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

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

(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 $-AK \frac{\partial \theta}{\partial x}(x, t)$, where $A$ is the (constant) cross-sectional area and $k$ the (constant) thermal conductivity;

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

$$A \int_a^b \sigma \rho \theta(x, t) \, dx,$$

(2)

where $\sigma$ is the (constant) specific heat and $\rho$ the (constant) density, with its rate of change

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

(3)

being equal to the net heat flux in

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

(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 $\theta_0$, and that for $t \geq 0$, the temperature of one end ($x = 0$) is suddenly altered to a different value $\theta_1$ 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

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

(5)

and to the boundary conditions

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

(6)

and either

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

(7a)

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

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

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

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

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
\[
U_T = U_{XX} \quad \text{for} \quad T > 0 , \quad 0 < X < 1 , \tag{13}
\]
with initial condition
\[
U(X,0) = 0 \quad \text{for} \quad 0 < X < 1 , \tag{14}
\]
and boundary conditions
\[
U(0,T) = 1 \quad \text{for} \quad T > 0 , \tag{15}
\]
and either
\[
U_X(1,T) = 0 \quad \text{for} \quad T > 0 , \tag{16a}
\]
or
\[
U(1,T) = 0 \quad \text{for} \quad T > 0. \tag{16b}
\]

**Question 2**  
First find an analytic solution of the fixed-endpoint-temperature problem (13)–(15) and (16b) in the form
\[
U(X,T) = 1 - X + \sum_{n \geq 1} g_n(T) \sin(n\pi X) , \tag{17}
\]
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
\[
U(X,T) = U_s(X) + \sum_{n \geq 1} G_n(T) H_n(X) , \tag{18}
\]
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 \( X = 0.125n, n = 0, 1, \ldots, 8 \), 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 \( T = 0.0625, 0.125, 0.25, 0.5, 1.0 \) 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 \( T \geq 0.0625 \); 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 \( 0 \leq X \leq 1 \) 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:

\[
\frac{\partial U(X,T)}{\partial T} = \frac{U(X,T+\delta T) - U(X,T)}{\delta T} + O(\delta T),
\]

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

\[
\frac{\partial^2 U(X,T)}{\partial X^2} = \frac{U(X+\delta X,T) - 2U(X,T) + U(X-\delta X,T)}{(\delta X)^2} + O((\delta X)^2),
\]

giving the numerical scheme

\[
U^{m+1}_n = U^n_m + C [U^n_{m+1} - 2U^n_m + U^n_{m-1}],
\]

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 \( 1 \leq n \leq N \) with \( U^n_N+1 = U^n_N \) for all \( m \geq 0 \); why? You should take \( U^n_0 = 0 \); why?

**Question 3**

**Programming Task.** Write a program to implement this numerical scheme, and run it with \( N = 8, 16, 32 \) and \( C = \frac{1}{12}, \frac{1}{6}, \frac{1}{3}, \frac{1}{2} \) and \( \frac{2}{3} \). For the case \( N = 8, C = \frac{1}{2} \):

(i) tabulate both the analytic and the numerical solutions, and the value of the error, at \( T = 0.125, 0.25, 0.5 \) and 1.0;

(ii) plot on the same graph both the analytic and the numerical solutions for \( T = 0.0625, 0.125, 0.25, 0.5, 1.0 \) 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**


\[\text{†} \text{ Note that there is a MATLAB function erfc.}\]