2.1 The Diffusion Equation

IB Methods is relevant.

1 Background and Problem Formulation

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

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

where $\theta(x, t)$ is the temperature (in kelvin K) averaged over the cross-section A at distance x metres along the bar and time t seconds; κ is a positive constant, the so-called *thermal diffusivity* (measured in m² s⁻¹). 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 $-A k \partial \theta(x, t) / \partial x$ where A is the (constant) cross-sectional area and k the (constant) thermal conductivity, and

(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, 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 heat flux in across x = a less the heat flux out across x = b

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

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

Suppose that for t < 0, the bar is at a uniform temperature θ_0 , and that for $t \ge 0$, the temperature at one end (x = 0) experiences an increase proportional to time, while the other end (x = L) is either maintained at a constant temperature or insulated. 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

$$\theta(0,t) = \theta_0 + \alpha t \quad \text{for } t > 0, \tag{6}$$

where α is a positive constant (measured in K s⁻¹), and either

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

or

$$\frac{\partial \theta}{\partial x}(L,t) = 0$$
 for $t > 0$ (i.e. vanishing heat flux at the insulated end). (8)

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

2 Analytic solutions

Question 1 First consider the case of a semi-infinite bar, for which the boundary condition (7) or (8) is replaced by

$$\theta \to \theta_0 \quad \text{or} \quad \frac{\partial \theta}{\partial x}(x,t) \to 0 \quad \text{as } x \to \infty.$$
 (9)

Substitute

$$\theta(x,t) = \theta_0 + \alpha t F(x,t) , \qquad (10)$$

and explain with the help of dimensional analysis why in both cases F is a function only of the similarity variable

$$\xi = \frac{x}{\left(\kappa t\right)^{1/2}} \,, \tag{11}$$

and independent of θ_0 and α . Find the equation and boundary conditions satisfied in each case by the function $F(\xi)$, and show that in both cases the *unique* solution is

$$F(\xi) = \left(1 + \frac{1}{2}\xi^2\right) \operatorname{erfc}\left(\frac{1}{2}\xi\right) - \pi^{-1/2}\xi e^{-\xi^2/4}$$
(12)

where

$$\operatorname{erfc}(s) = \frac{2}{\sqrt{\pi}} \int_{s}^{\infty} e^{-u^2} \mathrm{d}u$$
 (13)

[This might be done by differentiating the equation twice and proceeding to *derive* the solution, or by finding a second independent solution of the equation, say as a series.^{*}]

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

$$x = LX$$
, $t = L^2 \kappa^{-1}T$, $\theta(x,t) = \theta_0 + \alpha L^2 \kappa^{-1} U(X,T)$, (14)

in terms of which the diffusion equation (1) becomes

$$U_T = U_{XX} \quad \text{for } T > 0 , \quad 0 < X < 1 ,$$
 (15)

with initial condition

$$U(X,0) = 0 \quad \text{for } 0 < X < 1 \tag{16}$$

and boundary conditions

$$U(0,T) = T \text{ for } T > 0$$
 (17)

and either

$$U(1,T) = 0 \quad \text{for } T > 0.$$
 (18)

or

$$U_X(1,T) = 0 \text{ for } T > 0$$
 (19)

^{*}N.B. An n^{th} -order ODE with (ostensibly) n boundary conditions may have a non-unique solution, or no solution at all: consider, for example, $d^2y/dx^2 + 3dy/dx + 2y = 0$ with y = 1 at $x = 0, y \to 0$ as $x \to \infty$, or $d^2y/dx^2 - 3dy/dx + 2y = 0$ with the same conditions.

Question 2 Find an analytic solution (as an infinite series) of the first problem (15)–(18) as follows. Ignoring the initial condition (16) for the time being, subtract off the simplest function which satisfies the boundary conditions (17) and (18),

$$U(X,T) = T(1-X) + V(X,T)$$
(20)

$$\Rightarrow \quad 1 - X + V_T = V_{XX} , \quad V(0,T) = 0 , \quad V(1,T) = 0 , \qquad (21)$$

and noting that there is a particular solution with V independent of T, subtract that off,

$$V(X,T) = -\frac{1}{3}X + \frac{1}{2}X^2 - \frac{1}{6}X^3 + W(X,T) , \qquad (22)$$

to obtain the *homogeneous* problem

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$$W_T = W_{XX}$$
, $W(0,T) = 0$, $W(1,T) = 0$ (23)

which has separable solutions for W. Now construct a superposition of these separable solutions which satisfies the initial condition (16). Show that

$$W(X,T) \sim \frac{2}{\pi^3} \sin\left(\pi X\right) e^{-\pi^2 T} \quad \text{as } T \to \infty.$$
(24)

Adapt this method to obtain an (infinite-series) analytic solution of the second problem (15)-(17) and (19).

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 = 0.25and X = 0.125n, $n = 0, 1, \ldots, 8$ and also tabulate the semi-infinite solution (11)–(12) evaluated at these T- and X-values [note that there is a MATLAB function erfc]. Plot the non-dimensionalised temperature profiles, U against X, for all three at T = 0.03125, 0.125, 0.25, 0.375, 0.75 and 1.5; also plot the non-dimensionalised heat flux $-\partial U/\partial X$ 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 $T \ge 0.03125$; 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.

3 Numerical Integration

The first problem (15)–(18) is now to be solved numerically as follows. Let the domain $0 \leq X \leq 1$ be divided into N intervals, each of length $\delta X = 1/N$, and let U_T be approximated by a forward difference in time:

$$\frac{\partial U(X,T)}{\partial T} = \frac{U(X,T+\delta T) - U(X,T)}{\delta T} + O\left(\delta T\right) , \qquad (25)$$

and U_{XX} by a centred difference in space at the current time:

$$\frac{\partial^2 U(X,T)}{\partial X^2} = \frac{U(X+\delta X,T) - 2U(X,T) + U(X-\delta X,T)}{\left(\delta X\right)^2} + O\left(\left(\delta X\right)^2\right) , \qquad (26)$$

giving the numerical scheme

$$U_n^{m+1} = U_n^m + C \left[U_{n+1}^m - 2U_n^m + U_{n-1}^m \right],$$
(27)

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).

Question 3

Programming Task: Write a program to implement this numerical scheme, and run it with N = 4, 8, 16, 32 and $C = \frac{2}{3}, \frac{1}{2}, \frac{1}{3}, \frac{1}{6}$ and $\frac{1}{12}$. For the case $N = 4, C = \frac{1}{2}$, tabulate both the analytic and the numerical solutions, and the value of the error, at T = 0.125, 0.25 and 0.375.

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

Reference

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