2.3 The Diffusion Equation

2 Analytic solution

Question 1: Performing dimensional analysis:

$[\theta] = (Temperature); [x] = (Length); [t] = (Time); [\lambda] = \frac{(Length)^2}{(Time)}; [k] = \frac{(Temperature)}{(Time)}$

Eliminating length:

$[\theta] = (Temperature); [t] = (Time); \left[\frac{\lambda}{x^2}\right] = \frac{1}{(Time)}; [k] = \frac{(Temperature)}{(Time)}$

Eliminating temperature:

$[t] = (Time); \left[\frac{\lambda}{x^2}\right] = \frac{1}{(Time)}; \left[\frac{k}{\theta}\right] = \frac{1}{(Time)}$.

Eliminating time it is found that $\frac{x}{\sqrt{\lambda t}}$ and $\frac{\theta}{kt}$ are dimensionless. Thus $(\exists F)\ \frac{\theta}{kt} = F\left(\frac{x}{\sqrt{\lambda t}}\right)$, where F is independent of k by construction. Since physical laws are independent of system of measurement it is possible to change the origin of the variable θ so that $\theta - \theta_0 = ktF\frac{x}{\sqrt{\lambda t}}$, and make F independent of θ_0.

Now substituting

$\theta(x,t) = \theta_0 + ktF(\xi)$

$\theta_t = kF(\xi) + ktF'(\xi)\left(\frac{-x}{2\lambda^{\frac{1}{2}}t^{\frac{3}{2}}}\right)$

$\theta_{xx} = \frac{k}{\lambda}F''(\xi)$

By the Diffusion Equation:

$F''(\xi) + \frac{1}{2}\xi F'(\xi) - F(\xi) = 0$. Differentiating this twice:

$F^{(4)}(\xi) + \frac{1}{2}\xi F'''(\xi) = 0 \Rightarrow F'''(\xi) = Ae^{-\frac{\xi^2}{4}}$.

$F''(\xi) = A\int_0^\xi e^{-\frac{a^2}{4}}da.$

$F'(\xi) = A\xi\int_0^\xi e^{-\frac{a^2}{4}}da + 2Ae^{-\frac{\xi^2}{4}}$

$F(\xi) = A\left[\left(1+\frac{\xi^2}{2}\right)\left(\int_0^\xi e^{-\frac{a^2}{4}}da\right) + \xi e^{-\frac{\xi^2}{4}}\right] + c$

$= A\left[\xi e^{-\frac{\xi^2}{4}} - \left(1+\frac{\xi^2}{2}\right)\int_\xi^\infty e^{-\frac{a^2}{4}}da\right] + A\int_0^\infty e^{-\frac{a^2}{4}}da + c$

$= A\left[\xi e^{-\frac{\xi^2}{4}} - \left(1+\frac{\xi^2}{2}\right)\int_\xi^\infty e^{-\frac{a^2}{4}}da\right] + A\sqrt{\pi} + c$

Now use the boundary conditions.

$\theta(x,t) \to \theta_0$ as $x \to \infty$ means that $F \to 0$ as $\xi \to \infty$. Thus $c = -A\sqrt{\pi}$.

Also, $\theta(0,t) = \theta_0 + kt \Rightarrow F(0) = 1$ so $1 = A\left(-\int_0^\infty e^{-\frac{a^2}{4}}da\right) \Rightarrow A = \frac{-1}{\sqrt{\pi}}$. That is:

$F(\xi) = \frac{1}{\sqrt{\pi}}\left[\left(1+\frac{1}{2}\xi^2\right)\int_\xi^\infty e^{-\frac{a^2}{4}}da - \xi e^{-\frac{\xi^2}{4}}\right].$

Question 2: $U(X,T) = T(1-X) + V(X,T) \Rightarrow$

$U_T = 1 - X + V_T$

$U_{XX} = V_{XX}$

By the Diffusion Equation: $U_T = 1 - X + V_T = V_{XX} = U_{XX}$. Now let $V = \sum_{n=1}^\infty q_n(T)\,sin(n\pi x)$. Expanding $1-X$ also: $1 - X = \sum_{n=1}^\infty Q_n(T)\,sin(n\pi X) \Rightarrow \frac{1}{2}Q_n(T) = \int_0^1(1-X)\,sin(n\pi X)\,dX = \frac{1}{n\pi}$.

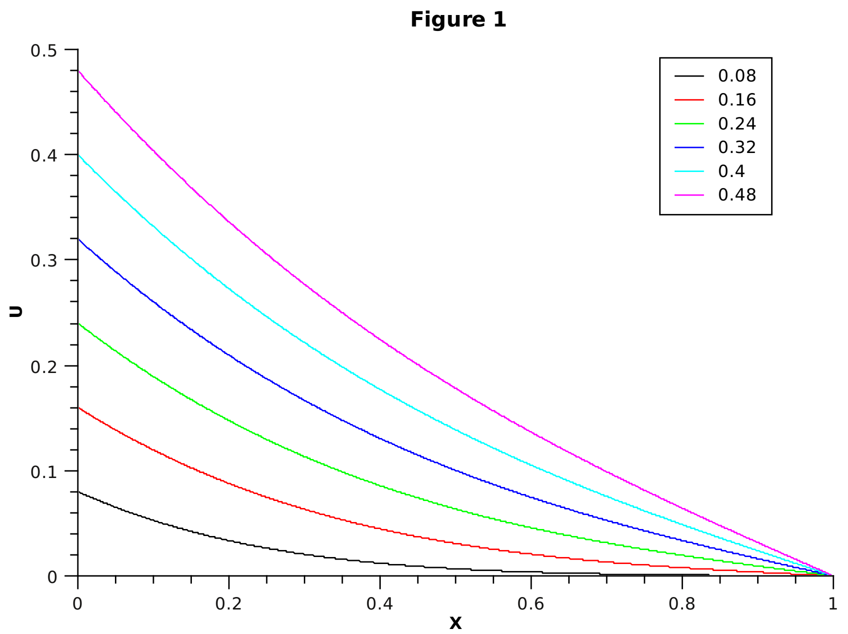
So: $(\forall X)\sum_{n=1}^\infty\left(\frac{2}{n\pi} + \dot{q}(T) + n^2\pi^2q_n(T)\right)sin(n\pi X) = 0.$

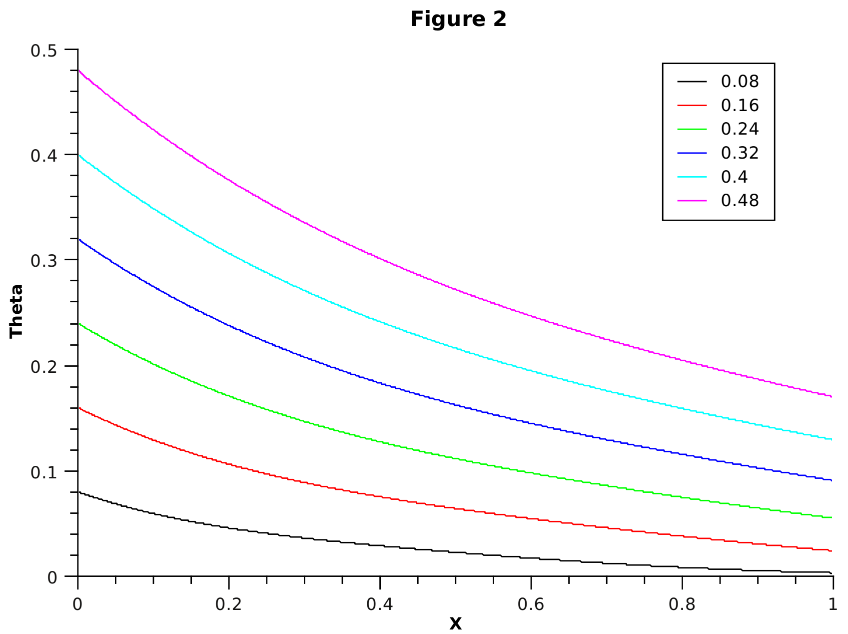
That is $\frac{2}{n\pi} + \dot{q}(T) + n^2\pi^2q_n(T) = 0$. Solving gives: $q_n(T) = \frac{-2}{n^3\pi^3} + c_ne^{-n^2\pi^2T}$. So $V = \sum_{n=1}^\infty\left(\frac{-2}{n^3\pi^3}\right)sin(n\pi X) + \sum_{n=1}^\infty c_ne^{-n^2\pi^2T}sin(n\pi X)$. Using the condition $U(X,0) = 0$, $c_n = \frac{2}{n^3\pi^3}$. So as $T \to \infty$, $V \to \sum_{n=1}^\infty\left(\frac{-2}{n^3\pi^3}sin(n\pi X)\right)$. It remains to show that this is equal to $\frac{-1}{3}X + \frac{1}{2}X^2 - \frac{1}{6}X^3$.

$2\int_0^1\left(\frac{-1}{3}X + \frac{1}{2}X^2 - \frac{1}{6}X^3\right)sin(n\pi X)$

$$= 2\left[\left(\frac{-1}{3}X + \frac{1}{2}X^2 - \frac{1}{6}X^3\right)\left(\frac{-1}{n\pi}\right) cos\left(n\pi X\right)\right]_0^1 - 2\int_0^1 \left(\frac{-1}{3} + X - \frac{1}{2}X^2\right)\left(\frac{-1}{n\pi} cos(n\pi X\right) dX$$
$$= -2\left[\left(\frac{-1}{3} + X - \frac{1}{2}X^2\right)\left(\frac{-1}{n^2\pi^2}\right) sin\left(n\pi X\right)\right]_0^1 + 2\int_0^1 (1-X)\left(\frac{-1}{n^2\pi^2}\right) sin\left(n\pi X\right) dX$$
$$= 2\left[(1-X)\left(\frac{1}{n^3\pi^3}\right) cos\left(n\pi X\right)\right]_0^1 = \left(\frac{-2}{n^3\pi^3}\right).$$

Programming Task 1: The source and header files are in Appendix B (files _____). The full printouts are in Appendix A (printouts _____). The output of my program is six decimal places. Firstly, $\frac{1}{10}e^{-n^2\pi^2 T} > e^{-(n+1)^2\pi^2 T} \iff n > \frac{log(\frac{1}{10})+1}{2} = 0.65(2d.p.)$. Secondly, $e^{-n^2\pi^2 T} < 0.0000001 \iff n^2 > 7\frac{log(10)}{\pi^2 T}$. In the worst case, $T = 0.08$, so $n > 4.52(2d.p.)$. So if $n = 5$, then my answers will be accurate to six decimal places. Figure 1 shows U against X at various values of T (the case of the finite bar). Figure 2 shows θ against X for the same values of T. In this latter case (of the semi-infinite bar) I chose $\theta_0 = 0$ and $k = 1$ so that the initial conditions (apart from (4)) are the same.





The behaviour is similar in that the temperature decreases as X increases. Also, in both cases, the temperature decreases more rapidly (at a given value of X) for larger values of T. The difference is that (for a given value of T) in the case of the finite bar, the temperature decreases more rapidly as X increases and at X=1, the temperature is 0 at any time. In the case of the semi-infinite bar, the temperature is strictly positive at all time greater than 0, with larger values of T having the higher temperatures.

Question 3: The source and header files are in Appendix B (files ___). Using the Taylor expansion:

$\frac{U(X,T+\delta T)-U(X,T)}{\delta T} = \frac{\partial U}{\partial T} + \frac{\delta T}{2!}\frac{\partial^2 U}{\partial T^2} + \frac{(\delta T)^2}{3!}\frac{\partial^3 U}{\partial T^3} + ...$

$\frac{U(X+\delta X,T)-2U(X,T)+U(X-\delta X,T)}{(\delta X)^2} = \frac{\partial^2 U}{\partial X^2} + \frac{(\delta X)^2}{12}\frac{\partial^4 U}{\partial X^4} + \frac{(\delta X)^4}{360}\frac{\partial^6 U}{\partial X^6} + ...$

If sufficient differentiability is assumed, then $\frac{\partial^n U}{\partial T^n} = \frac{\partial^{2n} U}{\partial X^{2n}}$. So the discretization error is:

$Error = \left(\frac{\delta T}{2!}\frac{\partial^2 U}{\partial T^2} - \frac{(\delta X)^2}{12}\frac{\partial^4 U}{\partial X^4}\right) + \left(\frac{(\delta T)^2}{3!}\frac{\partial^3 U}{\partial T^3} - \frac{(\delta X)^4}{360}\frac{\partial^6 U}{\partial X^6}\right) + ... = \frac{\partial^4 U}{\partial X^4}(\delta X)^2\left(\frac{\nu}{2!} - \frac{1}{12}\right) + \frac{\partial^6 U}{\partial X^6}(\delta X)^4\left(\frac{\nu^2}{3!} - \frac{1}{360}\right) + ...$

So the order of the error is $\mathcal{O}\left((\delta X)^2\right)$, unless $\nu = \frac{1}{6}$, when it is $\mathcal{O}\left((\delta X)^4\right)$.

For the case $N = 5$ and $\nu = \frac{1}{2}$, the tables of the analytic and numerical solutions and the value of the error at the specified values of T are in Appendix A (printouts _____). Now I will investigate the theoretical stability of the method.

Let ξ be a constant (independent of m and n) defined by $U_n^{m+1} = \xi U_n^m$. i.e. $U_i^m = \xi^m U_i^0$. Now express U_i^0 in a complex Fourier series: $U_i^0 = \sum_{k=0}^{N} A_k e^{ik\pi\left(\frac{n}{N}\right)}$. Since the finite difference equation is linear, it is only neccessary to consider a general term of this. It is seen that there is stability if and only if $|\xi| \leq 1$. For the scheme in equation (11),

$e^{ik\pi\left(\frac{n}{N}\right)}\xi^{m+1} = e^{ik\pi\left(\frac{n}{N}\right)}\xi^m + \nu\left(e^{ik\pi\left(\frac{n-1}{N}\right)}\xi^m - 2e^{ik\pi\left(\frac{n}{N}\right)}\xi^m + e^{ik\pi\left(\frac{n+1}{N}\right)}\xi^m\right)$

$\xi = 1 + \nu\left(e^{-\frac{ik\pi}{N}} - 2 + e^{\frac{ik\pi}{N}}\right) = 1 + \nu\left(2cos\left(\frac{k\pi}{N}\right) - 2\right) = -4\nu sin^2\left(\frac{k\pi}{2N}\right)$. So the condition for stability is:

$|\xi| = \left|1 - 4\nu sin^2\left(\frac{k\pi}{2N}\right)\right| \leq 1$. Since $\nu > 0$, $1 - 4\nu sin^2\left(\frac{k\pi}{2N}\right) \leq 1$ for all ν. So:

$1 - 4\nu sin^2\left(\frac{k\pi}{2N}\right) \geq -1 \Rightarrow \nu \leq \frac{1}{2sin^2\left(\frac{k\pi}{2N}\right)}$. Now, the summation is over $k = 0, 1...N$, so $\nu \leq \frac{1}{2}$ is the condition for stability. The tables of the analytic and numerical solutions and the value of the error at $\nu = \frac{1}{2}$ and $\nu = \frac{2}{3}$ illustrate this. I have chosen $N = 10$ and $T = 0.48$ for this comparison, as it gives concise clear results. For $\nu = \frac{1}{2}$:

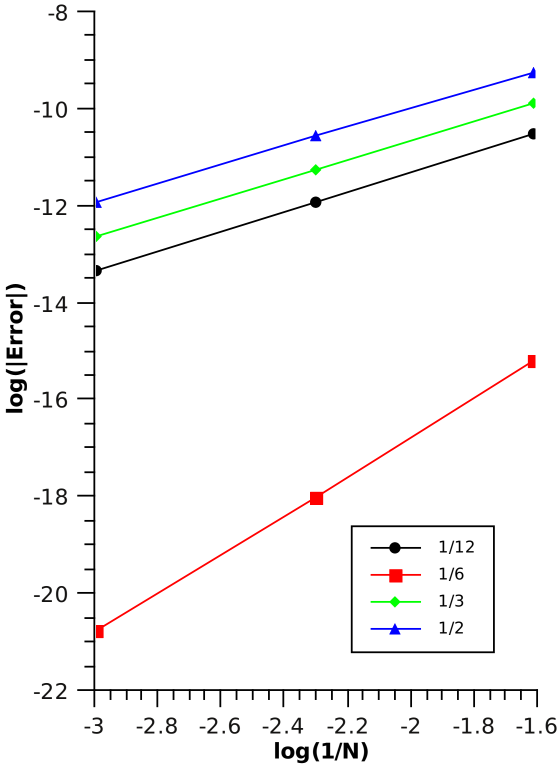
X	U	Analytic	Error
0.000000	0.480000	0.480000	-0.000000
0.100000	0.403661	0.403675	0.000013
0.200000	0.336306	0.336332	0.000026
0.300000	0.276922	0.276957	0.000035
0.400000	0.224496	0.224537	0.000042
0.500000	0.178022	0.178065	0.000043
0.600000	0.136496	0.136537	0.000042
0.700000	0.098922	0.098957	0.000035
0.800000	0.064306	0.064332	0.000026
0.900000	0.031661	0.031675	0.000013
1.000000	0.000000	0.000000	0.000000

For $\nu = \frac{2}{3}$:

X	U	Analytic	Error
0.000000	0.480000	0.480000	0.000000
0.100000	6649117093.816221	0.403675	-6649117093.412546
0.200000	-12646450638.164291	0.336332	12646450638.500624
0.300000	17404370237.482307	0.276957	-17404370237.205349
0.400000	-20457137568.822617	0.224537	20457137569.047153
0.500000	21506496102.922276	0.178065	-21506496102.744209
0.600000	-20450648953.536060	0.136537	20450648953.672596
0.700000	17393871437.088352	0.098957	-17393871436.989395
0.800000	-12635951838.220335	0.064332	12635951838.284668
0.900000	6642628478.069665	0.031675	-6642628478.037991
1.000000	0.000000	0.000000	0.000000

Figure 3 is the plot of $log\left(|Error|\right)$ against $log\left(\frac{1}{N}\right)$ for each of the different values of ν. Again, I chose $T = 0.48$.

Figure 3



Where the gradients of the lines are the orders of the methods (GIVE SIMILAR PROOF TO BEFORE...). Modelling the graphs in Figure 3 as straight lines, the gradient (measured between the two extreme data points) of the lines representing $\nu = \frac{1}{12}$, $\frac{1}{3}$ and $\frac{1}{2}$ are 2.03(2d.p.), 1.99(2d.p.) and 1.94(2d.p.) respectively. The gradient of the line representing $\nu = \frac{1}{6}$ is 4.03(2d.p.). Thus my results are consistent with the theoretical orders of accuracy of the scheme.