Problem Discretization using Approximation Theory II

Discretization using Finite Difference Method SKG

To begin with we present an application of scalar Taylor series expansion to discretization of ODE-BVP and PDEs. Even when the domain of the function under consideration is multivariate, the Taylor series approximation is applied locally by considering one variable at a time.

1 Local Approximation of Derivatives using Taylor Series Expansion

Let function $u(z)$ denote an n-times differentiable function where the independent $z \in [a,b]$. Consider the problem of developing a local approximation of derivatives of $u(z)$ at a point, say $z = \overline{z}$, in (a,b).

Let $\Delta z > 0$ represent a small perturbation from $z = \overline{z}$ such that $[\overline{z} - \Delta z, \overline{z} + \Delta z] \in [a,b]$. If Δz is sufficiently small, then, using the Taylor Series expansion, we can write

$$u(\overline{z} + \Delta z) = u(\overline{z}) + \left[\frac{du(\overline{z})}{dz}\right](\Delta z) + \frac{1}{2!}\frac{d^2u(\overline{z})}{dz^2}(\Delta z)^2 + \frac{1}{3!}\frac{d^3uu(\overline{z})}{dz^3}(\Delta z)^3 + r_4(\overline{z},\Delta z) \quad (22)$$

Similarly, using the Taylor series expansion , we can express $u(\overline{z} - \Delta z)$ as follows

$$u(\overline{z} - \Delta z) = u(\overline{z}) - \frac{du(\overline{z})}{dz}(\Delta z_i) + \frac{1}{2!}\frac{d^2u(\overline{z})}{dz^2}(\Delta z)^2 - \frac{1}{3!}\frac{d^3u(\overline{z})}{dz^3}(\Delta z)^3 + \widetilde{r}_4(\overline{z},\Delta z) \quad (23)$$

From equations (22) and (23) we can arrive at several approximate expressions for $\left(\frac{du}{dz}\right)$ at $z = \overline{z}$. Rearranging equation (22) we obtain

$$\frac{du(\overline{z})}{dz} = \frac{[u(\overline{z} + \Delta z) - u(\overline{z})]}{\Delta z} - \left[\frac{d^2u(\overline{z})}{dz^2}\left(\frac{\Delta z}{2}\right) + \ldots\right] \quad (24)$$

and, when Δz is sufficiently small, then neglecting the higher order terms we obtain *forward difference* approximation of the local first order derivative as follows

$$\frac{du(\overline{z})}{dz} \simeq \frac{u(\overline{z} + \Delta z) - u(\overline{z})}{\Delta z}$$

Similarly, starting from equation (23), we can arrive at *backward difference* approximation of the local first order derivative, i.e.

$$\frac{du(\overline{z})}{dz} \simeq \frac{u(\overline{z}) - u(\overline{z} - \Delta z)}{\Delta z}$$

It may be noted that the errors in the forward and the backward difference approximation are of the order of Δz, which is denoted as $O(\Delta z)$. Alternatively, subtracting equation (23) from (22) and rearranging we can arrive at the following expression

$$\frac{du(\overline{z})}{dz} = \frac{[u(\overline{z} + \Delta z) - u(\overline{z} - \Delta z)]}{2(\Delta z)} - \left[u_i^{(3)}\left(\frac{\Delta z^2}{3!}\right) + \ldots\right] \quad (25)$$

and, for sufficiently small Δz, we obtain *central difference* approximation of the local first order derivative by neglecting the terms of order higher than Δz^2 , i.e.

$$\frac{du(\overline{z})}{dz} \simeq \frac{[u(\overline{z} + \Delta z) - u(\overline{z} - \Delta z)]}{2(\Delta z)} \quad (26)$$

The central difference approximation is accurate to $O[(\Delta z)^2]$ and is more commonly used.

To arrive at an approximation for the second order derivatives at $z = \overline{z}$, adding equation (23) with (22) and rearranging, we have

$$\frac{d^2u(\overline{z})}{dz^2} = \frac{[u(\overline{z} + \Delta z) - 2u(\overline{z}) + u(\overline{z} - \Delta z)]}{(\Delta z)^2} - \left[2\frac{d^4u(\overline{z})}{dz^4}\frac{(\Delta z)^2}{4!} + \ldots\right] \quad (27)$$

When Δz is sufficiently small, we obtain the following approximation for the second derivative

$$\frac{d^2u(\overline{z})}{dz^2} \simeq \frac{u(\overline{z} + \Delta z) - 2u(\overline{z}) + u(\overline{z} - \Delta z)}{(\Delta z)^2} \quad (28)$$

Note that errors in the approximations (26) and (28) are of order $O[\Delta z)^2]$. This process can be continued to arrive at approximations of higher order derivatives at $z = \overline{z}$.

The approach developed for function of one independent variables can easily be extended to arrive at local approximations to partial derivatives of a continuously differential function in multiple variables. For example, Let function $u(x,y)$ denote an n-times differentiable function where the independent

$x \in (a,b)$ and $z \in (c,d)$. Consider the problem of developing a local approximation of partial derivatives of $u(x,y)$ at a point, say $x = \overline{x} \in (a,b)$ and $y = \overline{y} \in (c,d)$. Let $\Delta x > 0, \Delta y > 0$ represent a small perturbations from $x = \overline{x}, y = \overline{y}$ such that $[\overline{x} - \Delta x, \overline{x} + \Delta x] \in [a,b]$ and $[\overline{y} - \Delta y, \overline{y} + \Delta y] \in [c,d]$. Then, using similar argumemnts, we can arrive at the following approximations of the first and the second order partial derivatives and so on.

$$\frac{du(\overline{x},\overline{y})}{dx} \simeq \frac{[u(\overline{x} + \Delta x, \overline{y}) - u(\overline{x} - \Delta\overline{x}, \overline{y})]}{2(\Delta x)} \quad (29)$$

$$\frac{du(\overline{x},\overline{y})}{dy} \simeq \frac{[u(\overline{x}, \overline{y} + \Delta y) - u(\overline{x}, \overline{y} - \Delta\overline{y})]}{2(\Delta y)} \quad (30)$$

$$\frac{d^2(\overline{x},\overline{y})}{dx^2} \simeq \frac{u(\overline{x} + \Delta x, \overline{y}) - 2u(\overline{x} + \Delta x, \overline{y}) + u(\overline{x} - \Delta\overline{x}, \overline{y})}{(\Delta x)^2} \quad (31)$$

2 Discretization of ODE-BVPs

Consider the following general form of 2^{nd} order ODE-BVP problem frequently encountered in engineering problems

$$\Psi\left[\frac{d^2u}{dz^2}, \frac{du}{dz}, u, z\right] = 0 \; for \; z \in \; (0,1) \quad (32)$$

$$B.C.\ 1\ (at\ z = 0) : f_1\left[\frac{du}{dz}, u, 0\right] = 0 \quad (33)$$

$$B.C.\ 2\ (at\ z = 1) : f_2\left[\frac{du}{dz}, u, 1\right] = 0 \quad (34a)$$

Let $u^*(z) \in C^{(2)}[0,1]$ denote the exact / true solution to the above ODE-BVP. Depending on the nature of operator Ψ,it may or may not be possible to find the true solution to the problem. In the present case, however, we are interested in finding an approximate numerical solution, say $u(z)$, to the above ODE-BVP. The basic idea in finite difference approach is to convert the ODE-BVP into a set of coupled linear or nonlinear algebraic equations using local approximation of the derivatives based on the Taylor series expansion. In order to achieve this, the domain $0 \leq z \leq 1$ is divided into $(n+1)$ grid points $z_1, \ldots, z_n, z_{n+1}$ located such that

$$z_1 = 0 < z_2 < z_3 \ldots < \; z_{n+1} = 1$$

The simplest option is to choose them equidistant, i.e.

$$z_i = (i-1)(\Delta z) = (i-1)/(n) \text{ for } i = 1, 2, \ldots, n+1$$

which is considered for the subsequent development. Let the value of the approximate solution, $u(z)$, at location z_i be denoted as $u_i = u(z_i)$. If Δz is sufficiently small, then the Taylor Series expansion based approximations of the local derivatives presented in the previous sub-section can be used to discretize the ODE-BVP. The basic idea is to enforce the approximation of equation (32) at each internal grid point. The remaining equations are obtained from discretization of the boundary conditions. While discretizing the ODE, it is preferable to use the approximations having similar accuracies. Thus, central difference approximation of the first derivative is preferred over the forward or the backward difference approximations as order of error in approxmations is $O[(\Delta z)^2]$, which is similar to the order of errors in the approximation of the second order derivatives. The steps involved in the discretization can be summarized as follows:

- **Step 1 :** Force residual R_i at each internal grid point to zero,i.e.,

$$R_i = \Psi\left[\frac{(u_{i+1} - 2u_i + u_{i-1})}{(\Delta z)^2}, \frac{(u_{i+1} - u_{i-1})}{2(\Delta z)}, u_i, z_i\right] = 0 \quad (35 \& 36)$$

$$i = 2, 3 \ldots, n.$$

This gives rise to $(n-1)$ equations in $(n+1)$ unknowns $\{u_i : i = 1, 2, \ldots, n+1\}$.

- **Step 2:** Use boundary conditions to generate the remaining algebraic equations. This can be carried out using either of the following two approaches
  - **Approach 1:** Use one-sided derivatives only at the boundary points, i.e.,

    $$f_1\left[\frac{(u_2 - u_1)}{\Delta z}, u_1, 0\right] = 0 \quad (37)$$

    $$f_2\left[\frac{(u_{n+1} - u_n)}{\Delta z}, u_{n+1}, 1\right] = 0 \quad (38)$$

    This gives remaining two equations.

  - **Approach 2:** This approach introduces two more variables u_0 and u_{n+2} at two hypothetical grid points, which are located at

    $$z_0 = z_1 - \Delta z = -\Delta z$$

    $$z_{n+2} = z_{n+1} + \Delta z = 1 + \Delta z$$

    With the introduction of these hypothetical points, the boundary conditions are evaluated as

    $$f_1\left[\frac{(u_2 - u_0)}{(2\Delta z)}, u_1, 0\right] = 0 \quad (39)$$

    $$f_2\left[\frac{u_{n+2} - u_n}{(\Delta z)}, u_{n+1}, 1\right] = 0 \quad (40)$$

    Now we have $n+3$ variables and $n+1$ algebraic constraints. Two additional algebraic equations are generated by setting the residual at the boundary points to zero,i.e., at z_1 and z_{n+1} ,i.e.,

    $$R_1(z=0) = \Psi\left[\frac{(u_2 - 2u_1 + u_0)}{(\Delta z)^2}, \frac{(u_2 - u_0)}{2(\Delta z)}, u_1, 0\right] = 0$$

    $$R_{n+1}(z=1) = \Psi\left[\frac{(u_{n+2} - 2u_{n+1} + u_n)}{(\Delta z)^2}, \frac{(u_{n+2} - u_n)}{2(\Delta z)}, u_{n+1}, 1\right] = 0$$

    This results in $(n+3)$ equations in $(n+3)$ unknowns $\{u_i : i = 0, 1, 2, \ldots, n+2\}$.

It may be noted that the local approximations of the derivatives are developed under the assumption that Δz is chosen sufficiently small. Consequently, it can be expected that the quality of the approximate solution would improve with the increase in the number of grid points.

Example 9 Consider steady state heat transfer/conduction in a slab of thickness L, in which energy is generated at a constant rate of q W/m^3. The boundary at $z = 0$ is maintained at a constant temperature T^*,while the boundary at $z = L$ dissipates heat by convection with a heat transfer coefficient h into the ambient temperature at T_∞. The mathematical formulation of the conduction problem is represented as a ODE-BVP of the form

$$k\frac{d^2T}{dz^2} + q = 0 \quad for \ 0 < z < L \quad (41)$$

$$B.C.\ at\ z=0 : T(0)=T^* \qquad \textbf{(42)}$$

$$B.C.\ at\ z=L : k\left[\frac{dT}{dz}\right]_{z=L} = h[T_\infty - T(L)] \ \textbf{(43)}$$

Note that this problem can be solved analytically. However, it is used here to introduce the concepts of discretization by finite difference approach. Dividing the region $0 \le z \le L$ into n equal subregions with $\Delta z = L/n$ and setting residuals zero at the internal grid points, we have

$$\frac{(T_{i+1} - 2T_i + T_{i-1})}{(\Delta z)^2} + \frac{q}{k} = 0 \quad (44)$$

for $i = 2, 3, \ldots n$. Using the boundary condition ($bc1_1$) i.e. ($T_1 = T^*$), the residual at z_2 reduces to

$$-2T_2 + T_3 = -(\Delta z)^2\left(\frac{q}{k}\right) - T^* \quad (45)$$

Using one sided derivative at $z = L$, boundary condition (43) reduces to

$$k\frac{(T_{n+1} - T_n)}{(\Delta z)} = h(T_\infty - T_{n+1}) \quad (46)$$

or

$$T_{n+1}\left(1 + \frac{h\Delta z}{k}\right) - T_n = h\Delta z\frac{T_\infty}{k} \quad (47)$$

Rearranging the equations in the matrix form, we have

$$\mathbf{A}\widetilde{\mathbf{x}} = \widetilde{\mathbf{y}}$$

$$\widetilde{\mathbf{x}} = \begin{bmatrix} T_2 & T_3 & \ldots & T_{n+1} \end{bmatrix}^T$$

$$\widetilde{\mathbf{y}} = \begin{bmatrix} -(\Delta z)^2(q/k) - T^* & -(\Delta z)^2(q/k) & \ldots & +h(\Delta z)T_\infty/k \end{bmatrix}^T$$

$$\mathbf{A} = \begin{bmatrix} -2 & 1 & 0 & 0 & .. & 0 \\ 1 & -2 & 1 & 0 & .. & 0 \\ 0 & 1 & -2 & 1 & .. & 0 \\ .. & .. & .. & .. & .. & .. \\ .. & .. & .. & .. & -2 & 1 \\ 0 & 0 & .. & .. & -1 & (1 + h\Delta z/k) \end{bmatrix}$$

Thus, after discretization, the ODE-BVP is reduced to a set of linear algebraic equation and the transformation operator $\mathcal{T} = \mathbf{A}$. It may also be noted that we end up with a tridiagonal matrix $\mathbf{A}$, which is a sparse matrix i.e. it contains large number of zero elements.

Example 10 Consider the ODE-BVP describing the steady state conditions in a tubular reactor with axial mixing (TRAM) in which an irreversible 2nd order reaction is carried out at a constant temperature. The steady state behavior can be modelled using the following ODE-BVP:

$$\frac{1}{Pe}\frac{d^2C}{dz^2} - \frac{dC}{dz} - DaC^2 = 0 \qquad (0 \le z \le 1) \quad (48)$$

$$B.C.\, at\; z = 0 : \frac{dC}{dz} = Pe(C-1) \qquad at \quad z = 0; \quad \textbf{(49)}$$

$$B.C.\, at\; z = 1 : \frac{dC}{dz} = 0 \qquad at \quad z = 1; \quad \textbf{(50)}$$

Forcing residuals at (n-1) internal grid points to zero, we have

$$\frac{1}{Pe}\frac{C_{i+1} - 2C_i + C_{i-1}}{(\Delta z)^2} - \frac{C_{i+1} - C_{i-1}}{2(\Delta z)} = DaC_i^2$$

$$i = 2, 3, \ldots n$$

Defining

$$\alpha = \left(\frac{1}{(\Delta z)^2 Pe} - \frac{1}{2(\Delta z)}\right) \; ; \; \beta = \left(\frac{2}{Pe(\Delta z)^2}\right), \gamma = \left(\frac{1}{(\Delta z)^2 Pe} + \frac{1}{2(\Delta z)}\right)$$

the above set of nonlinear equations can be rearranged as follows

$$\alpha C_{i+1} - \beta C_i + \gamma C_{i-1} = DaC_i^2$$

$$i = 2, 3, \ldots n$$

The two boundary conditions yield two additional equations

$$\frac{C_2 - C_1}{\Delta z} = Pe(C_1 - 1)$$

$$\frac{C_{n+1} - C_n}{\Delta z} = 0$$

The resulting set of nonlinear algebraic equations can be arranged as follow

$$\mathcal{T}(\widetilde{\mathbf{x}}) = \mathbf{A}\widetilde{\mathbf{x}} - \mathbf{G}(\widetilde{\mathbf{x}}) = \overline{\mathbf{0}} \quad (51)$$

where

$$\widetilde{\mathbf{x}} = \begin{bmatrix} C_1 \\ C_2 \\ \ldots \\ \ldots \\ C_{n+1} \end{bmatrix} ; \; \mathbf{G}(\widetilde{\mathbf{x}}) = \begin{bmatrix} -Pe(\Delta z) \\ DaC_2^2 \\ \ldots\ldots \\ DaC_n^2 \\ 0 \end{bmatrix}$$

$$\mathbf{A} = \begin{bmatrix} -(1 + \Delta z Pe) & 1 & 0. & \ldots & \ldots & 0 \\ \gamma & -\beta & \alpha & \ldots & \ldots & .. \\ \ldots. & \ldots & .. & \ldots & \ldots & 0. \\ \ldots.. & \ldots & .. & \ldots & -\beta & \alpha \\ 0 & \ldots & .. & \ldots & -1 & 1 \end{bmatrix} \quad (52)$$

Thus, the ODE-BVP is reduced to a set of coupled nonlinear algebraic equations after discretization.

To provide some insights into how the approximate solutions change as a function of the choice of n, we have carried out simulation studies on the TRAM problem (with Pe = 6 and Da = 2). Figure 2 demonstrates how the approximate solutions behave as a function of number of grid points. As can be expected, more and more refined solutions are obtained as number of grid points increase.

3 Discretization of PDEs using Finite Difference [2]

Typical second order PDEs that we encounter in engineering problems are of the form

$$\frac{\partial u}{\partial t} - \left[a\nabla^2 u + b\nabla u + cg(u)\right] = f(x,y,z,t)$$

$$x_L < x < x_H \;\; ; \;\; y_L < y < y_H \;\; ; \;\; z_L < z < z_H$$

subject to appropriate boundary conditions and initial conditions. For example, the Laplacian operators ∇^2 and gradient operator ∇ are defined in the Cartesian coordinates as follows

$$\nabla u = \frac{\partial u}{\partial x} + \frac{\partial u}{\partial y} + \frac{\partial u}{\partial z}$$

$$\nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}$$

In Cartesian coordinate system, we construct grid lines parallel to x, y and z axis and force the residuals to zero at the internal grid points. For example,adopting notation

$$u_{i,j,k} = u(x_i, y_j, z_k)$$

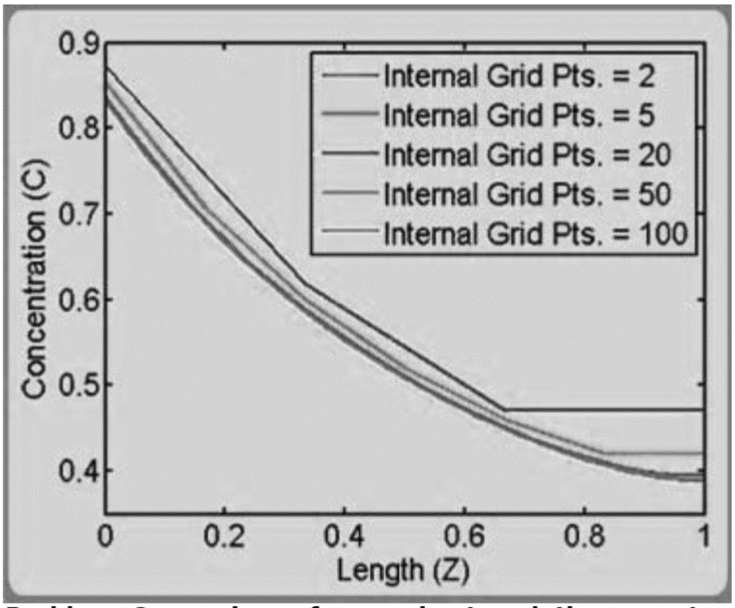

Figure 2: TRAM Problem: Comparison of approximate solutions constructed using finite difference approach with different number of grid points (n)

the partial derivative of the dependent variable u with respect to x at grid point (x_i, y_j, z_k) can be approximated as follows

$$\left(\frac{\partial u}{\partial x}\right)_{ijk} = \frac{(u_{i+1,j,k} - u_{i-1,j,k})}{2(\Delta x)}$$

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_{ijk} = \frac{(u_{i+1,j,k} - 2u_{i,j,k} + u_{i-1,j,k})}{(\Delta x)^2}$$

The partial derivatives in the remaining directions can be approximated in analogous manner. It may be noted that the partial derivatives are approximated by considering one variable at a time and is equivalent to application of Taylor series expansion of a scalar function.

When the PDE involves only the spatial derivatives, the discretization process yields either coupled set of linear / nonlinear algebraic equations or an ODE-BVP. When the PDEs involve time derivatives, the discretization is carried out only in the spatial coordinates. As a consequence, the discretization process yields coupled nonlinear ODEs with initial conditions specified, i.e. an ODE-IVP.

Example 11 Consider the PDE describing the unsteady state condition in a tubular reactor with axial mixing (TRAM) in which an irreversible 2nd order reaction is carried out.

$$\frac{\partial C}{\partial t} = \frac{1}{Pe}\frac{\partial^2 C}{\partial z^2} - \frac{\partial C}{\partial z} - DaC^2 \quad in \quad (0 < z < 1) \quad (53)$$

$$t = 0 \ : \ c(z,0) = f(z) \quad in \quad (0 < z < 1) \quad (54)$$

$$B.C. at\ z = 0 : \frac{\partial C(0,t)}{\partial z} = Pe(C(0,t) - 1) \ for\ t \geq 0 \quad (55)$$

$$B.C. at\ z = 1 : \frac{\partial C(1,t)}{\partial z} = 0 \qquad for\ t \geq 0 \quad (56)$$

Using finite difference method along the spatial coordinate z with $n-1$ internal grid points, we have

$$\frac{dC_i(t)}{dt} = \frac{1}{Pe}\left(\frac{C_{i+1}(t) - 2C_i(t) + C_{i-1}(t)}{(\Delta z)^2}\right) \quad (57)$$

$$-\left(\frac{C_{i+1}(t) - C_{i-1}(t)}{2(\Delta z)}\right) - Da[C_i(t)]^2 \quad (58)$$

$$i = 2, 3, \ldots. n$$

The boundary conditions yield

$$B.C.1 \ : \ \frac{C_2(t) - C_1(t)}{\Delta z} = Pe(C_1(t) - 1)$$

$$\Rightarrow C_1(t) = \left[\frac{1}{\Delta z} + Pe\right]^{-1}\left[\frac{C_2(t)}{\Delta z} + Pe\right] \quad (59)$$

and

$$B.C.2 : \frac{C_{n+1}(t) - C_n(t)}{\Delta z} = 0 \Rightarrow C_{n+1}(t) = C_n(t) \quad (60)$$

These boundary conditions can be used to eliminate variables $C_1(t)$ and $C_{n+1}(t)$ from the set of ODEs (57). This gives rise to a set of (n-1) coupled ODEs together with the initial conditions

$$C_2(0) = f(z_2), C_3(0) = f(z_3), \ldots.. = C_n(0) = f(z_n) \quad (61)$$

Thus, defining vector $\widetilde{\mathbf{x}}$ of concentration values at the internal grid points as

$$\widetilde{\mathbf{x}} = \begin{bmatrix} C_2(t) & C_3(t) & \ldots & C_n(t) \end{bmatrix}^T$$

the discretized problem is an ODE-IVP of the form

$$\mathcal{T}(\widetilde{\mathbf{x}}) = \frac{d\widetilde{\mathbf{x}}}{dt} - F(\widetilde{\mathbf{x}}) = \overline{\mathbf{0}} \quad (62)$$

subject to the initial condition $\widetilde{\mathbf{x}}(0)$. Needless to say that better approximation is obtained if large number of grid points are selected.

Example 12 Laplace equation represents a prototype for steady state diffusion processes. For example 2-dimensional Laplace equation

$$\alpha\left[\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right] = f(x,y) \quad (63)$$

$$0 < x < 1 \, ; \, 0 < y < 1$$

where T is temperature and x, y are dimensionless space coordinates. Equations similar to this arise in many problems of fluid mechanics, heat transfer and mass transfer. In the present case , $T(x,y)$ represents the dimensionless temperature distribution in a furnace and represents thermal diffusivity.

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Three walls of the furnace are insulated and maintained at a constant temperature. Convective heat transfer occurs from the fourth boundary to the atmosphere. The boundary conditions are as follows:

$$x = 0 \; : \; T = T^* \quad ; \quad x = 1 : T = T^* \quad (64)$$

$$y = 0 \; : \; T = T^* \quad (65)$$

$$y = 1 : k\frac{dT(x,1)}{dy} = h[T_\infty - T(x,1)] \quad (66)$$

We construct the 2 -dimensional grid with $(n_x + 1)$ equispaced grid lines parallel to y axis and $(n_y + 1)$ equispaced grid lines parallel to x axis. The temperature T at (i,j) th grid point is denoted as $T_{ij} = T(x_i, y_j)$. We then force the residual to be zero at each internal grid point to obtain the following set of equations:

$$\frac{(T_{i+1,j} - 2T_{i,j} + T_{i-1,j})}{(\Delta x)^2} + \frac{(T_{i,j+1} - 2T_{i,j} + T_{i,j-1})}{(\Delta y)^2} = f(x_i, y_j)/\alpha \quad (67)$$

for $(i = 2,3,\ldots,n_x)$ and ($j = 2,3,\ldots,n_y)$. Note that regardless of the size of the system, each equation contains not more than five unknowns, resulting in a sparse linear algebraic system. Consider the special case when

$$\Delta x = \Delta y = \beta$$

For this case the above equations can be written as

$$T_{i-1,j} + T_{i,j-1} - 4T_{i,j} + T_{i,j+1} + T_{i+1,j} = \beta^2 f(x_i, y_j) \quad (68)$$

$$for \; (i = 2,3,\ldots,n_x) \; and \; (j = 2,3,\ldots,n_y)$$

Using the boundary conditions, we have additional equations

$$T_{1,j} = T^* \; ; \; T_{n_x+1,j} = T^* \quad for \;\; j = 1,2,\ldots,n_y$$

$$T_{i,0} = T^* \quad for \;\; i = 1,2,\ldots n_x + 1$$

$$k\frac{T_{i,n_y+1} - T_{i,n_y}}{\Delta y} = h[T_\infty - T_{i,n_y+1}]$$

$$\Rightarrow T_{i,n_y+1} = \frac{1}{(k/\Delta y) + h}[hT_\infty + (k/\Delta y)T_{i,n_y}]$$

$$for \;\; i = 1,2,\ldots,n_x + 1$$

that can be used to eliminate the boundary variables from the set of ODEs. Thus, we obtain $(n_x - 1) \times (n_y - 1)$ linear algebraic equations in $(n_x - 1) \times (n_y - 1)$ unknowns. Defining vector $\widetilde{\mathbf{x}}$ as

$$\widetilde{\mathbf{x}} = [T_{2,2} \;\; T_{2,3} \ldots\ldots T_{2,n_y}, \ldots, T_{n_x,2} \ldots\ldots T_{n_x,n_y}]^T$$

we can rearrange the resulting set of equations in form of $\mathbf{A}\widetilde{\mathbf{x}} = \mathbf{b}$, then $\mathbf{A}$ turns out to be a large sparse matrix. Even for modest choice of 10 internal grid lines in each direction, we would get a 100×100 sparse matrix associated with 100 variables.

Example 13 Converting a PDE to an ODE-BVP by method of lines [2]: Consider the 2-D steady state heat transfer problem in the previous example. By method of lines, we discretize only in one spatial direction. For example, we choose $n_x - 1$ internal grid points along x coordinate and construct $n_x - 1$ grid lines parallel to the y-axis. The temperature T along the i^{th} grid line is denoted as

$$T_i(y) = T(x_i, y) \quad (69)$$

Now, we equate residuals to zero at each internal grid line as

$$\frac{d^2 T_i}{dy^2} = -\frac{1}{(\Delta x)^2}[T_{i+1}(y) - 2T_i(y) + T_{i-1}(y)] + f(x_i, y)/\alpha \quad (70)$$

$$i = 2, 3, \ldots . n_x$$

The boundary conditions at $x = 0$ and $x = 1$ yield

$$T_1(y) = T^* \quad ; \quad T_{n_x+1}(y) = T^*$$

which can be used to eliminate variables in the above set of ODE that lie on the corresponding edges. The boundary conditions at $y = 0$ and $y = 1$ are:

$$T_i(0) = T^* \; (71)$$

$$k\frac{dT_i(1)}{dy} = h(T_\infty - T_i(1)) \; (72)$$

$$i = 2, 3, \ldots . n_x$$

Thus, defining

$$\widetilde{\mathbf{u}} = \begin{bmatrix} T_2(y) & T_3(y) & \ldots & T_n(y) \end{bmatrix}^T$$

discretization of the PDE using the method of lines yields OBE-BVP of the form

$$\mathcal{T}(\widetilde{\mathbf{u}}) = \frac{d^2\widetilde{\mathbf{y}}}{dy^2} - F[\widetilde{\mathbf{u}}] = \overline{\mathbf{0}}$$

subject to the boundary conditions

$$\widetilde{\mathbf{u}}(0) = T^*$$

$$\frac{d\widetilde{\mathbf{u}}(1)}{dy} = G[\widetilde{\mathbf{u}}(1)]$$

Example 14 Consider the 2-dimensional unsteady state heat transfer problem

$$\frac{\partial T}{\partial t} = \alpha[\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}] + f(x, y, t) \quad (73)$$

$$t = 0 : T = H(x, y) \quad (74)$$

$$x = 0 : T(0, y, t) = T^*; \; x = 1 : T(1, y, t) = T^* \quad (75)$$

$$y = 0 \quad : T(x, 0, t) = T^*; \; (76)$$

$$y = 1 \; : \; k\frac{dT(x, 1, t)}{dy} = h(T_\infty - T(x, 1, t)) \; (77)$$

where $T(x, y, t)$ is the temperature at locations (x, y) at time t and α is the thermal diffusivity. By finite difference approach, we construct a 2-dimensional grid with $n_x - 1$ equispaced grid lines parallel to the y-axis and $n_y - 1$ grid lines parallel to the x-axis. The temperature T at the (i, j)'th grid point is given by

$$T_{ij}(t) = T(x_i, y_i, t) \quad (78)$$

Now, we force the residual to zero at each internal grid point to generate a set of coupled ODE-IVP's as

$$\begin{aligned} \frac{dT_{ij}}{dt} &= \frac{\alpha}{(\Delta x)^2}[T_{i+1,j} - 2T_{i,j} + T_{i-1,j}] \\ &+ \frac{\alpha}{(\Delta y)^2}[T_{i,j+1} - 2T_{i,j} + T_{i,j-1}] + f(x_i, y_j, t) \end{aligned} \quad (79)$$

$$\text{for } i = 2,3,\ldots,n_x \qquad \text{and} \qquad j = 2,3,\ldots,n_y$$

Using the boundary conditions, we have constraints at the four boundaries

$$T_{0,j}(t) = T^* \;;\; T_{n_x+1,j}(t) = T^* \quad for \quad j = 1,2,\ldots n_y + 1$$

$$T_{i,0}(t) = T^* \quad for \quad i = 1,2,\ldots .n_x + 1$$

$$k\frac{T_{i,n_y+1} - T_{i,n_y}}{\Delta y} = h[T_\infty - T_{i,n_y+1}]$$

$$\Rightarrow T_{i,n_y+1}(t) = \frac{1}{(k/\Delta y) + h}[hT_\infty + (k/\Delta y)T_{i,n_y}(t)]$$

$$for \quad i = 2,\ldots .n_x$$

These constraints can be used to eliminate the boundary variables from the set of ODEs ODEij. Thus, defining vector

$$\widetilde{\mathbf{x}}(t) = [T_{2,2}(t) \;\; T_{2,3}(t) \ldots . T_{2,n_y}(t) \ldots , T_{n_x,2}(t) \ldots \ldots T_{n_x,n_y}(t)]^T$$

the PDE after discretization is reduced to a set of coupled ODE-IVPs of the form

$$\mathcal{T}(\widetilde{\mathbf{x}}) = \frac{d\widetilde{\mathbf{x}}}{dt} - F(\widetilde{\mathbf{x}}, t) = \overline{\mathbf{0}}$$

subject to the initial condition $\widetilde{\mathbf{x}}(0)$

$$\widetilde{\mathbf{x}}(0) = [H(x_2, y_2) \;\; H(x_2, y_3) \ldots . H(x_{n_x}, y_2) \ldots . H(x_{n_x}, y_{n_y})]^T$$

4 Newton's Method for Solving Nonlinear Algebraic Equations

The most prominent application of the multivariate Taylor series expansion in the numerical analysis is arguably the Newton's method, which is used for solving a set of simultaneous nonlinear algebraic equations. Consider set of n coupled nonlinear equations of the form

$$f_i(\mathbf{x}) = 0 \text{ for } i = 1,\ldots .,n \quad (80)$$

which have to be solved simultaneously. Here, each $f_i(.) : R^n \to R$ is a scalar function. Defining a function vector

$$\mathbf{F}(\mathbf{x}) = \begin{bmatrix} f_1(\mathbf{x}) & f_2(\mathbf{x}) & \ldots & f_n(\mathbf{x}) \end{bmatrix}^T$$

the problem at hand is to solve vector equation

$$\mathbf{F}(\mathbf{x}) = \overline{\mathbf{0}}$$

Suppose $\mathbf{x}^*$ is a solution such that $F(\mathbf{x}^*) = \overline{0}$. If each function $f_i(\mathbf{x})$ is continuously differentiable, then, in the neighborhood of $\mathbf{x}^*$ we can approximate its behavior by Taylor series, as

(81)

$$\mathbf{F}(\mathbf{x}^*) = \mathbf{F}[\widetilde{\mathbf{x}}+(\mathbf{x}^*-\widetilde{\mathbf{x}})] = \mathbf{F}(\widetilde{\mathbf{x}}) + \left[\frac{\partial F}{\partial x}\right]_{\mathbf{x}=\widetilde{\mathbf{x}}} (\mathbf{x}^*-\widetilde{\mathbf{x}}) + \mathbf{R}_2(\mathbf{x}^*, \mathbf{x}^*-\widetilde{\mathbf{x}})$$

where $\widetilde{\mathbf{x}}$ represents a guess solution. If the guess solution is sufficiently close to the true solution, then, neglecting terms higher than the first order, we can locally approximate the nonlinear transformation $\mathbf{F}(\mathbf{x}^*)$ as follows

$$\mathbf{F}(\mathbf{x}^*) \simeq \widetilde{\mathbf{F}}(\mathbf{x}^*) = \mathbf{F}(\widetilde{\mathbf{x}}) + \left[\frac{\partial F}{\partial x}\right]_{\mathbf{x}=\widetilde{\mathbf{x}}} \Delta\widetilde{\mathbf{x}}$$

$$\Delta\widetilde{\mathbf{x}} = \mathbf{x}^*-\widetilde{\mathbf{x}}$$

and solve for

$$\widetilde{\mathbf{F}}(\mathbf{x}^*) = \overline{0}$$

The approximated operator equation can be rearranged as follows

$$\left[\frac{\partial F}{\partial x}\right]_{\mathbf{x}=\widetilde{\mathbf{x}}} [\Delta\widetilde{\mathbf{x}}] = -\mathbf{F}(\widetilde{\mathbf{x}})$$

$$(n \times n)\ matrix \times (n \times 1)\ vector = (n \times 1)\ vector$$

which corresponds to the standard form $\mathbf{Ax} = \mathbf{b}$. Solving the above linear equation yields $\Delta\widetilde{\mathbf{x}}$ and, if the guess solution $\widetilde{\mathbf{x}}$ is sufficiently close to true solution, then

$$\mathbf{x}^* \approx \widetilde{\mathbf{x}}+\Delta\widetilde{\mathbf{x}} \quad (82)$$

However, we may not reach the true solution in a single iteration. Thus, equation (82) is used to generate a new guess solution, say $\widetilde{\mathbf{x}}_{New}$, as follows

$$\widetilde{\mathbf{x}}_{New} = \widetilde{\mathbf{x}} + \Delta\widetilde{\mathbf{x}} \quad (83)$$

This process is continued till

$$\left\|\widetilde{\mathbf{F}}(\widetilde{\mathbf{x}}_{\mathbf{New}})\right\| < \varepsilon_1$$

or

$$\frac{\|\widetilde{\mathbf{x}}_{\mathbf{New}} - \widetilde{\mathbf{x}}\|}{\|\widetilde{\mathbf{x}}_{\mathbf{New}}\|} < \varepsilon_2$$

where tolerances ε_1 and ε_2 are some sufficiently small numbers. The above derivation indicates that the Newton's method is likely to converge only when the guess solution is *sufficiently close* to the true solution, $\mathbf{x}^*$, and the term $\mathbf{R}_2(\mathbf{x}^*, \mathbf{x}^*-\widetilde{\mathbf{x}})$ can be neglected.

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