He who can, does.
He who cannot teaches.

— GEORGE BERNARD SHAW

Chapter 7

Ordinary differential equations - Boundary value problems

In the present chapter we develop algorithms for solving systems of (linear or nonlinear) ordinary differential equations of the *boundary value type*. Such equations arise in describing *distributed, steady state* models in one spatial dimension. The differential equations are transformed into systems of (linear and nonlinear) algebraic equations through a discretization process. In doing so, we use the tools and concepts developed in Chapter 5. In particular we will develop (i) *finite difference* methods using the difference approximations given in Table 5.4, (ii) shooting methods based on *methods for initial value problems* seen in chapter 6 and (iii) the *method of weighted residuals* using notions of functional approximation developed in Chapter 5.

We will conclude this chapter with an illustration of a powerful software package called COLSYS that solves a system of multi-point boundary value problems using the collocation method, cubic splines and adaptive mesh refinement. It is available from NETLIB.

7.1 Model equations and boundary conditions

Consider the model for heat transfer through a fin developed in section §1.5.1. We will consider three specific variations on this model equation (1.22) and the associated boundary conditions. First let us scale the problem by introducing the following dimensionless temperature and distance variables,

$$\theta = \frac{T - T_\infty}{T_0 - T_\infty} \qquad \xi = \frac{x}{L}$$

Using these definitions, equation (1.22) can be rewritten as,

$$\frac{d}{d\xi}\left[kA\frac{d\theta}{d\xi}\right] - hPL^2\theta = 0 \tag{7.1}$$
$$\theta(\xi = 0) = 1 \qquad \theta(\xi = 1) = 0$$

where the objective is to find the continuous function $\theta(\xi)$ over the domain of interest, viz. $\xi \in [0,1]$ for a prescribed set of parameters $\{k, A, h, P, L\}$. All of these parameters can be constants, or some of them might be dependent on the position ξ (*e.g.*, $A(\xi)$) or on the unknown temperature itself (*e.g.*, $k(\theta)$). We examine each case next.

For constant area, A and thermal conductivity, k, equation (7.1) results in a second order *linear differential equation* with *constant* coefficients for which an analytical solution is possible. But we focus only on developing methodologies for obtaining a numerical solutions.

$$\frac{d^2\theta}{d\xi^2} - \frac{hPL^2}{kA}\theta = 0 \tag{7.2}$$
$$\theta(\xi = 0) = 1, \qquad \theta(\xi = 1) = 0$$

When the values of the dimensionless temperature, θ on the boundary are specified, the boundary condition is called the *Dirichlet* boundary conditions.

In a variation of the above model, if we let the area be a variable $A(\xi)$ (*i.e.*, tapered fin), but keep the thermal conductivity, k, constant, we obtain a *variable coefficient*, linear boundary value problem, still of second order.

$$A(\xi)\frac{d^2\theta}{d\xi^2} + \frac{dA(\xi)}{d\xi}\frac{d\theta}{d\xi} - \frac{hPL^2}{k}\theta = 0 \tag{7.3}$$
$$\theta(\xi = 0) = 1, \qquad \left.\frac{d\theta}{d\xi}\right|_{\xi=1} = 0$$

In the above model, we have also introduced a variation on the boundary condition at $\xi = 1$. Such boundary conditions, where the derivatives are specified, are called *Newman* boundary conditions. The temperature value at $\xi = 1$ is an unknown and must be found as part of the solution procedure.

In yet another variation, consider the case where the thermal conductivity is a function of temperature, viz. $k(\theta) = \alpha + \beta\theta^2$ where α and β are experimentally determined constants. Let the area, A be a constant. The equation is nonlinear and must be solved numerically.

$$\begin{aligned} k(\theta)\frac{d^2\theta}{d\xi^2} + \frac{dk(\theta)}{d\theta}\left[\frac{d\theta}{d\xi}\right]^2 - \frac{hPL^2}{A}\,\theta &= 0 \qquad (7.4) \\ \theta(\xi = 0) = 1, \qquad \left[k\frac{d\theta}{d\xi} + h\theta\right]_{\xi=1} &= 0 \end{aligned}$$

At this opportunity a third variation on the boundary condition, called the mixed or *Robin* boundary condition has been used. Once again, the temperature value at $x = L$ is an unknown and must be found as part of the solution procedure.

All of these problems can be represented symbolically as,

$$\begin{aligned} \mathcal{D}\theta &= f \qquad \text{on } \Omega \\ \mathcal{B}\theta &= g \qquad \text{on } \partial\Omega \end{aligned}$$

where $\mathcal{D}$ and $\mathcal{B}$ are differential operators, Ω is the domain of interest and $\partial\Omega$ represents its boundary. Our task is to obtain an *approximate solution*, $\tilde{\boldsymbol{\theta}}$ to the above problem. The approximation consists in constructing a *discrete* version of the differential equations which results in a system algebraic equations. If the differential equations are *linear* (as in equations (7.2,7.3), then the resulting discrete, algebraic equations will also be linear of the type $\boldsymbol{\mathcal{A}}\tilde{\boldsymbol{\theta}} = \boldsymbol{b}$ and methods of Chapter 3 can be used to obtain the final approximate solution. If the differential equations are *nonlinear* (as in equation (7.4)) then the resulting discrete, algebraic equations will also be nonlinear of the type $\boldsymbol{\mathcal{F}}(\tilde{\boldsymbol{\theta}}) = \mathbf{0}$ and methods of Chapter 4 can be used to obtain the final approximate solution.

In the following sections we develop various schemes for constructing approximate solutions.

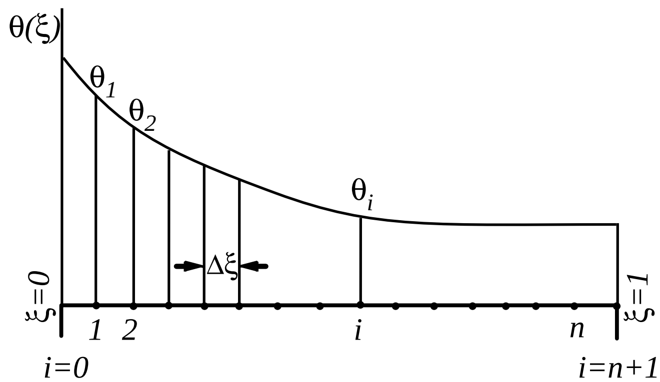

Figure 7.1: One dimensional finite difference grid of equally spaced data points

7.2 Finite difference method

7.2.1 Linear problem with constant coefficients

Let us consider equation (7.2) which is a linear problem subject to Dirichlet boundary conditions. In solving equation (7.2) by the finite difference method, we divide the domain $\Omega = \xi \in [0,1]$ into $(n+1)$ equally spaced subdivisions as shown in figure 7.1. The distance between the two grid points is denoted by $\Delta\xi$. The grid spacing $\Delta\xi$ and the value of the independent variable ξ at the nodal point i are given by,

$$\Delta\xi = \frac{1-0}{n+1} \qquad \xi_i = i\,\Delta\xi \qquad i = 0, 1, \cdots (n+1)$$

Next, instead of attempting to find a solution $\theta(\xi)$ as a continuous function of ξ that satisfies the differential equation (7.2) exactly at *every* ξ, we content ourselves with finding an approximate solution at the selected nodal points shown in the figure - *i.e.*, $\{\theta(\xi_i) = \tilde{\theta}_i | i = 1, 2, \cdots n\}$, where n is the number of *interior* grid points. Note that for the *Dirichlet* type of boundary conditions θ_0 and θ_{n+1} are known. Hence, it remains to determine only n unknowns at the interior points. We obtain n equations by evaluating the differential equation (7.2) at the interior nodal points. In doing this we replace all the derivatives by the corresponding *finite difference approximation* from Table 5.4. Clearly, we have several choices; but it is important to match the truncation error in every term to be of the same order. We illustrate this process using *central difference approximations.*

Using the central difference approximation for the second derivative in equation (7.2), we obtain,

$$\left[\frac{\tilde{\theta}_{i-1} - 2\tilde{\theta}_i + \tilde{\theta}_{i+1}}{(\Delta\xi)^2} + \mathcal{O}((\Delta\xi)^2)\right] - \frac{hPL^2}{kA}\tilde{\theta}_i = 0 \qquad i = 1, 2, \cdots n$$

The term in the square brackets is the central difference approximation for the second derivative and $\mathcal{O}((\Delta\xi)^2)$ is included merely to remind us of the order of the truncation error. We now have a system of n linear algebraic equations. Let us write these out explicitly for $n = 4$.

$$\begin{aligned}
\tilde{\theta}_0 - 2\tilde{\theta}_1 + \tilde{\theta}_2 - \left[\frac{hPL^2}{kA}(\Delta\xi)^2\right]\tilde{\theta}_1 &= 0 \\
\tilde{\theta}_1 - 2\tilde{\theta}_2 + \tilde{\theta}_3 - \left[\frac{hPL^2}{kA}(\Delta\xi)^2\right]\tilde{\theta}_2 &= 0 \\
\tilde{\theta}_2 - 2\tilde{\theta}_3 + \tilde{\theta}_4 - \left[\frac{hPL^2}{kA}(\Delta\xi)^2\right]\tilde{\theta}_3 &= 0 \\
\tilde{\theta}_3 - 2\tilde{\theta}_4 + \tilde{\theta}_5 - \left[\frac{hPL^2}{kA}(\Delta\xi)^2\right]\tilde{\theta}_4 &= 0
\end{aligned}$$

$\tilde{\theta}_0$ in the first equation and $\tilde{\theta}_5$ in the last equation are known from the *Dirichlet* boundary conditions. The above equations can be expressed in matrix notation as, $\boldsymbol{\mathcal{T}}\tilde{\boldsymbol{\theta}} = \boldsymbol{b}$,

$$\begin{bmatrix} -(2+\alpha) & 1 & 0 & 0 \\ 1 & -(2+\alpha) & 1 & 0 \\ 0 & 1 & -(2+\alpha) & 1 \\ 0 & 0 & 1 & -(2+\alpha) \end{bmatrix} \begin{bmatrix} \tilde{\theta}_1 \\ \tilde{\theta}_2 \\ \tilde{\theta}_3 \\ \tilde{\theta}_4 \end{bmatrix} = \begin{bmatrix} -\tilde{\theta}_0 \\ 0 \\ 0 \\ -\tilde{\theta}_5 \end{bmatrix} \tag{7.5}$$

where $\alpha = \frac{hPL^2}{kA}(\Delta\xi)^2$. Note that the boundary values $\tilde{\theta}_0$ and $\tilde{\theta}_5$ appear as forcing terms on the right hand side. Equation (7.5) is the *discrete* version of equation (7.2). Once the structure is apparent, we can increase n to reduce $(\Delta\xi)$ and hence reduce the truncation error. In the limit of $\Delta\xi \to 0$ the solution to equations (7.5) will approach that of equation (7.2). The matrix size will increase with decreasing $\Delta\xi$ and increasing n. The matrix $\boldsymbol{\mathcal{T}}$ is tridiagonal and hence the Thomas algorithm developed in section §3.4.4 can be used to get the solution.

7.2.2 Linear problem with variable coefficients

Next we consider equation (7.3) which is also a linear problem subject to Dirichlet condition at $\xi = 0$ and Neuman boundary condition at $\xi =$

1. It also has variable coefficients, $A(\xi)$ and $A'(\xi)$ - *i.e.*, A is a known function of ξ. The discretization procedure remains the same as seen in the previous section §7.2.1, with the exception that $\tilde{\theta}_{n+1}$ is now included in the unknown set

$$\tilde{\boldsymbol{\theta}} = \{\tilde{\theta}_1, \tilde{\theta}_2, \cdots, \tilde{\theta}_{n+1}\}.$$

But we have the Neuman boundary condition as an extra condition that will provide the additional equation. Using the central difference approximations for both the second and first derivatives in equation (7.3), we obtain,

$$A(\xi_i)\left[\frac{\tilde{\theta}_{i-1} - 2\tilde{\theta}_i + \tilde{\theta}_{i+1}}{(\Delta\xi)^2} + \mathcal{O}((\Delta\xi)^2)\right]$$
$$A'(\xi_i)\left[\frac{\tilde{\theta}_{i+1} - \tilde{\theta}_{i-1}}{2(\Delta\xi)} + \mathcal{O}((\Delta\xi)^2)\right] - \frac{hPL^2}{k}\tilde{\theta}_i = 0 \qquad i = 1, 2, \cdots n+1$$

Once again the truncation error term has been retained at this stage, only to emphasize that it should preferably be of the same order for every derivative that has been replaced by a difference approximation; otherwise the effective error is of the same order as the term with the lowest order truncation error. Multiplying throughout by $(\Delta\xi)^2$ and collecting like terms together, we get,

$$\left[A(\xi_i) - A'(\xi_i)\frac{(\Delta\xi)}{2}\right]\tilde{\theta}_{i-1} + \left[-2A(\xi_i) - \frac{hPL^2(\Delta\xi)^2}{k}\right]\tilde{\theta}_i +$$
$$\left[A(\xi_i) + A'(\xi_i)\frac{(\Delta\xi)}{2}\right]\tilde{\theta}_{i+1} = 0, \qquad i = 1, 2, \cdots n+1$$

Letting

$$\begin{aligned} a_i &= \left[A(\xi_i) - A'(\xi_i)\frac{(\Delta\xi)}{2}\right] \\ d_i &= \left[-2A(\xi_i) - \frac{hPL^2(\Delta\xi)^2}{k}\right] \qquad i = 1, \cdots n+1 \\ c_i &= \left[A(\xi_i) + A'(\xi_i)\frac{(\Delta\xi)}{2}\right] \end{aligned}$$

we can rewrite the equation as,

$$a_i\tilde{\theta}_{i-1} + d_i\tilde{\theta}_i + c_i\tilde{\theta}_{i+1} = 0, \qquad i = 1, 2, \cdots n+1$$

Observe that the coefficients $\{a_i, d_i, c_i\}$ in the above equations are known. However, unlike in equation (7.5), they vary with the grid point location i. Also, for $i = 1$, $\tilde{\theta}_0$ on the left boundary is known through the Dirichlet boundary condition. The last equation for $i = n + 1$ needs special attention since it contains the unknown $\tilde{\theta}_{n+2}$ which lies outside the domain of interest. So far we have not used the Neuman boundary condition at the right boundary $\xi_{n+1} = 1$. Using the central difference approximation for the first derivative to discretize the Neuman boundary condition we get,

$$\left.\frac{d\theta}{d\xi}\right|_{\xi_{n+1}=1} \approx \left[\frac{\tilde{\theta}_{n+2} - \tilde{\theta}_n}{2\Delta\xi}\right] = 0$$

which implies $\tilde{\theta}_{n+2} = \tilde{\theta}_n$. This can be used to eliminate $\tilde{\theta}_{n+2}$ from the last equation, which becomes,

$$(a_i + c_i)\tilde{\theta}_n + d_i\tilde{\theta}_{n+1} = 0, \text{ for } \qquad i = n + 1$$

Thus we obtain a tridiagonal system of linear equation of the form $\boldsymbol{\mathcal{T}}\tilde{\boldsymbol{\theta}} = \boldsymbol{b}$. For $n = 4$, as an example, we get the follwoing five equations.

$$\begin{bmatrix} d_1 & c_1 & 0 & 0 & 0 \\ a_2 & d_2 & c_2 & 0 & 0 \\ 0 & a_3 & d_3 & c_3 & 0 \\ 0 & 0 & a_4 & d_4 & c_4 \\ 0 & 0 & 0 & a_5 + c_5 & d_5 \end{bmatrix} \begin{bmatrix} \tilde{\theta}_1 \\ \tilde{\theta}_2 \\ \tilde{\theta}_3 \\ \tilde{\theta}_4 \\ \tilde{\theta}_5 \end{bmatrix} = \begin{bmatrix} -a_1\tilde{\theta}_0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{7.6}$$

Equation (7.6) is the *discrete* version of equation (7.3). Once the structure is apparent, we can increase n to reduce $(\Delta\xi)$ and hence reduce the truncation error. In the limit of $\Delta\xi \to 0$ the solution to equations (7.6) will approach that of equation (7.3). The matrix size will increase with decreasing $\Delta\xi$ and increasing n. The matrix $\boldsymbol{\mathcal{T}}$ is tridiagonal and hence the Thomas algorithm developed in section §3.4.4 can be used to get the solution.

7.2.3 Nonlinear problem

Conceptually there is no difference in discretizing a linear or a non-linear differential equation. The process of constructing a grid and replacing the differential equations with the difference equations at each grid point is the same. The main difference lies in the choice of solution technique available for solving the nonlinear algebraic equations. Let us consider the nonlinear model represented by equation (7.4). In this case we have a *Robin* condition at $\xi = 1$ and hence $\tilde{\theta}_{n+1}$ is unknown. Thus the unknowns on the discrete grid consist of

$$\tilde{\boldsymbol{\theta}} = \{\tilde{\theta}_1, \tilde{\theta}_2, \cdots, \tilde{\theta}_{n+1}\}.$$

and we need $n + 1$ equations.

Discretizing equation (7.4) at a typical grid point i, we obtain the following $(n + 1)$ nonlinear algebraic equations.

$$f_i(\tilde{\boldsymbol{\theta}}) := k(\tilde{\theta}_i)\left[\frac{\tilde{\theta}_{i-1} - 2\tilde{\theta}_i + \tilde{\theta}_{i+1}}{(\Delta\xi)^2}\right] + k'(\tilde{\theta}_i)\left[\frac{\tilde{\theta}_{i+1} - \tilde{\theta}_{i-1}}{2(\Delta\xi)}\right]^2 - \frac{hPL^2}{A}\tilde{\theta}_i = 0 \qquad i = 1, 2, \cdots n + 1$$

In this set of equations $i = 1$ and $i = (n+1)$ require special consideration to incorporate the boundary conditions. Thus, making use of the left boundary condition, $\tilde{\theta}_0 = 1$, $f_1(\tilde{\boldsymbol{\theta}})$ becomes,

$$f_1(\tilde{\theta}_1, \tilde{\theta}_2) := k(\tilde{\theta}_1)\left[\frac{1 - 2\tilde{\theta}_1 + \tilde{\theta}_2}{(\Delta\xi)^2}\right] + k'(\tilde{\theta}_1)\left[\frac{\tilde{\theta}_2 - 1}{2(\Delta\xi)}\right]^2 - \frac{hPL^2}{A}\tilde{\theta}_1 = 0$$

At the right boundary, we discretize the Robin boundary condition as,

$$k(\tilde{\theta}_{n+1})\left[\frac{\tilde{\theta}_{n+2} - \tilde{\theta}_n}{2(\Delta\xi)}\right] + h\tilde{\theta}_{n+1} = 0$$

which can be rearranged as,

$$\tilde{\theta}_{n+2} = \left[\tilde{\theta}_n - \left(\frac{2(\Delta\xi)h}{k(\tilde{\theta}_{n+1})}\right)\tilde{\theta}_{n+1}\right] = \left[\tilde{\theta}_n - \beta\tilde{\theta}_{n+1}\right]$$

This can be used in the equation $f_{n+1}(\tilde{\boldsymbol{\theta}})$ to eliminate $\tilde{\theta}_{n+2}$.

$$f_{n+1}(\tilde{\theta}_n, \tilde{\theta}_{n+1}) := k(\tilde{\theta}_{n+1})\left[\frac{\tilde{\theta}_n - 2\tilde{\theta}_{n+1} + [\tilde{\theta}_n - \beta\tilde{\theta}_{n+1}]}{(\Delta\xi)^2}\right] + k'(\tilde{\theta}_{n+1})\left[\frac{[\tilde{\theta}_n - \beta\tilde{\theta}_{n+1}] - \tilde{\theta}_n}{2(\Delta\xi)}\right]^2 - \frac{hPL^2}{A}\tilde{\theta}_{n+1} = 0$$

The above equations $f_1 = 0, f_2 = 0, \cdots f_{n+1} = 0$ can be represented symbolically as a system of $(n + 1)$ nonlinear equations of the form, $\boldsymbol{\mathcal{F}}(\tilde{\boldsymbol{\theta}}) = \mathbf{0}$. These can be solved most effectively by the Newton method for the unknowns $\tilde{\boldsymbol{\theta}} = \{\tilde{\theta}_1, \tilde{\theta}_2, \cdots, \tilde{\theta}_{n+1}\}$.

$$\tilde{\boldsymbol{\theta}}^{p+1} = \tilde{\boldsymbol{\theta}}^p - \boldsymbol{J}^{-1}\boldsymbol{f}(\tilde{\boldsymbol{\theta}}^p) \qquad p = 0, 1, \cdots$$

The Jacobian matrix, $\boldsymbol{J} = \frac{\partial\boldsymbol{\mathcal{F}}}{\partial\tilde{\boldsymbol{\theta}}}$ has the following tridiagonal structure.

$$\boldsymbol{J} = \begin{bmatrix} \frac{\partial f_1}{\partial\tilde{\theta}_1} & \frac{\partial f_1}{\partial\tilde{\theta}_2} & 0 & 0 \\ \frac{\partial f_2}{\partial\tilde{\theta}_1} & \frac{\partial f_2}{\partial\tilde{\theta}_2} & \frac{\partial f_2}{\partial\tilde{\theta}_3} & 0 \\ 0 & \frac{\partial f_3}{\partial\tilde{\theta}_2} & \frac{\partial f_3}{\partial\tilde{\theta}_3} & \frac{\partial f_3}{\partial\tilde{\theta}_4} \\ 0 & 0 & \frac{\partial f_4}{\partial\tilde{\theta}_3} & \frac{\partial f_4}{\partial\tilde{\theta}_4} \end{bmatrix}$$

7.3 Quasilinearization of nonlinear equations

Recall the Newton method applied to a system of nonlinear algebraic equations:

$$\boldsymbol{f}(\boldsymbol{x}) = \mathbf{o} \tag{7.7}$$

A solution is sought by linearizing the equations using

$$\boldsymbol{x} = \boldsymbol{x}_a + \boldsymbol{\delta} \tag{7.8}$$

where $\boldsymbol{x}_a$ is an approximate solution and $\boldsymbol{\delta}$ is the correction vector. Hence the original equation becomes,

$$\boldsymbol{f}(\boldsymbol{x}_a + \boldsymbol{\delta}) = \boldsymbol{f}(\boldsymbol{x}_a) + \left.\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}}\right|_{x_a} \boldsymbol{\delta} + O(\delta^2) \tag{7.9}$$

Neglecting second and higher order terms, one gets the linearized equation,

$$\left.\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}}\right|_{x_a} \boldsymbol{\delta} = -\boldsymbol{f}(\boldsymbol{x}_a) \tag{7.10}$$

Similar concepts can be applied to a (system of) differential equations as well. Consider for example the equation given below

$$\frac{d}{d\xi}\left[k(\theta)\xi\frac{d\theta}{d\xi}\right] = 0 \tag{7.11}$$

with the boundary conditions

$$\theta(\xi = 1) = 1 \quad \text{inner wall;} \quad \theta(\xi = \xi_0) = 0 \quad \text{outer wall}$$

The thermal conductivity is given by $k(\theta) = \alpha + \gamma\theta^2$ The equation can be written as,

$$f(\theta) := k(\theta)\xi\frac{d^2\theta}{d\xi^2} + k(\theta)\frac{d\theta}{d\xi} + \xi\frac{dk}{d\theta}\left[\frac{d\theta}{d\xi}\right]^2 = 0 \tag{7.12}$$

The solution to this nonlinear problem can be obtained by successive iteration from an initial guess $\theta_a(\xi)$. Let the actual solution be written as

$$\theta(\xi) = \theta_a(\xi) + \delta(\xi) \tag{7.13}$$

where $\delta(\xi)$ is a small correction to be obtained by solving a linearized form of equation (7.12). The linearized equation is derived by substituting equation (7.13) in equation (7.12), expanding the resulting expression and neglecting quadratic and higher order terms in $\delta(\xi)$ in the expansion.

$$k(\theta_a+\delta)\xi\frac{d^2(\theta_a+\delta)}{d\xi^2}+k(\theta_a+\delta)\frac{d(\theta_a+\delta)}{d\xi}+\xi\left.\frac{dk}{d\theta}\right|_{\theta_a+\delta}\left[\frac{d(\theta_a+\delta)}{d\xi}\right]^2=0 \quad (7.14)$$

Note that each nonlinear term must now be expanded in Taylor series, e.g.

$$k(\theta_a+\delta)\approx k(\theta_a)+\left.\frac{dk}{d\theta}\right|_{\theta_a}\delta+\cdots$$
$$\left.\frac{dk}{d\theta}\right|_{\theta_a+\delta}\approx\left.\frac{dk}{d\theta}\right|_{\theta_a}+\left.\frac{d^2k}{d\theta^2}\right|_{\theta_a}\delta+\cdots \quad (7.15)$$

etc. Hence the expanded form of the equation is,

$$\xi\left[k(\theta_a)\frac{d^2\theta_a}{d\xi^2}+k(\theta_a)\frac{d^2\delta}{d\xi^2}+\left.\frac{dk}{d\theta}\right|_{\theta_a}\delta\frac{d^2\theta_a}{d\xi^2}+\left.\frac{dk}{d\theta}\right|_{\theta_a}\delta\frac{d^2\delta}{d\xi^2}+\cdots\right]$$
$$k(\theta_a)\frac{d\theta_a}{d\xi}+k(\theta_a)\frac{d\delta}{d\xi}+\left.\frac{dk}{d\theta}\right|_{\theta_a}\delta\frac{d\theta_a}{d\xi}+\left.\frac{dk}{d\theta}\right|_{\theta_a}\delta\frac{d\delta}{d\xi}+\cdots$$
$$\xi\left\{\left.\frac{dk}{d\theta}\right|_{\theta_a}+\left.\frac{d^2k}{d\theta^2}\right|_{\theta_a}\delta+\cdots\right\}\left[\left\{\frac{d\theta_a}{d\xi}\right\}^2+\left\{\frac{d\delta}{d\xi}\right\}^2+2\left\{\frac{d\theta_a}{d\xi}\frac{d\delta}{d\xi}\right\}\right]=0 \quad (7.16)$$

Now, terms of order δ^2 and higher are neglected since δ is small. The terms that are evaluated at the current guess θ_a are moved to the right hand side. Hence we get,

$$k(\theta_a)\xi\frac{d^2\delta}{d\xi^2}+\xi\left.\frac{dk}{d\theta}\right|_{\theta_a}\delta\frac{d^2\theta_a}{d\xi^2}+k(\theta_a)\frac{d\delta}{d\xi}+\left.\frac{dk}{d\theta}\right|_{\theta_a}\delta\frac{d\theta_a}{d\xi}+$$
$$\xi\left.\frac{d^2k}{d\theta^2}\right|_{\theta_a}\delta\left\{\frac{d\theta_a}{d\xi}\right\}^2+2\xi\left.\frac{dk}{d\theta}\right|_{\theta_a}\left\{\frac{d\theta_a}{d\xi}\frac{d\delta}{d\xi}\right\}$$
$$=-\left[k(\theta_a)\xi\frac{d^2\theta_a}{d\xi^2}+k(\theta_a)\frac{d\theta_a}{d\xi}+\xi\left.\frac{dk}{d\theta}\right|_{\theta_a}\left\{\frac{d\theta_a}{d\xi}\right\}^2\right] \quad (7.17)$$

Note that the right hand side of equation (7.17) is the same as equation (7.12) evaluated at θ_a and when it is zero the problem is solved! The left hand side of equation (7.17) is linear in δ subject to homogeneous boundary condition of $\delta(1)=0$ and $\delta(\xi_0)=0$. Hence the solution (or correction) $\delta(\xi)$ will be zero when the iteration is converged. Now one can discretize equation (7.17) and solve for the correction iteratively. Equation (7.17) can also be written in operator form as,

$$\boldsymbol{D}_\theta\delta=-f(\theta)$$

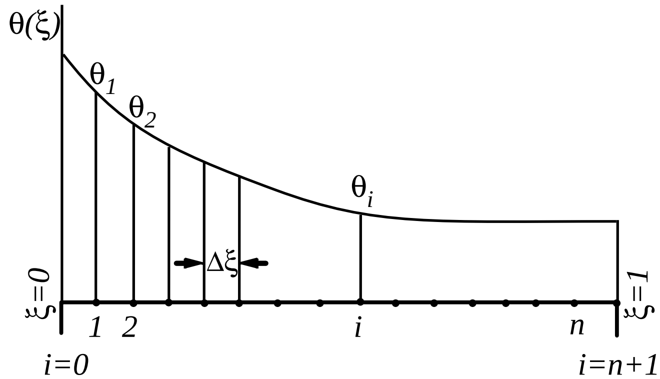

Figure 7.2: One dimensional control volume discretization

where the linear operator $\boldsymbol{D}_\theta$, called the Fréchet derivative is given by,

$$k(\theta_a)\xi \frac{d^2 \cdot}{d\xi^2} + \left[k(\theta_a) + 2\xi \left.\frac{dk}{d\theta}\right|_{\theta_a} \left\{ \frac{d\theta_a}{d\xi} \right\} \right] \frac{d\cdot}{d\xi} +$$
$$\left[\xi \left.\frac{dk}{d\theta}\right|_{\theta_a} \frac{d^2\theta_a}{d\xi^2} + \left.\frac{dk}{d\theta}\right|_{\theta_a} \frac{d\theta_a}{d\xi} + \xi \left.\frac{d^2 k}{d\theta^2}\right|_{\theta_a} \left\{ \frac{d\theta_a}{d\xi} \right\}^2 \right] \cdot$$

7.4 Control volume method

7.5 Shooting method

7.6 Collocation methods

7.7 Method of weighted residuals