Diffusion Equation with Finite Element Method TF4062

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1 Steady heat equation

Consider steady heat equation:

$$-k\frac{\mathrm{d}^2T}{\mathrm{d}x^2} = Q\tag{1}$$

for 0 < x < L and boundary conditions:

$$-k\frac{\mathrm{d}T}{\mathrm{d}x} = q \quad \text{at } x = 0 \tag{2}$$

and

$$T = T_L$$
 at $x = L$ (3)

The analytical solution to this problem can be expressed as [1]:

$$T(x) = T_L + \frac{q}{k}(L - x) + \frac{1}{k} \int_{-\infty}^{L} \left(\int_{0}^{y} Q(z) dz \right) dy \tag{4}$$

For constant Q, this equation reduces to

$$T(x) = T_L + \frac{q}{k}(L - x) + \frac{Q}{2k}(L^2 - x^2)$$
 (5)

1.1 Discretization and approximation

The FEM procedure start by discretizing the spatial domain into elements e_i where:

$$e_i: \{x_i \le x \le x_{i+1}\}, \quad i = 1, 2, \dots, n$$
 (6)

The points x_i are also called *nodes*. If we have n elements then we have n + 1 nodes (or nodal points). The solution to the PDE can be approximated as:

$$T(x) \approx \sum_{i}^{n+1} T_i N_i(x) \tag{7}$$

where T_i are (unknown) nodal values of T(x) and $N_i(x)$ are shape functions (also called *trial functions* or *basis functions*) associated with each node.

1.2 Linear shape functions

The shape functions are defined such that $N_i(x_i) = 1$ and $N_i(x_j) = 0$ if $j \neq i$. In FEM, they are usually chosen to be low order, piecewise polynomials. As an example, we will consider the case of one element, n = 1, or two nodes. The shape functions can be defined as:

$$N_1(x) = 1 - \frac{x}{L} \tag{8}$$

$$N_2(x) = \frac{x}{L} \tag{9}$$

An illustration of this case is shows in Figure 1.

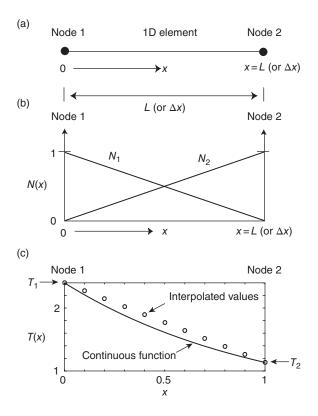


Figure 1: The case of one element with linear shape functions. (from [2])

For general case of linear elements we have the following shape functions. For left boundary points:

$$N_1(x) = \begin{cases} \frac{x_2 - x}{h_1} & x_1 \le x \le x_2 \\ 0 & \text{otherwise} \end{cases}$$
 (10)

For interior points:

$$N_{i}(x) = \begin{cases} \frac{x - x}{h_{i-1}} & x_{i-1} \le x \le x_{i} \\ \frac{x_{i+1} - x}{h_{i}} & x_{i} \le x \le x_{i+1}, \quad i = 2, 3, \dots, n \\ 0 & \text{otherwise} \end{cases}$$
 (11)

And for right boundary points:

$$N_{n+1}(x) = \begin{cases} \frac{x - x_n}{h_n} & x_n \le x \le x_{n+1} \\ 0 & \text{otherwise} \end{cases}$$
 (12)

where h_i are the spacings between nodal points.

$$h_i = x_{i+1} - x_i (13)$$

1.3 Weighted residuals

When we approximate the solution as ??ref??, in general, we cannot obtain the true solution to the differential equation. So, we will not get an exact equality but some *residual* associated with the error in the approximation. This residual can be defined as:

$$R(T,x) \equiv -k\frac{\mathrm{d}^2 T}{\mathrm{d}x^2} - Q \tag{14}$$

where T in the above equation is the approximation to the true solution T^* for which we have:

$$R(T^*, x) \equiv 0 \tag{15}$$

However, for any $T \neq T^*$, we cannot force the residual to vanish at every point x, no matter how small we make the grid or long the series expansion. The idea of the *weighted residuals method* is that we can multiply the residual by a *weighting function* and force the integral of the weighted expression to vanish:

$$\int_0^L w(x)R(T,x)\mathrm{d}x = 0 \tag{16}$$

where w(x) is the weighting function. Choosing different weighting functions and replacing each of them in ??ref??, we can then generate a system of linear equations in the unknown parameters T_i that will determine an approximation T of the form of the finite series given in Equation ??ref??. This will satisfy the differential equation in an "average" or "integral" sense. The type of weighting function chosen depends on the type of weighted residual technique selected. In the *Galerkin procedure*, the weights are set equal to the shape functions N_i , that is

$$w_i(x) = N_i(x) \tag{17}$$

So we have:

$$\int_0^L N_i \left[-k \frac{\mathrm{d}^2 T}{\mathrm{d}x^2} - Q \right] \, \mathrm{d}x = 0 \tag{18}$$

Since the temperature distribution must be a continuous function of x, the simplest way to approximate it would be to use piecewise polynomial interpolation over each element, in particular, piecewise linear approximation (by using linear shape functions as in ??ref??) provides the simplest approximation with a continuous function. Unfortunately, the first derivatives of such functions are not continuous at the elements' ends and, hence, second derivatives do not exist there; furthermore, the second derivative of \mathcal{T} would vanish inside each element. However, to require the second-order derivatives to exist everywhere is too restrictive. We can weaken this requirement by application of integration by parts to the second derivative:

$$\int_0^L N_i \left[-k \frac{\mathrm{d}^2 T}{\mathrm{d} x^2} \right] \, \mathrm{d} x = \int_0^L k \frac{\mathrm{d} N_i}{\mathrm{d} x} \frac{\mathrm{d} T}{\mathrm{d} x} \mathrm{d} x - \left[k N_i \frac{\mathrm{d} T}{\mathrm{d} x} \right]_0^L \tag{19}$$

Substituting the Equation ??ref?? to the integral term at the RHS:

$$\int_0^L k \frac{\mathrm{d}N_i}{\mathrm{d}x} \frac{\mathrm{d}}{\mathrm{d}x} \left(\sum_{j=1}^{n+1} T_j N_j \right) \mathrm{d}x = \int_0^L k \frac{\mathrm{d}N_i}{\mathrm{d}x} \left(\sum_{j=1}^{n+1} \frac{\mathrm{d}N_j}{\mathrm{d}x} T_j \right) \mathrm{d}x \tag{20}$$

$$= \int_0^L k \left(\sum_{j=1}^{n+1} \frac{\mathrm{d}N_i}{\mathrm{d}x} \frac{\mathrm{d}N_j}{\mathrm{d}x} T_j \right) \, \mathrm{d}x \tag{21}$$

The Equation ??ref?? can be rewritten as

$$\int_0^L k \left(\sum_{j=1}^{n+1} \frac{\mathrm{d} N_i}{\mathrm{d} x} \frac{\mathrm{d} N_j}{\mathrm{d} x} T_j \right) \, \mathrm{d} x - \int_0^L N_i Q \, \mathrm{d} x - \left[k N_i \frac{\mathrm{d} T}{\mathrm{d} x} \right]_0^L = 0 \tag{22}$$

for i = 1, 2, ..., n + 1. The quantities k, Q, N_i are known. The terms containing T_i can be isolated to the LHS and the known quantities can be moved to the RHS. This is a system of linear equations with T_i as the unknown variables. In matrix form:

$$Ku = f (23)$$

where K is a matrix arising from the integral terms, f are column vector whose elements arise from the integrals of source term and boundary terms, and \mathbf{u} is column vector of the unknown T_i . These linear equations can be solved by standard method such as Gaussian elimination and LU decomposition.

In practice, the integral in Equation ??ref?? can be calculated analytically or by numerical methods such as Gaussian quadrature. In the present case, the integral can be calculated analytically. The integral over all spatial domain can be divided into integrals over elements:

$$\int_0^L = \int_{x_1=0}^{x_2} + \int_{x_2}^{x_3} + \dots + \int_{x_n}^{x_{n+1}=L}$$
 (24)

For simplicity, let's consider two elements with equal spacing $h_1 = h_2$ with nodes

$$x_1 = 0, x_2 = L/2, x_3 = L$$
 (25)

The first integral is done over the first element. In the first element, only N_1 and N_2 contributes to the integrals because N_3 is zero in this interval. So the index i and j are limited to 1 and 2 only. This also applies to other elements.

These integrals can be written as a matrix:

$$\mathbf{K}^{e_1} = \int_0^{L/2} k \begin{bmatrix} \frac{\mathrm{d}N_1}{\mathrm{d}x} \frac{\mathrm{d}N_1}{\mathrm{d}x} & \frac{\mathrm{d}N_1}{\mathrm{d}x} \frac{\mathrm{d}N_2}{\mathrm{d}x} \\ \frac{\mathrm{d}N_2}{\mathrm{d}x} \frac{\mathrm{d}N_1}{\mathrm{d}x} & \frac{\mathrm{d}N_2}{\mathrm{d}x} \frac{\mathrm{d}N_2}{\mathrm{d}x} \end{bmatrix} \mathrm{d}x$$
 (26)

The needed integrals are:

$$\int_{0}^{L/2} \frac{dN_{1}}{dx} \frac{dN_{1}}{dx} dx = \int_{0}^{L/2} \left(-\frac{1}{h_{1}}\right) \left(-\frac{1}{h_{1}}\right) dx$$

$$= \int_{0}^{L/2} \frac{1}{(L/2)^{2}} dx$$

$$= \left[\frac{4}{L^{2}}x\right]_{0}^{L/2}$$

$$= \frac{2}{L}$$

and

$$\int_0^{L/2} \frac{\mathrm{d}N_1}{\mathrm{d}x} \frac{\mathrm{d}N_2}{\mathrm{d}x} \, \mathrm{d}x = \int_0^{L/2} \left(-\frac{1}{h_1} \right) \left(\frac{1}{h_1} \right) \, \mathrm{d}x$$
$$= -\frac{2}{L}$$

So the matrix elements can be written as

$$\mathbf{K}^{e_1} = \frac{k}{L/2} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \tag{27}$$

For more general case where $h_1 \neq h_2$, we obtain:

$$\mathbf{K}^{\mathbf{e}_1} = \frac{k}{h_1} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \tag{28}$$

Source term for the first element:

$$\mathbf{f}^{e_1,s} = \begin{bmatrix} f_1^{e_1,s} \\ f_2^{e_1,s} \end{bmatrix} \tag{29}$$

$$f_1^{e_1,s} = Q \int_0^{L/2} N_1(x) \, \mathrm{d}x = Q \int_0^{L/2} \left(1 - \frac{2x}{L} \right) \, \mathrm{d}x = Q \left[x - \frac{1}{L} x^2 \right]_0^{L/2} = Q \frac{L}{4} = Q \frac{h_1}{2}$$
 (30)

$$f_2^{e_1,s} = Q \int_0^{L/2} N_2(x) \, dx = Q \int_0^{L/2} \left(\frac{2x}{L}\right) \, dx = Q \left[\frac{1}{L}x^2\right]_0^{L/2} = Q \frac{L}{4} = Q \frac{h_1}{2}$$
 (31)

Boundary terms for the first element

$$\mathbf{f}^{e_1,b} = \begin{bmatrix} f_1^{e_1,b} \\ f_2^{e_1,b} \end{bmatrix} \tag{32}$$

By using boundary condition at x = 0 and using the fact that $N_1(x = 0) = 1$ and $N_1(x = L/2) = 0$:

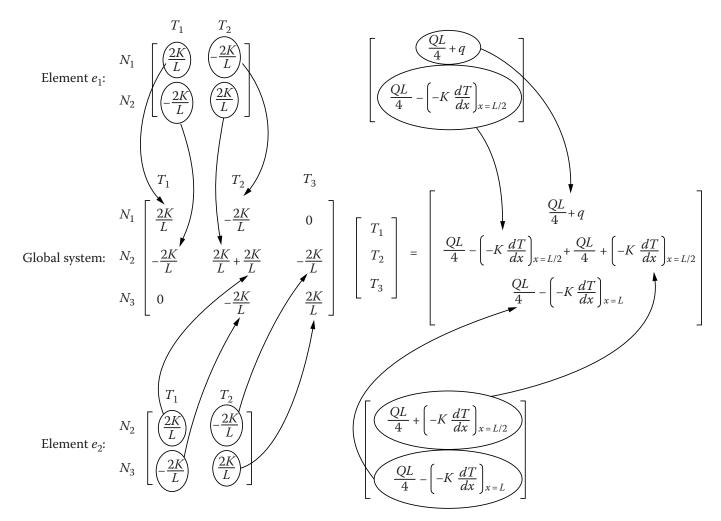
$$f_1^{e_1,b} = \left[N_1(x) \left(k \frac{dT}{dx} \right) \right]_0^{L/2} = N_1(L/2) \left(k \frac{dT}{dx} \right) \Big|_{x=L/2} - N_1(0) \left(k \frac{dT}{dx} \right) \Big|_{x=0} = q$$
 (33)

Meanwhile using using the fact that $N_2(x=0)=0$ and $N_2(x=L/2)=1$:

$$f_2^{e_1,b} = \left[N_2(x) \left(k \frac{\mathrm{d}T}{\mathrm{d}x} \right) \right]_0^{L/2} = N_2(L/2) \left(k \frac{\mathrm{d}T}{\mathrm{d}x} \right) \bigg|_{x=L/2} - N_2(0) \left(k \frac{\mathrm{d}T}{\mathrm{d}x} \right) \bigg|_{x=0} = \left(k \frac{\mathrm{d}T}{\mathrm{d}x} \right) \bigg|_{x=L/2}$$
(34)

Local stiffness matrix

The matrix \mathbf{K}^{e_2} associated with the second element also has similar form. The matrix \mathbf{K}^{e_2}



2 Time-dependent problem

Consider the unsteady heat PDE in one spatial dimension x:

$$\frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial t^2} + Q \tag{35}$$

where k is thermal diffusivity constant and Q is a constant heat source. The initial conditions is

$$T(x, t = 0) = 0, \qquad \forall x \in [0, L]$$
(36)

and the boundary conditions are

$$T(x = 0, t) = 0$$
 and $T(x = L, t) = 0$ (37)

3 Test

Test cite: [1]

Test code:

$$\alpha + \beta$$

References

- [1] Darrel W. Pepper and Juan C. Heinrich. *The Finite Element Method: Basic Concepts and Applications with MATLAB, MAPLE, and COMSOL*. CRC Press, Boca Raton, 3rd edition, 2017.
- [2] Guy Simpson. *Practical Finite Element Modeling in Earth Science using MATLAB*. Wiley Blackwell, Geneva, Switzerland, 2017.