=0.4; and solid curve for analytical solution.

21.4 Example of a boundary value problem

As a comparison, we shall solve the same differential equation as a boundary value problem.

$$\frac{d^2\phi}{dx^2} + k^2\phi = 0$$

We just use position x instead of time t. For simplicity, we consider $x = [0, l]$. The finite different equations are

$$\phi(x_{i+1}) + \left(h^2k^2 - 2\right)\phi(x_i) + \phi(x_{i-1}) = 0$$

where $i = 1, 2, \cdots, N-1$. The boundary conditions are given

$$\phi(x = 0) = \phi(x = l) = p$$

In the discrete space,

$$\phi(x_0) = \phi(x_N) = p$$

We can use the same approach to transform the differential equation into a finite difference equation. However since we do not have enough information at either end of interval to start propagating the solution, a different method is needed to solve the algebraic equations. The equations can be written in a matrix form,

$$A\Phi = B$$

Here $d = h^2k^2 - 2$

$$A = \begin{pmatrix} d & 1 & 0 & \cdots & 0 \\ 1 & d & 1 & & 0 \\ 0 & 1 & \ddots & \ddots & \vdots \\ \vdots & & \ddots & \ddots & 1 \\ 0 & 0 & \cdots & 1 & d \end{pmatrix}$$

and

$$B = \begin{pmatrix} -p \\ 0 \\ \vdots \\ 0 \\ -p \end{pmatrix} \qquad \Phi = \begin{pmatrix} \phi(x_1) \\ \phi(x_2) \\ \vdots \\ \phi(x_{N-2}) \\ \phi(x_{N-1}) \end{pmatrix}$$

The matrix has a tridiagonal form. We can use the methods of matrix to solve it. To achieve good accuracy, the step size must be small. Consequently N must be quite large.

21.5 Stability and convergence

Besides the obvious demand of efficiency, a numerical method has to be stable and solution converges to that of differential equation. The importance of these two additional requirements can be seen from oscillator example we encountered earlier. Since the full solution is obtained by propagating from two initial values, the truncation error in all the steps can be cumulative and may make the numerical results meaningless.

22 Runge-Kutta methods

Ordinary differential equation of order N can always be reduced to a set of first order ones in the form

$$\frac{dy}{dt} = f(y(t), t) \tag{1}$$

where $y = \{y_1, y_2, \cdots\}$ and $f = \{f_1, f_2, \cdots\}$. For example, the equation for a damped oscillation is given by

$$\frac{d^2\phi}{dt^2} + 2\gamma\frac{d\phi}{dt} + \omega_0^2\phi = 0.$$

Let us define

$$\begin{aligned} y_1 &= \phi \\ y_2 &= \frac{d\phi}{dt} \end{aligned}$$

The equation can be written as

$$\begin{aligned} \frac{dy_1}{dt} &= y_2 \\ \frac{dy_2}{dt} &= -\omega_0^2 y_1 - 2\gamma y_2 \end{aligned}$$

Thus the equations can written in the form in Eq. 1.

Thus finite difference approximation for Eq.1 may be expressed in the form

$$\frac{1}{h}\{y(t_{k+1}) - y(t_k)\} = f(y(t_k), t_k) \tag{2}$$

Notice that the Taylor expansion of y at $t = t_{k+1}$ is, for example

$$y_1(t_{k+1}) = y_1(t_k) + h \left.\frac{dy_1}{dt}\right|_{t_k} + \frac{h^2}{2} \left.\frac{d^2 y_1}{dt^2}\right|_{t_k} + \cdots$$

$$\left.\frac{dy_1}{dt}\right|_{t_k} = \frac{y_1(t_{k+1}) - y_1(t_k)}{h} - \frac{h}{2}\left.\frac{d^2y_1}{dt^2}\right|_{t_k} + \cdots$$

Thus the expression in Eq.2 is accurate to order of h. If we want to make any improvement of Eq.2, we must include additional "input" information on the right side. For example, we make use of

$$\begin{aligned} p &= f(y(t_k), t_k) \\ q &= f(y(t_k) + \alpha h p, t_k + \alpha h) \end{aligned}$$

where α is adjustable parameter. The equation is corrected as

$$\frac{1}{h}\{y(t_{k+1}) - y(t_k)\} = \beta_1 p + \beta_2 q$$

Using a Taylor series expansion and eliminating the term up to order of h, we have

$$q \approx \frac{dy}{dt} + \alpha h \frac{d^2y}{dt^2} + \frac{1}{2}(\alpha h)^2 \left\{ \frac{d^3y}{dt^3} - \frac{\partial f}{\partial y}\frac{d^2y}{dt^2} \right\}$$

The truncation error is then

$$\begin{aligned} E &= (1-\beta_1-\beta_2)\left.\frac{dy}{dt}\right|_{t_k} + h(\frac{1}{2}-\alpha\beta_2)\left.\frac{d^2y}{dt^2}\right|_{t_k} \\ &\quad + h^2\left\{\left(\frac{1}{6}+\frac{1}{2}\alpha^2\beta_2\right)\left.\frac{d^3y}{dt^3}\right|_{t_k} - \frac{\partial f}{\partial y}\left.\frac{d^2y}{dt^2}\right|_{t_k}\right\} + \cdots \end{aligned}$$

We can take α and β to reduce the possible error. It is not possible to eliminate all h^2 dependence for an arbitrary function. There are however several choices available to make E as small as possible. For instance,

$$\begin{aligned} 1-\beta_1-\beta_2 &= 0 \\ \frac{1}{2}-\alpha\beta_2 &= 0 \end{aligned}$$

We can take $\alpha = 1$ and $\beta_1 = \beta_2 = 1/2$, or $\alpha = 1/2$, $\beta_1 = 0$ and $\beta_2 = 1$.

The idea can be generalized to the order of h^4. One result commonly used

in practical application is the fourth-order Runge-Kutta formula

$$y(t_{k+1}) = y(t_k) + \frac{1}{6}h(p + 2q + 2r + s)$$

where

$$\begin{aligned} p &= f(y(t_k), t_k) \\ q &= f(y(t_k) + \frac{1}{2}hp, t_k + \frac{1}{2}h) \\ r &= f(y(t_k) + \frac{1}{2}hq, t_k + \frac{1}{2}h) \\ s &= f(y(t_k) + hr, t_k + h) \end{aligned}$$

In this case, the finite difference equation is accurate to order h^4.

The statement "fourth-order Runge-Kutta is generally superior to second-order" is a true one, but you should recognize it as a statement about the comtemporary practice of science rather than as a statement about

strict mathematics. That is, it reflects the nature of the problem that contemporary scientists like to solve.

Application to damped oscillation

The equation for a damped oscillator is

$$\mu\frac{d^2\phi}{dt^2} + b\frac{d\phi}{dt} + k\phi = 0$$

where b is the constant of proportionality for the damping term due to friction. In general

$$\frac{d^2\phi}{dt^2} + 2\gamma\frac{d\phi}{dt} + \omega_0^2\phi = 0.$$

To solve the problem numerically it can be written as

$$\frac{df}{dt} = f(y(t), t)$$

$$\begin{aligned} f_1 &= y_2 \\ f_2 &= -2\gamma y_2 - \omega_0^2 y_1 \end{aligned}$$

where $y_1 = \phi$, and $y_2 = d\phi/dt$. At $t = 0$, the initial conditions are

$$\begin{aligned} y_1 &= \phi_0 \\ y_2 &= \left.\frac{d\phi}{dt}\right|_{t=0} \end{aligned}$$

It is well known that there are three types of solution depending on the size of γ relative to that of ω_0.

To solve problem, we assume $\phi = e^{-\lambda t}$. Then the characteristic equation is

$$\lambda^2 - 2\gamma\lambda + \omega_0^2 = 0.$$

We have two solutions

$$\begin{aligned} \lambda_1 &= \gamma + (\gamma^2 - \omega_0^2)^{1/2} \\ \lambda_2 &= \gamma - (\gamma^2 - \omega_0^2)^{1/2} \end{aligned}$$

The general solution for ϕ becomes

$$\phi = c_1 e^{-\lambda_1 t} + c_2 e^{-\lambda_2 t}.$$

1. Heavy damping: $\gamma^2 > \omega_0^2$ gives a solution

$$\phi(t) = \frac{\phi_0 + \xi}{2} e^{-(\gamma - \zeta)t} + \frac{\phi_0 - \xi}{2} e^{-(\gamma + \zeta)t}$$

where

$$\begin{aligned} \zeta &= (\gamma^2 - \omega_0^2)^{1/2}; \\ \xi &= \frac{1}{\zeta} \left\{ \frac{d\phi}{dt}\Big|_{t=0} + \gamma \phi_0 \right\}. \end{aligned}$$

2. The critical damping: $\gamma^2 = \omega_0^2$ gives a solution,

$$\phi(t) = e^{-\gamma t}\left\{\phi_0 + \left(\left.\frac{d\phi}{dt}\right|_{t=0} + \gamma\phi_0\right) t\right\}$$

3. The underdamping, $\gamma^2 < \omega_0^2$ gives an analytical solution

$$\phi(t) = e^{-\gamma t}\left(\phi_0 \cos\omega t + \xi \sin\omega t\right)$$

where

$$\begin{aligned} \omega &= (\omega_0^2 - \gamma^2)^{1/2} \\ \xi &= \frac{1}{\omega}\left\{\left.\frac{d\phi}{dt}\right|_{t=0} + \gamma\phi_0\right\} \end{aligned}$$

The accuracy of numerical solution by the Runge-Kutta method is relatively poor. This is an example of a stiff differential equation, arising from the fact that there are two time constants in the solution ω and γ, and their

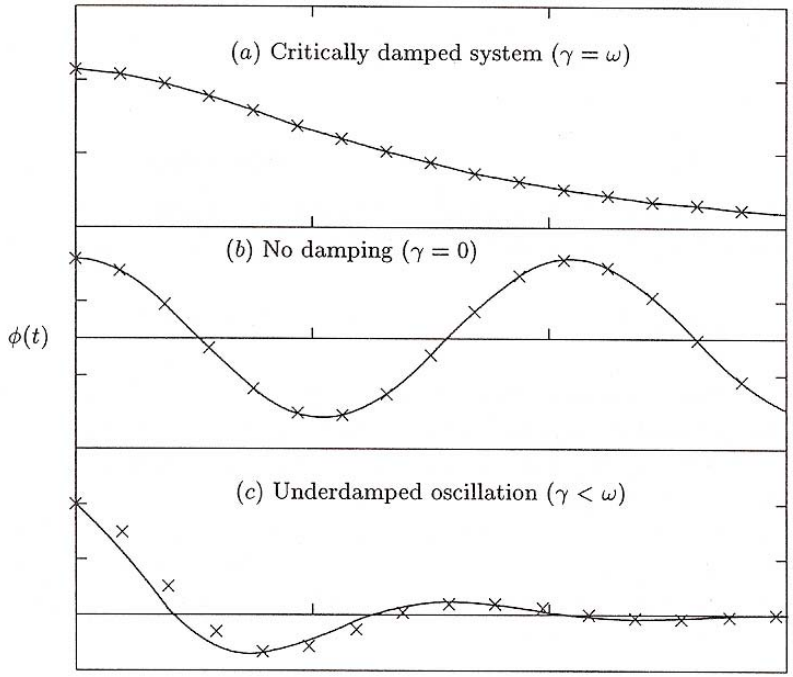
(a) Critically damped system ($\gamma = \omega$)
(b) No damping ($\gamma = 0$)
$\phi(t)$
(c) Underdamped oscillation ($\gamma < \omega$)

Figure 2:

values are rather different. As a result the numerical solution becomes unstable.

The solution to this problem is to introduce transformation,

$$\phi(t) = e^{-\gamma t} y(t)$$

On substituting this form of ϕ into the equation, we obtain

$$\frac{d^2 y}{dt^2} + \left(\omega_0^2 - \gamma^2\right) y = 0.$$

There is only one time scale here, and we should have no difficulty in solving the equation numerically.

Variable step size:

$$\mathbf{Y}_{2h}(t_k + 2h_t) = \mathbf{y}(t_k) + \frac{1}{3} h_t (\mathbf{p}_{2h} + 2\mathbf{q}_{2h} + 2\mathbf{r}_{2h} + \mathbf{s}_{2h})$$

The value of $\mathbf{y}(t)$ at $t = t_k + 2h_t$ can be also be obtained in two separate steps. First, we take a step of h_t. This gives us the result,

$$\mathbf{z}(t_k + h_t) = \mathbf{y}(t_k) + \frac{1}{6} h_t(\mathbf{p}_{h1} + 2\mathbf{q}_{h1} + 2\mathbf{r}_{h1} + \mathbf{s}_{h1})$$

Second, we start with $\mathbf{z}(t_k + h_t)$ and make another step of size h_t

$$\mathbf{Y}_{1h}(t_k + 2h_t) = \mathbf{z}(t_k + h_k) + \frac{1}{6} h_t(\mathbf{p}_{h2} + 2\mathbf{q}_{h2} + 2\mathbf{r}_{h2} + \mathbf{s}_{h2})$$

Since $\mathbf{Y}(t_k + 2h_t)$ and $\mathbf{Y}_{2h}(t_k + 2h_t)$ are obtained using a fourth-order Runge-Kutta method, we expect the difference between them to be on the order h_y^5.

$$\mathbf{\Delta}(t_k, h_t) = \mathbf{Y}_{2h}(t_k + 2h_t) - \mathbf{Y}_{1h}(t_k + 2h_t) \sim O(h_t^5)$$

The value of $\mathbf{\Delta}(t_k, h_t)$ is useful for two related purposes. First, we can compare the value with the maximum truncation error we can tolerate,

ε_{max}. If $|\mathbf{\Delta}(t_k, h_t)| < \varepsilon_{\text{max}}$, the step size of h_t is acceptable. Second, we can use $\mathbf{\Delta}(t_k, h_t)$ to estimate the optimal step size h_0 for the subinterval $[t_{k+1}, t_{k+2}]$.

$$h_0 = h_t \left| \frac{\varepsilon_{\text{max}}}{\mathbf{\Delta}(t_k, h_t)} \right|^{1/5}$$

If, on the other hand, the trial step size h_t produces a truncation error that is larger than ε_{max}, we must go back to take a smaller h_t

23 Relaxation Method

One approach to boundary value problems is to solve the finite difference equations in matrix method. To be more specific, we shall use the second

order differential equation

$$\frac{d^2\phi}{dx^2} + g(x)\phi(x) = 0$$

in the interval $[x_0, x_N]$. The two boundary conditions for this problem may be taken as

$$\phi(x_0) = \alpha_0, \quad \phi(x_N) = \alpha_N$$

The factor $g(x)$ can be either constant or function of x. The interval $[x_0, x_N]$ is divided into N subinterval and we just consider a constant step size

$$h = x_{k+1} - x_k$$

The second order derivative is written as

$$\left.\frac{d^2\phi}{dx^2}\right|_{x=x_k} \rightarrow \frac{1}{h^2}\left\{\phi(x_{k+1}) - 2\phi(x_k) + \phi(x_{k-1})\right\}$$

The equation is reduced to a discrete form

$$\frac{1}{h^2}\left\{\phi(x_{k+1}) - 2\phi(x_k) + \phi(x_{k-1})\right\} + g(x_k)\phi(x_k) = 0$$

$$\phi(x_{k+1}) + \left[h^2 g(x_k) - 2\right]\phi(x_k) + \phi(x_{k-1}) = 0$$

where $k = 1, 2, \cdots N-1$. Thus there are $N-1$ equations. Combining with the boundary conditions we can write the equations in a compact form

$$Ay = B$$

Here A is a $(N-1) \times (N-1)$ matrix

$$A = \begin{pmatrix} d_1 & -1 & & & \\ -1 & d_2 & -1 & & \\ & -1 & \ddots & \ddots & \\ & & \ddots & \ddots & -1 \\ & & & -1 & d_{N-1} \end{pmatrix}$$

and

$$d_k = 2 - h^2 g(x_k)$$

$$B = \begin{pmatrix} \alpha_0 \\ 0 \\ \vdots \\ 0 \\ \alpha_N \end{pmatrix}$$

The main feature is that the nonvanishing elements in A is very small. We can use an iterative method to solve this equation.

23.1 Iterative Method

To illustrate the method we just consider a system with three equations

$$\begin{aligned} A_{11}y_1 + A_{12}y_2 + A_{13}y_3 &= b_1 \\ A_{21}y_1 + A_{22}y_2 + A_{23}y_3 &= b_2 \\ A_{31}y_1 + A_{32}y_2 + A_{33}y_3 &= b_3 \end{aligned}$$

It is always possible to arrange the equations in such a way that all diagonal elements are nonvanishing

$$\begin{aligned} y_1 &= \frac{1}{A_{11}}\{b_1 - A_{12}y_2 - A_{13}y_3\} \\ y_2 &= \frac{1}{A_{22}}\{b_2 - A_{21}y_1 - A_{23}y_3\} \\ y_3 &= \frac{1}{A_{33}}\{b_3 - A_{31}y_1 - A_{32}y_2\} \end{aligned}$$

This is the starting point for iterative method to solve this equation.

An iterative solution begins with a set of initial estimate $y^{(0)}$. From the $y^{(0)}$, we can construct an approximate solution $y^{(1)}$, which may be closer to the real solution. Then, we can evaluate $y^{(2)}, y^{(3)}, \cdots y^{(n)}$ and so on. The convergence reaches if the difference between $y^{(k+1)}$ and $y^{(k)}$ are less than the tolerance or precision ϵ as required. In formula,

$$\begin{aligned} y_1^{(i+1)} &= \frac{1}{A_{11}}\left\{b_1 - A_{12}y_2^{(i)} - A_{13}y_3^{(i)}\right\} \\ y_2^{(i+1)} &= \frac{1}{A_{22}}\left\{b_2 - A_{21}y_1^{(i)} - A_{23}y_3^{(i)}\right\} \\ y_3^{(i+1)} &= \frac{1}{A_{33}}\left\{b_3 - A_{31}y_1^{(i)} - A_{32}y_2^{(i)}\right\} \end{aligned}$$

or

$$y_j^{(i+1)} = \frac{1}{A_{jj}}\left\{b_j - \sum_{i=1}^{j-1} A_{jk}y_k^{(i)} - \sum_{i=j+1}^{N} A_{jk}y_k^{(i)}\right\}$$

A slight improvement is made in following way: once the $y_1^{(i+1)}$ is evaluated in the first step, the result may be used in the calculation of other $y_k^{(i+1)}$ i.e.,

$$\begin{aligned} y_1^{(i+1)} &= \frac{1}{A_{11}}\left\{b_1 - A_{12}y_2^{(i)} - A_{13}y_3^{(i)}\right\} \\ y_2^{(i+1)} &= \frac{1}{A_{22}}\left\{b_2 - A_{21}y_1^{(i+1)} - A_{23}y_3^{(i)}\right\} \\ y_3^{(i+1)} &= \frac{1}{A_{33}}\left\{b_3 - A_{31}y_1^{(i+1)} - A_{32}y_2^{(i+1)}\right\} \end{aligned}$$

or

$$y_j^{(i+1)} = \frac{1}{A_{jj}}\left\{b_j - \sum_{i=1}^{j-1} A_{jk}y_k^{(i+1)} - \sum_{i=j+1}^{N} A_{jk}y_k^{(i)}\right\}$$

Alternatively,

$$y_j^{(i+1)} = y_j^{(i)} + \frac{1}{A_{jj}} \left\{ b_j - \sum_{i=1}^{j-1} A_{jk} y_k^{(i+1)} - \sum_{i=j}^{N} A_{jk} y_k^{(i)} \right\}$$

The second term in the right-hand side may be taken as the correction to $y_j^{(i)}$. As a result, it may be possible to modify the rate of convergence by introducing a relaxation parameter ω as the weighting factor

$$y_j^{(i+1)} = y_j^{(i)} + \frac{\omega}{A_{jj}} \left\{ b_j - \sum_{i=1}^{j-1} A_{jk} y_k^{(i+1)} - \sum_{i=j}^{N} A_{jk} y_k^{(i)} \right\}$$

For $\omega < 1$, it is known as the under-relaxation method; for $\omega = 1$, the Gauss-Sedel method; and for $\omega > 1$, the over-relaxation method.

Convergence

For a discussion on the convergence criteria, it is more convenient to write the equation as

$$y^{(i+1)} = Py^{(i)} + q$$

Assume y is the exact solution

$$y = Py + q$$

Then,

$$(y - y^{(k+1)}) = P(y - y^{(k)}) = P^k(y - y^{(0)})$$

For a large k, if $y^{(k+1)}$ approaches to the exact solution y, we require

$$\lim_{k \to \infty} P^k = 0$$

Assume v_l and λ_l the eigenvectors of P, and

$$y - y^{(0)} = \sum_l c_l v_l$$

then

$$y - y^{(k+1)} = \sum_l c_l \lambda_l^k v_l$$

If, in general, all eigenvalues λ_l satisfy

$$|\lambda_l| < 1$$

we have

$$\lim_{k \to \infty} \left(y - y^{(k+1)} \right) = 0.$$

Otherwise the solution becomes divergent.

Alternatively, we define a quantity for the matrix P called spectral radius, given by the maximum absolute value of the eigenvalues

$$\rho(P) = \max_{l=1,2,\cdots,N} |\lambda_l|$$

The condition of the convergence for our iterative method may be stated now as the reqquirement for the spectral radius of the corresponding point interation matrix to be less than unity.

Optimum relaxation parameter ω

As the condition of convergence is determined by the largest absolute value of the eigenvalues for $P(\omega)$, the role of the relaxation parameter ω is to change the largest absolute value.

$$\omega_x = \frac{2}{1 + (1 - \rho^2(P))^{1/2}}$$

24 Boundary value problems in partial differential equations

The relaxation methods developed in the last section were aimed at ordinary differential equations. With only minor modifications, they may also be used to solve partial differential equations (PDFs) where we have more than one independent variable. For simplicity we shall restrict ourselves to two spatial dimensions.

$$\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} = -\rho(x, y)$$

It describes the situation where the charge distribution is independent of the z-directions. To simplify the problem, we just consider the boundary

condition as

$$V(x = \pm l, y) = V(x, y = \pm l) = V_0$$

To solve this problem we first discrete the space as two-dimensional mesh as shown in Fig. The second-order derivative is written as

$$\left.\frac{\partial^2 V}{\partial x^2}\right|_{x=x_i, y=y_j} = \frac{1}{\Delta x^2}\left[V(x_{i+1}, y_j) - 2V(x_i, y_j) + V(x_{i-1}, y_j)\right]$$

$$\left.\frac{\partial^2 V}{\partial y^2}\right|_{x=x_i, y=y_j} = \frac{1}{\Delta y^2}\left[V(x_i, y_{j+1}) - 2V(x_i, y_j) + V(x_i, y_{j-1})\right]$$

If we take $\Delta x = \Delta y = h$, the equation simplifies to

$$V(x_{i+1}, y_j) + V(x_{i-1}, y_j) + V(x_i, y_{j+1}) + V(x_i, y_{j-1}) - 4V(x_i, y_j) = -h^2 \rho(x_i, y_j)$$

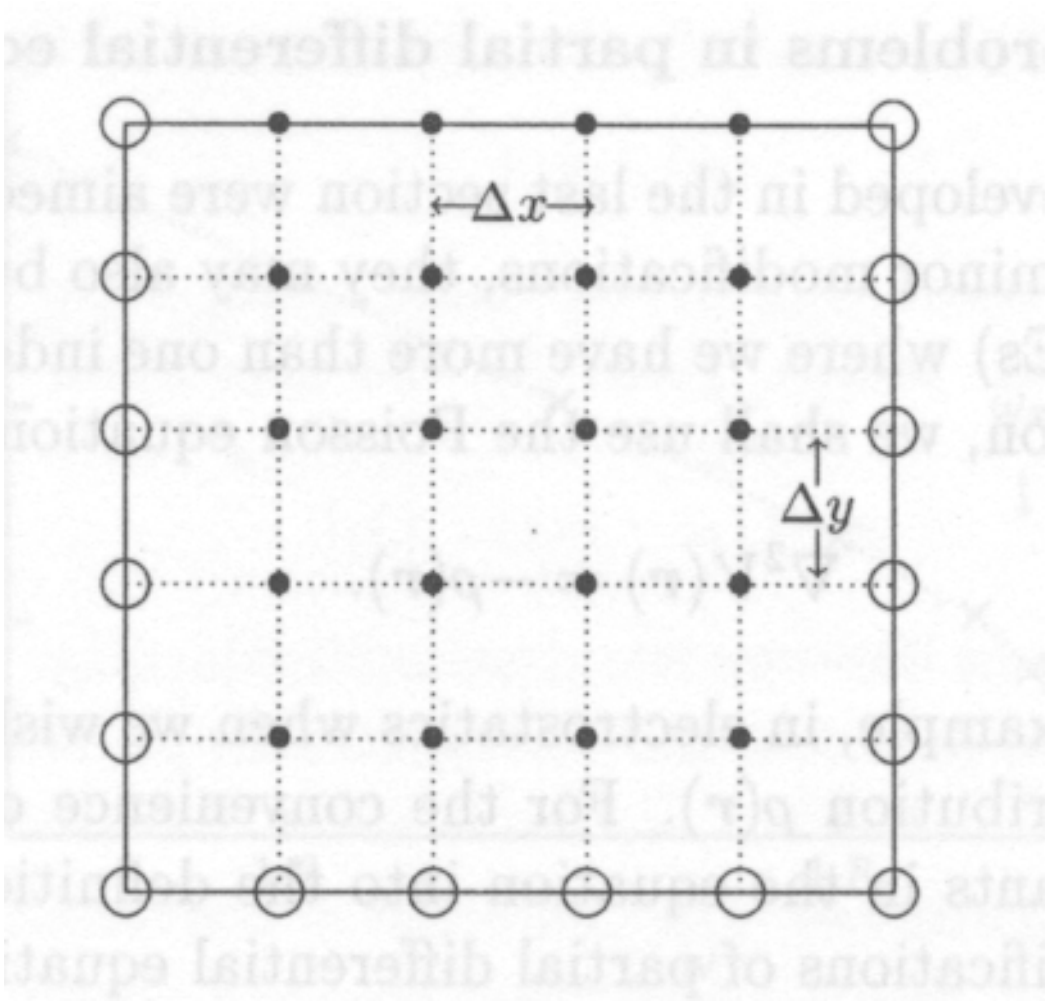

Figure 3: A two dimensional mesh of points to transform a PDF of two independent variables into a set of PDFs. In general, $\Delta x \neq \Delta y$. Circles

It is fairly straightforward to rewrite the equation as a recursion equation in this way

$$\begin{aligned} V^{(k+1)}(x_i, y_j) &= \frac{1}{4}\Big\{V^{(k)}(x_{i+1}, y_j) + V^{(k)}(x_{i-1}, y_j) \\ &\quad + V^{(k)}(x_i, y_{j+1}) + V^{(k)}(x_i, y_{j-1}) + h^2\rho(x_i, y_j)\end{aligned}$$

Alternatively, we can find the recursion relation by using Gauss-Seidel and successive overrelation method. The essential philosophy is to calculate $V^{(k+1)}(x, y)$ in the $(k+1)^{th}$ iteration using the updated values which are obtained in the $(k+1)^{th}$ iteration. For our purpose here, we shall take the simplest approach by working on all the elements of one row at a time, from the left to right in the order of increasing index i, before proceeding to the next row (increasing j). The resulting equation has the form

$$\begin{aligned} &V^{(k+1)}(x_i, y_j) = V^{(k)}(x_i, y_j) \\ &-\frac{\alpha}{4}\Big\{h^2\rho(x_i, y_j) + V^{(k+1)}(x_{i-1}, y_j) + V^{(k+1)}(x_i, y_{j-1})\end{aligned}$$

$$+ V^{(k)}(x_i, y_{j+1}) + V^{(k)}(x_{i+1}, y_j) - 4V^{(k)}(x_i, y_j)\Big\}$$

where α is the relaxation parameter.

$\rho(x, y)$

The point charge: $\rho(x, y) = \delta(x)\delta(y)$

25 Partial Differential Equations

In studying ordinary differential equations, we were motivated by the fact that many of the basic equations encountered in nature are cast in a form

where the rate of change in the function depends on the function itself. An example of this was Newton's laws of motion, where, in general, the acceleration can depend on the position. There are other fundamental relationships in physics; relationships that do not have as simple a structure.

Recall the first time you encountered the idea of potential energy. It was introduced for a number of reasons, one being that the potential energy is easier to calculate, since it is a scalar function and not a vector, allowing the force to be determined as

$$\hat{F} = -\frac{dU}{dx}\hat{x} \tag{3}$$

Unfortunately, while this was sufficient for one-dimensional problems, we live in a three dimensional world. Thus, the equation (3) very quickly became replaced with

$$\hat{F} = -\nabla U \tag{4}$$

where ∇ is the gradient, or directional derivative. In Cartesian coordinates, it is defined as

$$\nabla = \frac{\partial}{\partial x}\hat{x} + \frac{\partial}{\partial y}\hat{y} + \frac{\partial}{\partial z}\hat{z} \tag{5}$$

Notice that the derivatives in equation (5) are partial derivatives. This is a general trend. Moving from one to two, three or more dimensions inherently involves converting from ordinary derivatives to partial derivatives, and thus our equations transform from ordinary differential equations to partial differential equations.

Moving from ordinary differential equations to partial differential equations involves invoking a very different approach to their solution. In particular, whereas it was enough to specify the values of the function and its lesser derivatives to get an exact solution for an ODE, for a partial differential equation, an equivalent expression requires that the initial conditions must

be known throughout all of space. In addition, we usually want to constrain the solution of the PDE in some region of space. Thus, in order to solve a partial differential equation, we must specify either an initial condition function, or a boundary condition, or both.

25.1 Parabolic Equations

Let's start by looking at parabolic equations. These equations are the closest to ordinary differential equations, and thus are one of the easiest equations to understand. Parabolic equations usually use a mixed set of conditions, namely an initial configuration combined with a boundary condition. As a concrete example, consider the diffusion equation,

$$\frac{\partial T(x,t)}{\partial t} = \kappa \frac{\partial^2 T(x,t)}{\partial x^2} \tag{6}$$

where $T(x,t)$ is the temperature at location x and time t, and κ is the thermal diffusion coefficient. Assume that the temperature is known at time $t = 0$ to satisfy

$$T(x, t = 0) = T_0 \delta(x),$$

as well as the Dirichlet boundary conditions,

$$T(x = -L/2, t) = T(x = L/2, t) = 0.$$

To solve this problem numerically, we replace the continuous analytical variables x and t with a discrete grid covering space and time. In order to simplify the equations, let's introduce the shorthand notation,

$$T_{in} = T(x_i, t_n)$$

where $x_i = (i-1)h - L/2$ is the spatial step size, $t_n = (n-1)\tau$, and τ is the temporal step size. Notice that the spatial points are both positive and negative, while the time steps are strictly positive. Also note that the

boundary points correspond to $i = 1$ and $i = N$, thus forcing the spatial step size h to satisfy $h = L/(N - 1)$.

We still need to calculate the derivatives in equation (6). This can be done using equations associated with derivatives. In particular, the time derivative can be written as

$$\frac{\partial T(x,t)}{\partial t} \rightarrow \frac{T(x_i, t_n + \tau) - T(x_i, t_n)}{\tau} = \frac{T_{i,n+1} - T_{i,n}}{\tau} \tag{7}$$

You should recognize this as the definition of the forward derivative. We can use this form since we are interested in solutions that only travel forward in time.

The spatial derivative is a second order derivative, and so needs to be treated more carefully. Since the spatial shifts can go in both a positive and negative direction, we must choose a centrally located scheme.

Again borrowing from our previous work with derivatives, we see that this derivative can be written as

$$\begin{aligned} \frac{\partial^2 T(x,t)}{\partial x^2} &\rightarrow \frac{T(x_i+h,t_n)-2T(x_i,t_n)+T(x_i-h,t_n)}{h^2} \\ &= \frac{T_{i+1,n}-2T_{i,n}+T_{i-1,n}}{h^2} \end{aligned} \tag{8}$$

Substituting equations (7) and (8) into equation (6) yields

$$\frac{T_{i,n+1}-T_{i,n}}{\tau} = \kappa \frac{T_{i+1,n}-2T_{i,n}+T_{i-1,n}}{h^2}$$

Because the discrete version of the time derivative is a forward derivative while the discrete version of the spatial derivative is a central derivative, this method is known as the forward time centered space scheme.

Rearranging the equation to find the future value of the temperature yields

$$T_{i,n+1} = T_{i,n} + \frac{\tau\kappa}{h^2}\left(T_{i+1,n}-2T_{i,n}+T_{i-1,n}\right)$$

Notice that everything that depends on the time step n is on the right hand side, while only the future value of the temperature is on the left. Because of this, the forward time centered space scheme is an example of an explicit method for solving partial differential equations.

Returning to our specific problem, we need to cast the initial and boundary conditions into a discrete form. From the equation (6), we immediately see that the boundary conditions correspond to

$$T_{1,n} = T_{N,n} = 0$$

for all n. The initial condition, $T(x, 0) = T_0\delta(x)$, cannot be put into a program directly. Fortunately, the Kronecker delta function is defined at the limit of a number of functions. For our purposes it is sufficient to choose a function that has similar features, namely one where the value goes to infinity as the distance scale goes to zero while maintaining an enclosed

area of approximately unity. With this in mind, we can approximate the delta function as

$$\Delta(x) = \begin{cases} \frac{l+x}{l^2} & -l < x < 0 \\ \frac{l-x}{l^2} & 0 < x < l \\ 0 & otherwise \end{cases}$$

This is just a triangular spike with unit area. As l approaches zero, its value goes to infinity while the area remains constant. Thus, we see that

$$\lim_{h \to 0} \Delta(x) = \delta(x)$$

The last problem that needs to be solved before we can program the solution is determining the size of the time step. This is important since if we pick a step too small we use up significant computer resources before finding a solution, if indeed one is reached. Too large a step loses information relevant to the problem. So how do we determine this?

As we have done in the past, we again let the analytical solution guide us. Assuming that the solution can be separated into a product of a function that depends only on time and a function that depends only on position, we can use the separation of variables method to find a solution as

$$T_n(x,t) = T_0 \sum_{n=1}^{\infty} e^{-(2n-1)^2\pi^2\kappa t/L^2} \cos\left[(2n-1)\pi x/L\right]$$

In order to determine the step size, assume that the spread in T is to be minimized. The spread in T can be calculated by taking partial derivatives

$$\delta T_n(x,t) = T_0 \left(\frac{\partial T}{\partial t}\delta t + \frac{\partial T}{\partial x}\delta x\right).$$

This is minimized when δt satisfies

$$\delta t \approx -x\frac{\delta x}{\kappa} = -\frac{h^2}{\kappa}$$

where a spatial step size of h has been used for both x and δx. Since we are only interested in the size of the step, the negative sign can be ignored.

Notice that if this step size is substituted back into equation (11.16) it becomes

$$T_{i,n+1} = T_{i,n} + \left(T_{i+1,n} - 2T_{i,n} + T_{i-1,n}\right)$$

Thus, each component of the difference equation is approximately of the same weight, as we would expect.

Implicit and explicit method:

To construct the finite difference equation, we can make use of central difference for the second-order derivative

$$\left.\frac{\partial^2 T(x,t)}{\partial x^2}\right|_{x=x_i} \rightarrow \frac{T(x_i+h,t) - 2T(x_i,t) + T(x_i-h,t)}{h^2}$$

We can use forward difference to change the time derivative

$$\left.\frac{\partial T(x,t)}{\partial t}\right|_{t=t_n} \rightarrow \frac{T(x_i, t_n+\tau) - T(x_i, t_n)}{\tau} = \frac{T_{i,n+1} - T_{i,n}}{\tau}$$

Explicit method

$$\frac{T_{i,n+1} - T_{i,n}}{\tau} = D\frac{T_{i+1,n} - 2T_{i,n} + T_{i-1,n}}{h^2}$$

The advantage is that $T_{i,n+1}$ can be calculated from the values of $T_{i+1,n}$, $T_{i,n}$, and $T_{i-1,n}$. From the initial condition we can find all the values of $T_{i,n}$. The condition for stability

$$\frac{2D\tau}{h^2} < 1.$$

Implicit method

$$\frac{T_{i,n+1} - T_{i,n}}{\tau} = D\frac{T_{i+1,n+1} - 2T_{i,n+1} + T_{i-1,n+1}}{h^2}$$

The advantage is that the finite difference is unconditionally stable. Disadvantage is that the equations must be solved as a set of linear algebraic equations.

Crank-Nicholson method:

$$\begin{aligned}\frac{T_{i,n+1} - T_{i,n}}{\tau} = & \frac{D}{2}\frac{T_{i+1,n} - 2T_{i,n} + T_{i-1,n}}{h^2} \\ & + \frac{D}{2}\frac{T_{i+1,n+1} - 2T_{i,n+1} + T_{i-1,n+1}}{h^2}\end{aligned}$$

Example: the time-dependent Schrodinger equation

$$i\frac{\partial}{\partial t}\Psi(x,t) = H(x)\Psi(x,t)$$

where $H(x) = -\partial^2/\partial x^2 + V(x)$.

$$\Psi(x,t) = e^{-i(t-t_0)H}\Psi(x,t_0)$$

The propagator

$$\begin{aligned} e^{-i(t-t_0)H} &= 1 + \{-i(t-t_0)H\} \\ &\quad + \frac{1}{2!}\{-i(t-t_0)H\}^2 \\ &\quad + \frac{1}{3!}\{-i(t-t_0)H\}^3 + \cdots \end{aligned}$$

For an increment

$$\Psi(x, t + \Delta t) = e^{-i(\Delta t)H}\Psi(x, t)$$

On expressing all the quantities in terms of their values on the mesh points, we have

$$\begin{aligned}\Psi(x_j, t_{k+1}) &= e^{-i(\Delta t)H}\Psi(x_j, t_k) \\ &= [1 - i\Delta t H + \cdots]\Psi(x_j, t_k)\end{aligned}$$

$$\begin{aligned}\Psi(x_j, t_{k+1}) &\approx \Psi(x_j, t_k) - i\Delta t H\Psi(x_j, t_k) \\ &= \Psi(x_j, t_k) - i\Delta t(-\frac{\partial^2}{\partial x^2} + V(x))\Psi(x_j, t_k)\end{aligned}$$

$$\begin{aligned}\Psi(x_j, t_{k+1}) &\approx \Psi(x_j, t_k) - i\Delta t V(x)\Psi(x_j, t_k) \\ &\quad + i\frac{\Delta t}{(\Delta x)^2}(\Psi(x_{j+1}, t_k) - 2\Psi(x_j, t_k) + \Psi(x_{j-1}, t_k))\end{aligned}$$

This corresponds to the explicit method.

Alternatively, we can also start with the equation

$$\Psi(x_j, t_k) = e^{+i(\Delta t)H}\Psi(x_j, t_{k+1})$$

This corresponds to the implicit method.

The disadvantage is that the wave function is not preserved.

A different approach:

$$e^{-i\Delta tH} = \frac{1 - \frac{1}{2}i\Delta tH}{1 + \frac{1}{2}i\Delta tH}$$

$$e^{+i(\Delta t)H/2}\Psi(x_j, t_{k+1}) = e^{-i(\Delta t)H/2}\Psi(x_j, t_k)$$

$$[1 + i(\Delta t)H/2]\Psi(x_j, t_{k+1}) = [1 - i(\Delta t)H/2]\Psi(x_j, t_k)$$

This corresponds to the Crank-Nicholson method!

The finite difference equations are

$$\begin{aligned} RHS &= \Psi(x_j, t_k) - i\frac{\Delta t}{2}V(x)\Psi(x_j, t_k) \\ &\quad + i\frac{\Delta t/2}{(\Delta x)^2}(\Psi(x_{j+1}, t_k) - 2\Psi(x_j, t_k) + \Psi(x_{j-1}, t_k)) \\ LHS &= \Psi(x_j, t_{k+1}) + i\frac{\Delta t}{2}V(x)\Psi(x_j, t_{k+1}) \\ &\quad - i\frac{\Delta t/2}{(\Delta x)^2}(\Psi(x_{j+1}, t_{k+1}) - 2\Psi(x_j, t_{k+1}) + \Psi(x_{j-1}, t_{k+1})) \end{aligned}$$

Solve the equations?

Scattering of a wave packet

Potential:

Initial form:

25.2 Hyperbolic Equations

Hyperbolic equations take the form

$$\frac{\partial^2 f}{\partial q_1^2} - \frac{1}{\nu^2}\frac{\partial^2 f}{\partial q_2^2} = 0.$$

The best example of the application of this is as the wave equation. In particular, consider an ideal string, i.e. one that is perfectly elastic, offers

no resistance to bending, and is stretched between two immovable supports. Let the mass density of the string be uniform, and the tension in the string be much greater than the weight of the string. This will allow the effects of gravity to be ignored.

Freshman physics shows that, in this case, the wave equation can be written as

$$\frac{\partial^2 u}{\partial t^2} - \frac{T}{\mu}\frac{\partial^2 u}{\partial x^2} = 0. \tag{9}$$

where T is the tension in the string and μ is the mass density of the string. If we assume that the length of the string is L, then at the boundaries we have

$$u(0,t) = u(L,t) = 0$$

As a first attempt at converting this into a finite difference equation, use the second order central difference equation for the derivatives. This yields

$$\frac{\partial^2 u}{\partial x^2} \to \frac{u_{i+1,n} - 2u_{i,n} + u_{i-1,n}}{h^2}$$

and

$$\frac{\partial^2 u}{\partial t^2} \to \frac{u_{i,n+1} - 2u_{i,n} + u_{i,n-1}}{\tau^2}$$

Thus, the wave equation transforms into

$$\frac{u_{i,n+1} - 2u_{i,n} + u_{i,n-1}}{\tau^2} = \frac{T}{\mu}\frac{u_{i+1,n} - 2u_{i,n} + u_{i-1,n}}{h^2} \tag{10}$$

$$u_{i,n+1} - 2u_{i,n} + u_{i,n-1} = \frac{T\tau^2}{\mu h^2}\left(u_{i+1,n} - 2u_{i,n} + u_{i-1,n}\right)$$

Notice that we again have to use a two dimensional grid to solve this equation, only now we have to allow for the solution to move both forwards

and backwards in time. We may take $\frac{T\tau^2}{\mu h^2} = 1$ or $h = \frac{T}{\mu}\tau$ in the calculation.

In order to solve the hyperbolic equation, two sets of initial conditions must be specified. While they can take on many forms, for a traveling wave, the initial position and velocity of the wave pulse are the most frequently stated conditions.

25.2.1 Example:

Start with equation (9) and assume that the solution can be written as

$$u(x,t) = \chi(x)\tau(t)$$

Using separation of variables, equation (9) becomes

$$\begin{aligned}
\frac{\partial^2 u}{\partial t^2} &= \frac{T}{\mu}\frac{\partial^2 u}{\partial x^2} \\
\chi(x)\frac{\partial^2 \tau(t)}{\partial t^2} &= \frac{T}{\mu}\tau(t)\frac{\partial^2 \chi(x)}{\partial x^2} \\
\frac{1}{\tau(t)}\frac{\partial^2 \tau(t)}{\partial t^2} &= \frac{T}{\mu\chi(x)}\frac{\partial^2 \chi(x)}{\partial x^2} = -\omega^2
\end{aligned}$$

where ω is a constant. The last line consists of two ordinary differential equations,

$$\frac{\partial^2 \tau(t)}{\partial t^2} + \omega^2 \tau(t) = 0$$

and

$$\frac{T}{\mu}\frac{\partial^2 \chi(x)}{\partial x^2} + \omega^2 \chi(x) = 0$$

We can solve each one in turn.

It is easy to see that

$$\chi_n(x) = A_n \sin(k_n x)$$

where the sine function was picked to satisfy the boundary conditions $\chi(0) = \chi(l) = 0$, and

$$k_n = 2\pi(n+1)/l = \omega_n(\mu/T)^{1/2}$$

Similarly, the solution of $\tau(t)$ can be written as

$$\tau(t) = C_n \sin \omega_n t + D_n \cos \omega_n t.$$

The requirement that the string be released from rest forms the initial condition

$$0 = \left.\frac{\partial \tau}{\partial t}\right|_{t=0} = \omega_n C_n = 0$$

which means that $C_n = 0$. Thus, the general solution can be written as

$$u(x,t) = \sum_{n=0}^{\infty} B_n \sin k_n x \cos \omega_n t \tag{11}$$

In order to eliminate the last constant, B_n, we need to describe the form of the plucked string mathematically. We could assume that that $u(x,t) = u_0\delta(x)$, but this is not a very physical description. The next complication is to use a triangular pulse. Assuming that the pulse is symmetric about the peak and has a base twice the overall height, then this initial condition becomes

$$u(x, t = 0) = \begin{cases} x & 0 < x < 0.25m \\ -x + 0.5m & 0,25m < x < 0.5m \\ 0 & 0.5m < x < 5.00m \end{cases} \tag{12}$$

To find B_n, we multiply equation (11) on both sides by $\sin k_m x$ and integrate. The right hand side reduces to B_n due to the orthogonality of the sine functions, while the left hand side becomes

$$\int_0^l u(x,0)\sin k_m x dx = \frac{l^2}{2\pi^2(m+1)^2}\sin\frac{2\pi(m+1)x_0}{l}\left(1-\cos\frac{2\pi(m+1)x_0}{l}\right)$$

where $x_0 = 0.25m$ and $l = 5.00m$. Thus, the final analytical solution is

$$u(x,t) = \sum_{n=0}^{+\infty}\frac{2}{k_n^2}\sin(k_n x_0)\left[1-\cos(k_n x_0)\right]\sin(k_n x)\cos\left[(T/\mu)^{1/2}k_n t\right]$$

To solve this problem numerically, we must first specify a grid on which the solution will be found. The size of the position step can be estimated from equation (12). Since the initial pulse is assumed to be 0.5m in length, a step size of 1.00cm will give a reasonable approximation to the triangular

pulse. Since the overall length of the string is 5.00m, this translates to a total of 500 points in position space.

The temporal step can be determined be bound by the stability criteria associated with our numerical solution. In the case of a hyperbolic PDE, this criteria is that

$$(T/\mu)^{1/2} \leq \Delta x/\Delta t$$

where Δt is the time step and Δx is the spatial step. For the initial conditions associated with this problem,

$$\Delta t \leq \Delta x(T/\mu)^{1/2} \leq 4.52 \times 10^{-4} s$$

so a time step of $1.0 \times 10^{-4} s$ will satisfy this condition.

Once the grid has been specified, the initial conditions are encoded. The initial position can be determined directly from equation (12). The initial

velocity cannot be coded directly since it involves differentials. Translating this into a difference equation, the initial condition becomes

$$0 = \frac{\partial u(x, t = 0)}{\partial t} \cong \frac{u(x, \Delta t) - u(x, -\Delta t)}{2\Delta t}$$

$$u(x, \Delta t) = u(x, -\Delta t)$$

Substituting this into (10) yields

$$u_{i,1} = 2u_{i,0} + (\tau/h)^2(T/\mu)(u_{i+1,0} + u_{i-1,0} - 2u_{i,0})/2$$

for the first time step. Subsequent steps are determined from equation (10). A program to determine the evolution of the wave is shown in hyperbolic.c.

25.3 Elliptical Equations

Elliptical equations differ from the other two types of PDEs in that elliptical equations typically involve only spatial coordinates. Because of this, the initial conditions become boundary conditions, i.e., the value of the function along the boundaries is completely specified.

The most common example of elliptical PDEs comes from electricity and magnetism. Recall that, in differential form, Maxwell's equations are

$$\begin{aligned}
\nabla \cdot \mathbf{E} &= 4\pi\rho \\
\nabla \cdot \mathbf{B} &= 0 \\
\nabla \times \mathbf{E} &= -c\frac{\partial \mathbf{B}}{\partial t} \\
\nabla \times \mathbf{B} &= \frac{4\pi}{c} j + \frac{1}{c}\frac{\partial \mathbf{E}}{\partial t}
\end{aligned}$$

If we substitute the definition , where $E = -\nabla\varphi$ is the electric potential, into the first of these equations, we get Poisson's equation,

$$\nabla^2\varphi = -4\pi\rho \tag{13}$$

Depending upon the charge distribution, there are many ways to solve this analytically. In particular, when the charge distribution is zero, equation (13) reduces to Laplace's equation, which can then be solved via separation of variables.

In order to solve (13) numerically, we take advantage of the fact that the values on the boundaries are already specified. Since we are only concerned with the interior, we can immediately see that there are grid points on either side of any point being evaluated. Thus, a central difference approximation can be used and the derivative in the xith direction is approximated as

$$\frac{\partial^2\varphi}{\partial x_i^2} \approx \frac{\varphi(\cdots x_i + \Delta x_i \cdots) - 2\varphi(\cdots x_i \cdots) + \varphi(\cdots x_i - \Delta x_i \cdots)}{(\Delta x_i)^2}$$

Substituting this back into equation (13) converts Poisson's equation into a difference equation on a grid. This can then be solved to find the value of the potential at a particular grid point. For example, in two dimensions, the solution at (x_i, y_j) is:

$$\varphi(x_i, y_i) = \frac{1}{4}\left[\varphi(x_{i+1}, y_i) + \varphi(x_{i-1}, y_i) + \varphi(x_i, y_{i+1}) + \varphi(x_i, y_{i-1})\right]$$

It should be noted that this algorithm is not as sophisticated as we frequently want. This shows up through the large number of iterations needed to obtain convergence. If the amount of computer time needed to solve the problem becomes excessive, a more accurate and robust algorithm should be substituted.

26 Finite Element Solution to Partial Differential Equation

In boundary value problem, finite element methods (FEM) are often used instead of the finite difference methods.

26.1 Background

Example:

$$\frac{d\phi}{dt} + \phi = 0$$

with the boundary condition

$$\phi(t=0)=1$$

The analytical solution for this case is

$$\phi = e^{-t} = 1 - t + \frac{1}{2!}t^2 - \frac{1}{3!}t^3 + \cdots$$

26.1.1 Power series solution

Let us ignore the analytical solution for the momentum and instead, try to solve equation by using a trial solution consisting of a power series with n terms.

$$\tilde{\phi} = a_0 + a_1 t + a_2 t^2 + \cdots + a_n t^n.$$

To satisfy the initial value condition, it is necessary that $a_0 = 1$.For the convenience of discussion, let us take $n = 2$.

$$\tilde{\phi}_2(t) = 1 + a_1 t + a_2 t^2.$$

Obviously the result has a different form from the analytical solution of the problem. However, in practice, our interest is only in a restricted domain and we shall see soon it is possible to find a set of values for a_1 and a_2 such that $\tilde{\phi}_2(t)$ represent a very good approximation of the function e^{-t} with $t = [0, 1]$.For this purpose we introduce the residual,

$$R(t, a_1, a_2) = \frac{d\tilde{\phi}_2}{dt} + \tilde{\phi}_2 = 1 + (1 + t)a_1 + (2t + t^2)a_2.$$

More generally, if there are n parameters instead of 2, the residual may be defined as

$$R(t, \mathbf{a}) = \frac{d\tilde{\phi}_n}{dt} + \tilde{\phi}_n.$$

Since $\tilde{\phi}_n$ is not the solution to the equation, we do not expect the residue becomes zero everywhere in the range $t = [0, 1]$.

26.1.2 Determination of the parameters

To find the coefficients we can adjust them such that $\tilde{\phi}_2$ is as close to e^{-t} as possible in the range.

Method I: Collocation

In the collocation method, we require the residual to vanish at n points $t_1, t_2, \cdots, t_n$, within the domain of interest,

$$R(t_i, a) = 0$$

for $i = 1, 2, \cdots, n$. For $n = 2$, we can take two parameters t_1 and t_2 with $[0, 1]$, for example $t_1 = 1/3$, and $t_2 = 2/3$. This gives two equations, and their roots are

$$\begin{aligned} a_1 &= -\frac{27}{29} \\ a_2 &= +\frac{9}{29} \end{aligned}$$

And the solution is

$$\phi = 1 - \frac{27}{29}t + \frac{9}{29}t^2$$

Method II: Subdomain

Instead of insisting that the residual vanish at two points in the domain, we can also obtain the necessary equation to solve for a_1 and a_2 by setting

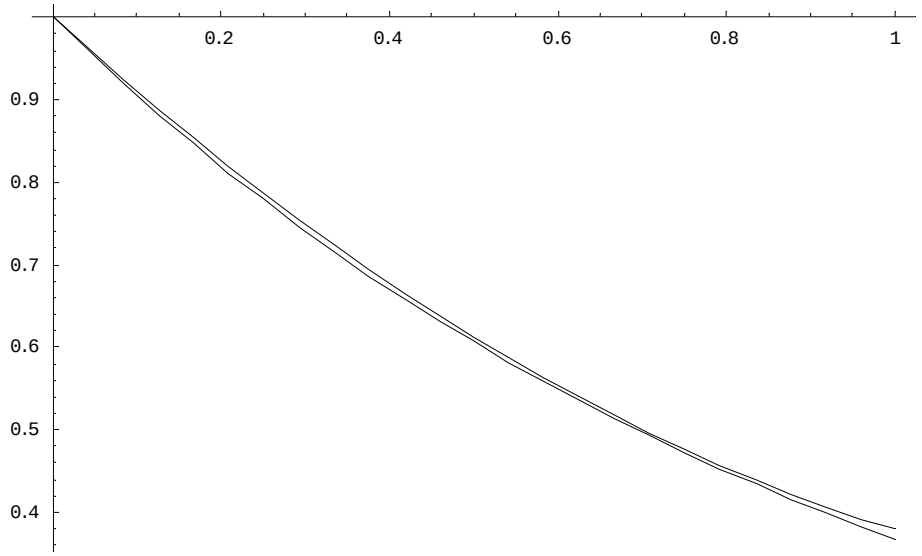

Figure 4:

the average value of R(t,a) in each of two different parts of the domain, Δt_1 and Δt_2 to vanish. That is

$$\frac{1}{\Delta t_i}\int_{\Delta t_i} R(t,a)dt = 0.$$

For $n = 2$, we take $\Delta t_1 = [0, 1/2]$ and $\Delta t_2 = [1/2, 1]$. The two average residuals are

$$\begin{aligned}
\frac{1}{\Delta t_1}\int_0^{1/2} R(t,a)dt &= 2\left\{\frac{1}{2} + \frac{5}{8}a_1 + \frac{7}{24}a_2\right\} \\
\frac{1}{\Delta t_2}\int_{1/2}^{1} R(t,a)dt &= 2\left\{\frac{1}{2} + \frac{7}{8}a_1 + \frac{25}{24}a_2\right\}
\end{aligned}$$

By requiring both to vanish, we obtain the result,

$$\begin{aligned}
a_1 &= -\frac{18}{19} \\
a_2 &= +\frac{6}{19}
\end{aligned}$$

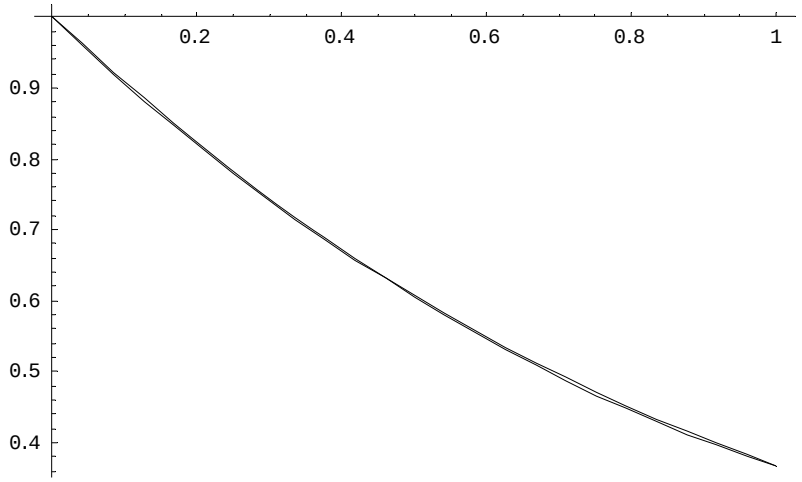

Figure 5:

Method III: Least-Squares

The coefficients a can be determined by making use of least-squares techniques.

$$\frac{\partial}{\partial a_i}\int_{\Delta t_i} R^2(t,a)dt = 2\int_{\Delta t_i} R(t,a)\frac{\partial}{\partial a_i}R(t,a)dt = 0$$

Method IV: Galerkin

In general,

$$\tilde{\phi}_n = \psi_0(t) + \sum_{i=1}^{n} a_n\psi_n(t)$$

$$\int_{\Delta} R(t,a)\psi_i(t)dt = 0$$

For $n = 2$, $\psi_0(t) = 1, \psi_1(t) = t$, and $\psi_2(t) = t^2$.

$$\begin{aligned} a_1 &= -\frac{32}{35} \\ a_2 &= +\frac{2}{7} \end{aligned}$$

26.2 Shape function and finite element approach

This idea can be applied to solve partial differential equation.

One-dimensional example

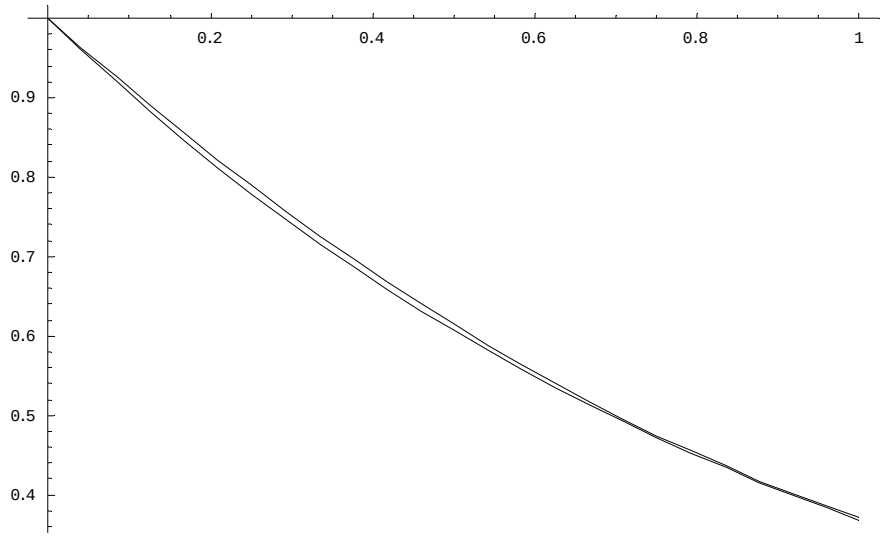

Figure 6:

$$
\begin{aligned}
f(x)_{[x_i,x_{i+1}]} &= f_i\lambda_i(x) + f_{i+1}\omega_i(x) \\
&\quad + f_i''\frac{(x_{i+1}-x_i)^2}{6}\{\lambda_i^3(x) - \lambda_i(x)\} \\
&\quad + f_{i+1}''\frac{(x_{i+1}-x_i)^2}{6}\{\omega_i^3(x) - \omega_i(x)\}
\end{aligned}
$$

Set $h = x_{i+1} - x_i$. We have

$$
\begin{aligned}
f(x)_{[x_i,x_{i+1}]} &= f_i\lambda_i(x) + f_{i+1}\omega_i(x) \\
&\quad + \frac{h^2}{6}f_i''\{\lambda_i^3(x) - \lambda_i(x)\} \\
&\quad + \frac{h^2}{6}f_{i+1}''\{\omega_i^3(x) - \omega_i(x)\}
\end{aligned}
$$

where

$$\begin{aligned} \lambda_i &= \frac{x_{i++1} - x}{h} \\ \omega_i &= 1 - \lambda_i = \frac{x - x_i}{h} \end{aligned}$$

Two-dimensional Poisson equation

27 Example

27.1 Fixed-Step Runge-Kutta 4 method

An example fixed-step RK4 routine

Listed below is an example fixed-step, fourth-order Runge-Kutta (RK4) integration routine which utilizes the Blitz++ library . see `rk4_fixed.cpp`