2.1 The Diffusion Equation

The Part IB Methods course is relevant.

1 Background

The conduction of heat down a lagged bar of length L metres may be described by the one-dimensional diffusion equation

$$\frac{\partial \theta}{\partial t} = K \frac{\partial^2 \theta}{\partial x^2} \quad (0 < x < L)\,, \tag{1}$$

where $\theta(x,t)$ is the temperature (in kelvin) averaged over the cross-section (at distance x metres along the bar and time t seconds), and K is a positive constant, the so-called *thermal diffusivity* (measured in metres-squared per second). This description is obtained on the basis that

(i) there is negligible heat flux through the sides;

(ii) the heat flux (in the positive x-direction) through the cross section at x is $-A\,k\,\partial\theta/\partial x(x,t)$, where A is the (constant) cross-sectional area and k the (constant) thermal conductivity;

(iii) the total heat in $a < x < b$ is

$$A\int_a^b \sigma\rho\theta(x,t)\,\mathrm{d}x\,, \tag{2}$$

where σ is the (constant) specific heat and ρ the (constant) density, with its rate of change

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[A\int_a^b \sigma\rho\theta(x,t)\,\mathrm{d}x\right] = A\sigma\rho\int_a^b \frac{\partial\theta}{\partial t}(x,t)\,\mathrm{d}x \tag{3}$$

being equal to the net heat flux in

$$-Ak\frac{\partial\theta}{\partial x}(a,t) + Ak\frac{\partial\theta}{\partial x}(b,t) = Ak\int_a^b \frac{\partial^2\theta}{\partial x^2}(x,t)\,\mathrm{d}x \tag{4}$$

for any a and b, implying (1) with $K = k/\sigma\rho$.

2 Formulation

Suppose that for $t < 0$, the bar is at uniform temperature θ_0, and that for $t \geqslant 0$, the temperature of one end ($x = 0$) is suddenly altered to a different value θ_1 and thereafter maintained at this value, while the other end ($x = L$) is either insulated or maintained at constant temperature. Equation (1) is therefore to be solved for $t > 0$ subject to the initial condition

$$\theta(x,0) = \theta_0 \quad \text{for } 0 < x < L\,, \tag{5}$$

and to the boundary conditions

$$\theta(0,t) = \theta_1 \quad \text{for } t > 0\,, \tag{6}$$

and either

$$\frac{\partial\theta}{\partial x}(L,t) = 0 \quad \text{for } t > 0 \tag{7a}$$

(i.e. vanishing heat flux at the insulated end), or

$$\theta(L,t) = \theta_0 \quad \text{for } t > 0\,. \tag{7b}$$

The aim of this project is to study the performance of a simple finite-difference method on this problem, for which numerical solutions can be compared with an analytic one.

3 Analytic Solutions

Question 1 First consider the case of a semi-infinite bar, for which the boundary condition (7a) or (7b) is replaced by

$$\frac{\partial \theta}{\partial x}(x,t) \to 0 \quad \text{or} \quad \theta(x,t) \to \theta_0 \quad \text{as } x \to \infty, \text{ respectively.} \tag{8}$$

If

$$\theta(x,t) = \theta_0 + (\theta_1 - \theta_0)\, F\,(x,t) \ , \tag{9}$$

explain with the help of dimensional analysis why in both cases F must have the 'similarity' form

$$F(x,t) = f(\xi) \ , \quad \xi = \frac{x}{(Kt)^{1/2}} \, . \tag{10}$$

Show that in both cases

$$f\,(\xi) = \operatorname{erfc}\left(\tfrac{1}{2}\xi\right) \equiv \frac{2}{\sqrt{\pi}} \int_{\xi/2}^{\infty} \exp\left(-u^2\right)\, du \ . \tag{11}$$

Now return to the case of a finite bar and define non-dimensional variables X, T and U by

$$x = LX \ , \quad t = L^2 K^{-1} T \ , \quad \theta(x,t) = \theta_0 + (\theta_1 - \theta_0)\, U(X,T) \ , \tag{12}$$

in terms of which the diffusion equation (1) becomes

$$U_T = U_{XX} \quad \text{for } T > 0 \ , \quad 0 < X < 1 \ , \tag{13}$$

with initial condition

$$U(X,0) = 0 \quad \text{for } 0 < X < 1 \, , \tag{14}$$

and boundary conditions

$$U(0,T) = 1 \quad \text{for } T > 0 \, , \tag{15}$$

and either

$$U_X(1,T) = 0 \quad \text{for } T > 0 \, , \tag{16a}$$

or

$$U(1,T) = 0 \quad \text{for } T > 0. \tag{16b}$$

Question 2 First find an analytic solution of the fixed-endpoint-temperature problem (13)–(15) and (16b) in the form

$$U(X,T) = 1 - X + \sum_{n \geqslant 1} g_n(T) \sin\left(n\pi X\right) , \tag{17}$$

where the $g_n(T)$ are to be found. Adapt this method to obtain an (infinite-series) analytic solution of the insulated-end problem (13)–(16a) of the form

$$U(X,T) = U_s(X) + \sum_{n \geqslant 1} G_n(T) H_n(X) \, , \tag{18}$$

for suitable functions $U_s(X)$, $G_n(T)$ and $H_n(X)$.

Programming Task. Write a program to evaluate both analytic solutions by summing a finite number of terms of each series. Tabulate $U(X,T)$ for both problems at $T = 0.25$

and $X = 0.125\,n$, $n = 0, 1, \ldots, 8$, and also tabulate the semi-infinite solution (10)–(11) evaluated at these values of T and X.† Plot the non-dimensionalised temperature profiles, U, against X, for all three at $T = 0.05$, 0.1, 0.2, 0.5, 1.0 and 2.0. Also plot the non-dimensionalised heat flux $-U_X$ at $X = 0$ for all three against T over this range.

Explain why you are satisfied that enough terms have been kept in the truncated series to provide 'sufficiently' accurate solutions (at least for $T \geqslant 0.05$; take into account what accuracy will be needed for Question 3 below). Compare how the three sets of temperature profiles evolve in time, and discuss.

4 Numerical Integration

The insulated-end problem (13)–(16a) is now to be solved numerically as follows. Let the domain $0 \leqslant X \leqslant 1$ be divided into N intervals, each of length $\delta X = 1/N$, and let U_T be approximated by a first-order forward difference in time:

$$\frac{\partial U(X,T)}{\partial T} = \frac{U(X, T+\delta T) - U(X,T)}{\delta T} + O(\delta T) \ , \tag{19}$$

and U_{XX} by a second-order central difference in space at the current time:

$$\frac{\partial^2 U(X,T)}{\partial X^2} = \frac{U(X+\delta X, T) - 2U(X,T) + U(X-\delta X, T)}{(\delta X)^2} + O\left((\delta X)^2\right) \ , \tag{20}$$

giving the numerical scheme

$$U_n^{m+1} = U_n^m + C\left[U_{n+1}^m - 2U_n^m + U_{n-1}^m\right] , \tag{21}$$

where U_n^m is an approximation to $U(n\delta X, m\delta T)$ and $C = \delta T/(\delta X)^2$ (the so-called *Courant number*). The derivative boundary condition (16a) can be incorporated by solving (21) for $1 \leqslant n \leqslant N$ with $U_{N+1}^m = U_{N-1}^m$ for all $m \geqslant 0$; why? You should take $U_0^0 = 0.5$; why?

Question 3

Programming Task. Write a program to implement this numerical scheme, and run it with $N = 10$, 20, 40 and $C = \frac{1}{20}, \frac{1}{10}, \frac{1}{5}, \frac{1}{4}, \frac{1}{2}$ and 1. For the case $N = 10$, $C = \frac{1}{2}$,

(i) tabulate both the analytic and the numerical solutions, and the value of the error, at $T = 0.1$, 0.2, 0.5 and 1.0;

(ii) plot on the same graph both the analytic and the numerical solutions for $T = 0.05$, 0.1, 0.2, 0.5, 1.0 and 2.0.

Discuss both the stability and the accuracy of the numerical scheme for the different values of N and C. Are your results consistent with the theoretical order of accuracy of the scheme? Illustrate your discussion with appropriate short tables and/or graphs.

Reference

Ames, W.F. *Numerical Methods for Partial Differential Equations*, Academic Press.

† Note that there is a MATLAB function `erfc`.