Subsections

Partial Differential Equations

An equation involving partial derivatives of an unknown function of two or more independent variables is called a partial differential equation, PDE. The order of a PDE is that of the highest-order partial derivative appearing in the equation.

A general linear second-order differential equation is

$$A\frac{\partial^2 u}{\partial x^2} + B\frac{\partial^2 u}{\partial x \partial y} + C\frac{\partial^2 u}{\partial y^2} + D = 0 \tag{8.1}$$

Depending on the values of the coefficients of the second-derivative terms eq. (8.1) can be classified int one of three categories.

- $B^2 - 4AC < 0$: Elliptic

  $$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$$

  Laplace equation(steady state with two spatial dimensions)
- $B^2 - 4AC = 0$: Parabolic

  $$\frac{\partial T}{\partial t} = k\frac{\partial^2 T}{\partial x^2}$$

  Heat conduction equation(time variable with one spatial dimension)
- $B^2 - 4AC > 0$: Hyperbolic

$$\frac{\partial^2 y}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 y}{\partial t^2}$$

Wave equation(time variable with one spatial dimension)

Finite Difference: Elliptic Equations

Elliptic equations in engineering are typically used to characterize steady-state, boundary-value problems.

The Laplace Equations

- The Laplace equation

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$$

- The Poisson equation

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = f(x, y)$$

Solution Techniques

- The Laplacian Difference Equation : use central difference based on the grid scheme

$$\frac{\partial^2 T}{\partial x^2} = \frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{\Delta x^2}$$

and

$$\frac{\partial^2 T}{\partial y^2} = \frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{\Delta y^2}$$

Substituting these equations into the Laplace equation gives

$$\frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{\Delta x^2} + \frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{\Delta y^2} = 0$$

For the square grid, $\Delta x = \Delta y$, and by collecting terms

$$T_{i+1,j} + T_{i-1,j} + T_{i,j+1} + T_{i,j-1} - 4T_{i,j} = 0$$

This relationship, which holds for all interior point on the plate, is referred to as the Laplacian difference equation.

This approach gives a large size of linear algebraic equations.

- The Liebmann Method : For larger-sized grids, a significant number of the terms will be zero. When applied to such sparse system, full-matrix elimination methods waste great amounts of computer memory storing these zeros. For this reason, approximate methods provide a viable approach for obtaining solutions for elliptical equation. The most commonly employed approach is Guass-Seidel, which when applied to PDEs is also referred to as Liebmann's method.

Boundary Conditions

- Derivative boundary conditions : including the derivative boundary conditions into the problem.
- Irregular boundaries : use contstants to depict the curvature.

The Control Volume Approach

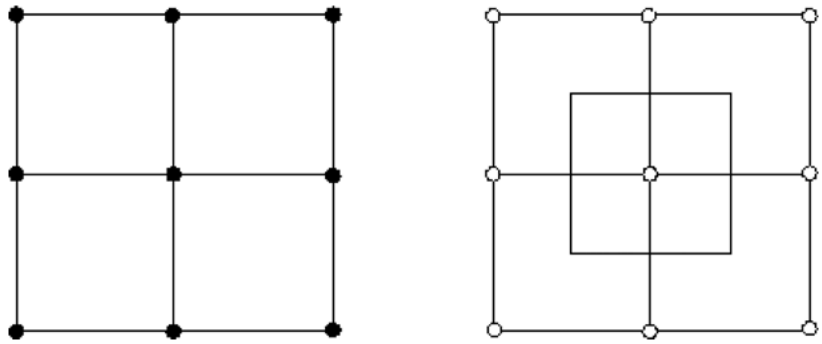

Figure 8.1: Two different perspectives for developing approximate solutions of PDEs.

Two different developing approximate solutions of PDEs

- Finite-difference : divides the continuum into nodes and convert the equations to an algebraic form.
- Control volume : approximates the PDEs with a volume surrounding the point.

Finite Difference: Parabolic Equations

The Heat Conduction Equation

Fourier's law of heat conduction

$$\frac{\partial T}{\partial t} = k\frac{\partial^2 T}{\partial x^2} \tag{8.11}$$

which is the heat-conduction equation.

Problems of parabolic equation

- consider changes in time as well as in space
- temporally open-ended
- consider the stability problem

Explicit Methods

With finite divided differences

$$\frac{\partial T}{\partial t} = \frac{T_i^{l+1} - T_i^l}{\Delta t} \tag{8.12}$$

and

$$\frac{\partial^2 T}{\partial x^2} = \frac{T^l_{i+1} - 2T^l_i + T^l_{i-1}}{(\Delta x)^2} \tag{8.13}$$

which give

$$T^{l+1}_i = T^l_i + \lambda(T^l_{i+1} - 2T^l_i + T^l_{i-1}) \tag{8.14}$$

where $\lambda = k\Delta t/(\Delta x)^2$.

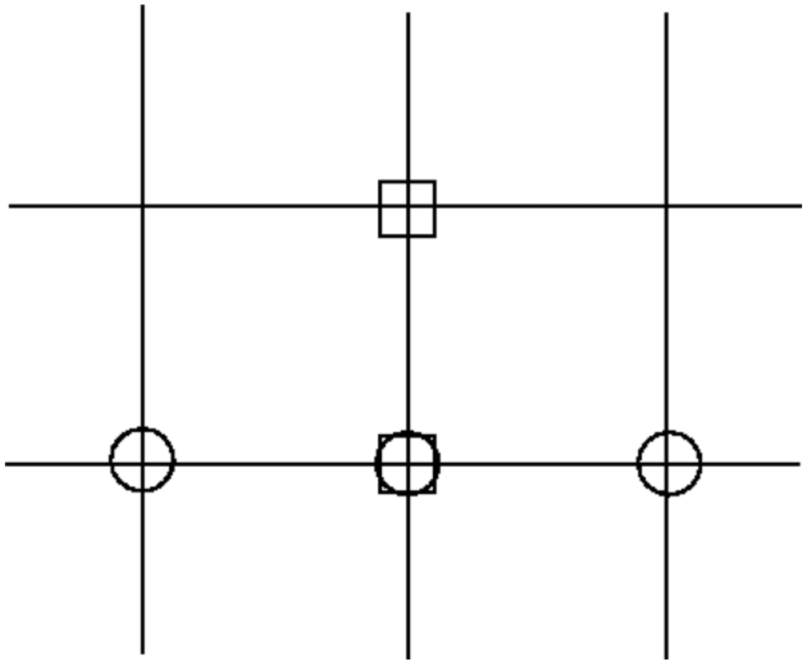

Figure 8.2: A computational modelcule for the explicit form.

Convergence and Stability

- Convergence : as Δx and Δt approach zero, the results of the finite-difference technique approach the true solution.
- Stability : errors at any stage of the computation are not amplified but are attenuated as the computation progresses.

Convergence: consider the following unsteady-state heat-flow equation in one dimension.

$$\frac{\partial U}{\partial t} = \frac{k}{c\rho}\frac{\partial^2 U}{\partial x^2} \tag{8.15}$$

Let the symbol U to represent the exact solution and u to represent the numerical solution. Let $e^j_i = U^j_i - u^j_i$, at the point $x = x_i$, $t = t_j$. By the explicit method,

$$u^{j+1}_i = r(u^j_{i+1} + u^j_{i-1}) + (1 - 2r)u^j_i \tag{8.16}$$

where $r = k\Delta t/c\rho(\Delta x)^2$. Substituting $u = U - e$ into the above equation,

$$e_i^{j+1} = r(e_{i+1}^j + e_{i-1}^j) + (1-2r)e_i^j - r(U_{i+1}^j + U_{i-1}^j) - (1-2r)U_i^j + U_i^{j+1} \tag{8.17}$$

By using Taylor series expansion,

$$U_{i+1}^j = U_i^j + \left(\frac{\partial U}{\partial x}\right)_{i,j} \Delta x + \frac{(\Delta x)^2}{2}\frac{\partial^2 U(\xi_1, t_j)}{\partial x^2}, \quad x_i < \xi_1 < x_{i+1} \tag{8.18}$$

$$U_{i-1}^j = U_i^j - \left(\frac{\partial U}{\partial x}\right)_{i,j} \Delta x + \frac{(\Delta x)^2}{2}\frac{\partial^2 U(\xi_2, t_j)}{\partial x^2}, \quad x_{i-1} < \xi_2 < x_i \tag{8.19}$$

$$U_i^{j+1} = U_i^j + \Delta t\frac{\partial U(x_i, \eta)}{\partial t}, \quad t_j < \eta < t_{j+1} \tag{8.20}$$

Substituting these into (8.17) and simplifying

$$e_i^{j+1} = r(e_{i+1}^j + e_{i-1}^j) + (1-2r)e_i^j + \Delta\left[\frac{\partial U(x_i, \eta)}{\partial t} - \frac{k}{c\rho}\frac{\partial^2 U(\xi, t_j)}{\partial x^2}\right],$$

$$t_j \le \eta \le t_{j+1}, x_{i-1} \le \xi \le x_{i+1} \tag{8.21}$$

Let E^j be the magnitude of the maximum error in the row of calculation for $t = t_j$, and let $M > 0$ be an upper bound for the magnitude of the expression. If $r \le \frac{1}{2}$, all the coefficients in the above equation are positive (or zero) and we may write the inequality

$$|e_i^{j+1}| \le 2rE^j + (1-2r)E^j + M\Delta t = E^j + M\Delta t \tag{8.22}$$

This is true for all the e_i^{j+1} at $t = t_{j+1}$, so

$$E^{j+1} \le E^j + M\Delta t \tag{8.23}$$

This is true at each time step,

$$E^{j+1} \le E^j + M\Delta t \le E^{j-1} + 2M\Delta t \le \cdots \le E^0 + Mt_{j+1} = Mt_{j+1} \tag{8.24}$$

because E^0, the errors at $t = 0$, are zero, as U is given by the initial conditions.

As $\Delta x \to 0$, $\Delta t \to 0$ if $k\Delta t/c\rho(\Delta x)^2 \le \frac{1}{2}$, and $M \to 0$, because, as both Δx and Δt get smaller

$$\left[\frac{\partial U(x_i, \eta)}{\partial t} - \frac{k}{c\rho}\frac{\partial^2 U(\xi, t_j)}{\partial x^2}\right] \to \left(\frac{\partial U}{\partial t} - \frac{k}{c\rho}\frac{\partial^2 U}{\partial x^2}\right)_{i,j} = 0 \tag{8.25}$$

Consequently, the explicit method is convergent for $r \le \frac{1}{2}$, because the errors approach zero as Δt and Δx are made smaller.

A Simple Implicit Method

The problems of explicit finite-difference formulation

- stability
- exclusion of information that has a bearing on the solution

See figure 30.6 at p838.

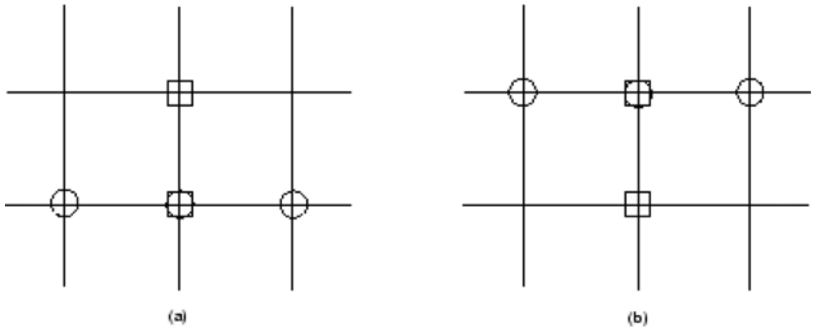

Figure 8.3: Computational molecules demonstrating the funcdamental differences.

In implicit methods, the spatial derivative is approximated at an advanced time level $l+1$.

$$\frac{\partial^2 T}{\partial x^2} \simeq \frac{T_{i+1}^{l+1} - 2T_i^{l+1} + T_{i-1}^{l+1}}{(\Delta x)^2} \tag{8.26}$$

When this relationship is substituted into the original PDE, the resulting difference equation contains several unknowns. Thus, it cannot be solved explicitly by simple algebraic rearrangement. Instead, the entire system of equations must be solved simultaneously. This is possible because, along with the boundary conditions, the implicit formulations result in a set of linear algebraic equations with the same number of unknowns.

The Crank-Nicholson Method

The Crank-Nicolson method provides an alternative implicit scheme that is second-order accurate in both space and time. To do this, develops difference approximations at the midpoint of the time increment.

$$\frac{\partial^2 T}{\partial x^2} = \frac{1}{2}\left[\frac{T_{i+1}^{l} - 2T_i^{l} + T_{i-1}^{l}}{(\Delta x)^2} + \frac{T_{i+1}^{l+1} - 2T_i^{l+1} + T_{i-1}^{l+1}}{(\Delta x)^2}\right] \tag{8.27}$$

Substituting and collecting terms gives

$$-\lambda T_{i-1}^{l+1} + 2(1+\lambda)T_i^{l+1} - \lambda T_{i+1}^{l+1} = \lambda T_{i-1}^{l} + 2(1-\lambda)T_i^{l} + \lambda T_{i+1}^{l} \tag{8.28}$$

Finite Element Method

- Finite-difference method
  - divide the solution domain into a grid of discrete points or nodes
  - write the PDE for each node and replace the derivative with finite divided differences
  - it is hard to apply for system with irregular geometry, unusual boundary conditions, or heterogeuous composition

- Finite-element method
  - divide the solution domain into simply shaped regions or ``elements''.
  - develop an approximate solution for the PDE for each of these elements.
  - link together the individiual solutions

Calculus of variation

The calculus of variations involves problems in which the quantity to be minimized appears as an integral. As the simplest case,

$$J = \int_{x_1}^{x_2} f(y, y_x, x) dx \tag{8.29}$$

Let J is the quantity that takes on an extreme value. Under the integral sign, f is a known function of the indicated variables $y(x)$, $y_x(x)$, and x but the dependence of y on x is not fixed: that is, $y(x)$ is unknown. Thus, the calculus of variation seeks to optimize a special class of functions called functionals. A functional can be thought of as a ``function of function.''

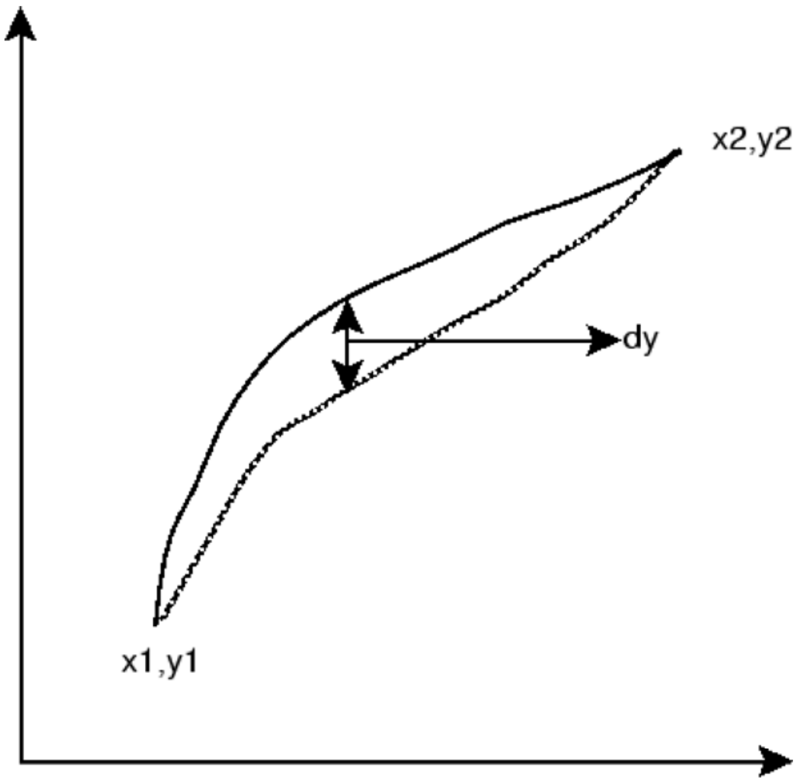

Figure 8.4: A varied path.

In figure 8.3.1 two possible paths are shown. The difference between these two for a given x is called the variation of y, δy, and introduce $\eta(x)$ to define the arbitrary deformation of the path and a scale factor α to give the magnitude of the variation. The function $\eta(x)$ is arbitrary except for two restrictions. First

$$\eta(x_1) = \eta(x_2) = 0 \tag{8.30}$$

which means that all varied paths must pass through the fixed end points. Second,

$$\begin{aligned}\eta(x) &= 1, \quad x = x_0 \\ &= 0, \quad x \neq x_0\end{aligned} \tag{8.31}$$

With the path described with α and $\eta(x)$,

$$y(x,\alpha) = y(x,0) + \alpha\eta(x) \tag{8.32}$$

and

$$\delta y = y(x,\alpha) - y(x,0) = \alpha\eta(x) \tag{8.33}$$

Let $y(x, \alpha = 0)$ be the unknown path that will minimize J. Then $y(x,\alpha)$ describes a neighboring path. Then J is now a function of new parameter α:

$$J(\alpha) = \int_{x_1}^{x_2} f[y(x,\alpha), y_x(x,\alpha), x]dx \tag{8.34}$$

and the extreme value is

$$\left[\frac{\partial J(\alpha)}{\partial x}\right]_{\alpha=0} = 0 \tag{8.35}$$

The partial derivative of J is

$$\frac{\partial J(\alpha)}{\partial \alpha} = \int_{x_1}^{x_2} \left[\frac{\partial f}{\partial y}\frac{\partial y}{\partial \alpha} + \frac{\partial f}{\partial y_x}\frac{\partial y_x}{\partial \alpha}\right] dx \tag{8.36}$$

From eq. (8.32)

$$\frac{\partial y(x,\alpha)}{\partial \alpha} = \eta(x) \tag{8.37}$$

$$\frac{\partial y_x(x,\alpha)}{\partial \alpha} = \frac{d\eta(x)}{dx} \tag{8.38}$$

Equation (8.36) becomes

$$\frac{\partial J(\alpha)}{\partial \alpha} = \int_{x_1}^{x_2} \left(\frac{\partial f}{\partial y}\eta(x) + \frac{\partial f}{\partial y_x}\frac{d\eta(x)}{dx}\right) dx \tag{8.39}$$

Integrating the second term by parts

$$\int_{x_1}^{x_2} \frac{d\eta(x)}{dx} \frac{\partial f}{\partial y_x} dx = \eta(x) \left. \frac{\partial f}{\partial y_x} \right|_{x_1}^{x_2} - \int_{x_1}^{x_2} \eta(x) \frac{d}{dx} \frac{\partial f}{\partial y_x} dx \tag{8.40}$$

The integrated part is zero and

$$\int_{x_1}^{x_2} \left[\frac{\partial f}{\partial y} - \frac{d}{dx} \frac{\partial f}{\partial y_x} \right] \eta(x) dx = 0 \tag{8.41}$$

Multiply α

$$\alpha \left[\frac{\partial J}{\partial \alpha} \right]_{\alpha=0} = \int_{x_1}^{x_2} \left[\frac{\partial f}{\partial y} - \frac{d}{dx} \frac{\partial f}{\partial y_x} \right] \delta y dx = \delta J = 0 \tag{8.42}$$

The condition for stationary is

$$\frac{\partial f}{\partial y} - \frac{d}{dx} \frac{\partial f}{\partial y_x} = 0 \tag{8.43}$$

which is known as the Euler(or Euler-Lagrange) equation.

Example: The shortest distance between two points

We have to determine the path that minimize the distance between two points which are given as (x_1, y_1) and (x_2, y_2).

$$\int_{x_1}^{x_2} \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2} = \int_{x_1}^{x_2} \sqrt{(dx)^2 + (dy)^2} = \int_{x_1}^{x_2} \sqrt{1 + \left(\frac{dy}{dx} \right)^2} dx \tag{8.44}$$

Equation (8.44) is a funtional that is a function of path $y(x)$ and our problem is to find $y = y(x)$ which will make

$$J = \sqrt{1 + y'^2} dx \tag{8.45}$$

as small as possible. And $y(x)$ is called an extremal. Assuming a neighboring line

$$Y(x) = y(x) + \alpha \eta(x) \tag{8.46}$$

Select a $Y(x)$ make

$$J = \sqrt{1 + Y'^2} dx \tag{8.47}$$

a minimum. Now I is a function of the parameter α; when $\alpha = 0$, $Y = y$. Our problem then is to make $I(\alpha)$ take its minimum value when $\alpha = 0$.

$$\frac{dJ}{d\alpha} = 0 \quad \textbf{when} \quad \alpha = 0 \tag{8.48}$$

Differentiating gives

$$\frac{dJ}{d\alpha} = \int_{x_1}^{x_2} \frac{1}{2} \frac{1}{\sqrt{1 + Y'^2}} 2Y' \left(\frac{dY'}{d\alpha} \right) dx \tag{8.49}$$

Y' is

$$Y'(x) = y'(x) + \alpha\eta'(x) \tag{8.50}$$

Then

$$\frac{dY'}{d\alpha} = \eta'(x) \tag{8.51}$$

Put $\alpha = 0$

$$\left(\frac{dI}{d\alpha} \right)_{\alpha=0} = \int_{x_1}^{x_2} \frac{y'(x)\eta'(x)}{\sqrt{1 + y'^2}} dx = 0 \tag{8.52}$$

Integrate by part

$$\left(\frac{dJ}{d\alpha} \right)_{\alpha=0} = \left. \frac{y'}{\sqrt{1 + y'^2}} \eta(x) \right|_{x_1}^{x_2} - \int_{x_1}^{x_2} \eta(x) \frac{d}{dx} \left(\frac{y'}{\sqrt{1 = y'^2}} \right) dx \tag{8.53}$$

The first term is zero and because $\eta(x)$ is arbitarary function,

$$\frac{d}{dx} \left(\frac{y'}{\sqrt{1 + y'^2}} \right) = 0 \tag{8.54}$$

In the Euler equation case,

$$F = \sqrt{1 + y'^2} \tag{8.55}$$

Then

$$\frac{\partial F}{\partial y'} = \frac{y'}{\sqrt{1+y'^2}}, \quad \frac{\partial F}{\partial y} = 0 \tag{8.56}$$

and the Euler equation gives

$$\frac{d}{dx}\left(\frac{y'}{\sqrt{1+y'^2}}\right) = 0 \tag{8.57}$$

From this

$$\frac{y'}{\sqrt{1+y'^2}} = c \tag{8.58}$$

Solving for y'

$$y' = \sqrt{\frac{c^2}{1-c^2}} = b \tag{8.59}$$

and

$$y = bx + a \tag{8.60}$$

The Rayleigh-Ritz Method

It is based on an elegant branch of methematics, the calculus of variations. With this method we solve a boundary-value problem by approximating the solution with a finite linear combination of simple basis functions that are chosen to fulfill certain ceiteria, including meeting the boundary conditions.

For example, consider the second-order linear boundary-value problem over $[a, b]$:

$$y'' + Q(x)y = F(x), \quad y(a) = y_0, \quad y(b) = y_n \tag{8.61}$$

The functional that corresponds to the above equation is

$$J[u] = \int_a^b \left[\left(\frac{du}{dx}\right)^2 - Qu^2 + 2Fu\right] dx \tag{8.62}$$

We can transform eq. (8.62) to eq. (8.61) through the Euler-Lagrange conditions, so optimizing (8.62) give the solution to eq. (8.61).

The benifits of operating with the functional rather than the original equation:

- only the first-order instead of second-order derivative
- simplify the mathematics and permits to find solutions even when there are discontinuities that cause y not to have sufficiently high

derivatives.

If we know the solution to our differential equation, substituting it for the solution will make J a minimum. Let $u(x)$, which is the approximation to $y(x)$, be a sum:

$$u(x) = c_0\nu_0(x) + c_1\nu_1(x) + \cdots + c_n\nu_n(x) = \sum_{i=0}^{n} c_i\nu_i(x) \tag{8.63}$$

Two conditions on the ν's which is called as trial function.

- chosen such that $u(x)$ meets the boundary conditions
- ν's are linearly independent.

Now fina a way of getting values fro the c's to force $u(x)$ to be close to $y(x)$ using the functional.

$$J(c_0, c_1, \ldots, c_n) = \int_a^b \left[\left(\frac{d}{dx} \sum c_i\nu_i \right)^2 - Q(\sum c_i\nu_i)^2 + 2F \sum c_i\nu_i \right] dx \tag{8.64}$$

To minimize J, take its partial derivatives with respect to each unknown c and set to zero.

$$\frac{\partial J}{\partial c_i} = \int_a^b 2 \left(\frac{du}{dx}\right) \frac{\partial}{\partial c_i} \left(\frac{du}{dx}\right) dx - \int_a^b 2Qu \left(\frac{\partial u}{\partial c_i}\right) dx + 2\int_a^b F \frac{\partial u}{\partial c_i} dx \tag{8.65}$$

The Collocation and Galerkin Method

The collocation method is another way to approximate $y(x)$ which is called a ``residual method."

$$R(x) = y'' - Qy - F \tag{8.66}$$

Algorithm of the collocation method:

- approximate $y(x)$ with $u(x)$ equal to a sum of trial function, usually chosen as linearly independent polynomials.
- substitute $u(x)$ int $R(x)$ and attempt to make $R(x) = 0$ by a suitable choice of the coefficients in $u(x)$.

Like collocation, Galerkin method is a ``residual method" that use the $R(x)$, except that now we multiply $R(x)$ by weighting function, $W_i(x)$.

(8.67)

$$\int_a^b W_i(x)R(x)dx = 0, \quad i = 0, 1, \ldots, n$$

The advantages of collocation and Galerkin method

- amount of arithmetic is cetainly less
- much easier and never have to find the variational form.

Finite elements for ordinary-differential equations

The disadvantages of the previous methods

- Find a good trial function(it it not so easy)
- polynomial may interpolate poorly.

The remedy to the above problems is based on the observation that even low-degree polynomials can reflect the behavior of a function if based on values that are closely spaced.

1. subdivide $[a, b]$ into n subintervals, called elements, that join at $x_1, x_2, \ldots, x_{n-1}$ which are called the nodes of the interval.
2. apply the Galerkin method to each element separately to interpolate between the end nodal values, $u(x_{i-1})$ and $u(x_i)$, where these u's are approximations to the $y(x_i)$'s.
3. use a low-degree polynomial for $u(x)$.
4. combine the separate element equations
5. adjust for the boundary conditions and solve equations to get approximations to $y(x)$ at the nodes.

Engineering Applications: Partial Differential Equations

Taechul Lee
2001-11-29