

Additional Project 2.1: The Diffusion Equation

Question 1

Rearranging the equation for $F(x,t)$:

$$F(x,t) = \frac{\theta(x,t) - \theta_0}{\theta_1 - \theta_0}$$

The RHS is a dimensionless quantity, hence F is dimensionless, for all x,t . Hence F must be a function of some dimensionless variables. The problem contains 3 variables; K , x , and t , with $[K] = L^2 T^{-1}$, $[x] = L$, $[t] = T$. Since we can only add quantities of the same dimension, the simplest relation we can have between variables is a power law. Letting $x^a t^b K^c$ be dimensionless, we find any dimensionless variable is some power of $\varepsilon = \frac{x}{\sqrt{Kt}}$, so we have $F(x,t) = f(\varepsilon)$ generally.

$$\theta_t = K\theta_{xx} \quad \text{and} \quad \theta(x,t) = \theta_0 + (\theta_1 - \theta_0)F(x,t)$$

imply

$$F_t = KF_{xx}$$

and we have new boundary conditions

$$F(x,0) = 0, \quad F(0,t) = 1 \quad \text{for } t > 0$$

and, as $x \rightarrow \infty$, either

$$(a) \quad \frac{\partial F}{\partial x}(x,t) \rightarrow 0 \quad \text{or} \quad (b) \quad F(x,t) \rightarrow 0$$

Now

$$\frac{\partial F}{\partial t} = \frac{df}{d\varepsilon} \frac{\partial \varepsilon}{\partial t} = \frac{df}{d\varepsilon} \frac{(-x)}{2K^{1/2}t^{3/2}} \quad \text{and similarly} \quad \frac{\partial F}{\partial x} = \frac{df}{d\varepsilon} \frac{1}{\sqrt{Kt}} \quad \text{and} \quad \frac{\partial^2 F}{\partial x^2} = \frac{d^2 f}{d\varepsilon^2} \frac{1}{Kt} \quad (*)$$

giving

$$\left(\frac{-\varepsilon}{2}\right) \frac{df}{d\varepsilon} = \frac{d^2 f}{d\varepsilon^2}$$

Integrating we get

$$\frac{df}{d\varepsilon} = C_1 \exp\left(-\frac{\varepsilon^2}{4}\right)$$

and by FTC we get

$$f(\varepsilon) = C_2 \int_{\varepsilon/2}^{\infty} \exp(-u^2) du + C_3$$

$F(x,0) = 0 \Rightarrow f(\varepsilon) \rightarrow 0$ as $\varepsilon \rightarrow \infty$ giving $C_3 = 0$. $F(0,t) = 1$ for $t > 0 \Rightarrow f(0) = 1 \Rightarrow C_2 = \frac{2}{\sqrt{\pi}}$. Hence

$$f(\varepsilon) = \frac{2}{\sqrt{\pi}} \int_{\varepsilon/2}^{\infty} \exp(-u^2) du = \text{erfc}(\varepsilon/2)$$

as required. Note we did not use conditions (a) or (b), but the solution satisfies both (a) and (b) by (*), as $x \rightarrow \infty \Rightarrow \varepsilon \rightarrow \infty$

Question 2

i) First consider the fixed-endpoint temperature problem. Write $\hat{U}(X,T) = U(X,T) - U_s(X)$, where $U_s(X)$ is the steady state solution $1 - X$, to convert the problem into one with homogeneous boundary conditions. We get

$$\begin{aligned} \hat{U}_T &= \hat{U}_{XX} \\ \hat{U}(0,T) &= 0 \quad \text{for } T > 0 \\ \hat{U}(1,T) &= 0 \quad \text{for } T > 0 \\ \hat{U}(X,0) &= X - 1 \end{aligned} \quad (**)$$

Now separate variables. Write $\hat{U}(X,T) = A(X)B(T)$. Plugging into the ODE, we get

$$\frac{\dot{B}}{B} = \frac{A''}{A}$$

where the LHS is a function only of T, and the RHS of only X, hence equal to a negative constant $-\lambda$ (the negative is required, else impossible for A(1) to be 0 below). Thus

$$A(X) = C_1 \sin(\sqrt{\lambda}X) + C_2 \cos(\sqrt{\lambda}X)$$

Using the boundary conditions, $A(0) = 0 \Rightarrow C_2 = 0$. Also $A(1) = 0 \Rightarrow \sin(\sqrt{\lambda}) = 0 \Rightarrow \lambda = n^2\pi^2$ for some $n \in \mathbb{N}$. This gives

$$A_n(X) = \sin(n\pi X) \quad \text{and} \quad B_n(T) = e^{-n^2\pi^2 T}$$

So the general solution is,

$$\hat{U}(X, T) = \sum_{n \geq 1} c_n \sin(n\pi X) e^{-n^2\pi^2 T}$$

We use the T=0 condition, along with orthogonality of eigenfunctions to calculate the $c_n = -\frac{2}{\pi n}$. Thus

$$U_{fixed}(X, T) = 1 - X - \frac{2}{\pi} \sum_{n \geq 1} \frac{1}{n} \sin(n\pi X) e^{-n^2\pi^2 T}$$

ii) For the insulated end problem, we proceed as above, but set our steady state solution to $U_s(X) = 1$, giving

$$\begin{aligned} \hat{U}_T &= \hat{U}_{XX} \\ \hat{U}(0, T) &= 0 \quad \text{for } T > 0 \\ \hat{U}(X, 0) &= -1 \quad \text{for } 0 < X < 1 \\ \hat{U}_X(1, T) &= 0 \end{aligned}$$

Following the same method, we get

$$A(X) = C_1 \sin(\sqrt{\lambda}X) + C_2 \cos(\sqrt{\lambda}X)$$

Using the boundary conditions, $A(0) = 0 \Rightarrow C_2 = 0$. Also $A_X(1) = 0 \Rightarrow \cos(\sqrt{\lambda}) = 0 \Rightarrow \lambda = (n + 1/2)^2\pi^2$ for $n = 0, 1, 2, 3, \dots$. Thus get

$$A_n(X) = \sin((n + 1/2)\pi X) \quad \text{and} \quad B_n(T) = e^{-(n+1/2)^2\pi^2 T}$$

and general solution

$$\hat{U}(X, T) = \sum_{n \geq 0} c_n \sin((n + \frac{1}{2})\pi X) e^{-(n+1/2)^2\pi^2 T}$$

and again, using the T=0 condition and orthogonality gives $c_n = -\frac{2}{\pi(n+1/2)}$. So have, rewriting from n=1,

$$U_{insulated}(X, T) = 1 - \frac{2}{\pi} \sum_{n \geq 1} \frac{1}{n - 1/2} \sin((n - \frac{1}{2})\pi X) e^{-(n-1/2)^2\pi^2 T}$$

Programming Task

The script *evaluateanalytic*, found on page 11 evaluates the analytic solutions U_{fixed} and $U_{insulated}$, up to n=25. We do the same for the derivatives in *evaluateanalyticflux.m* (see page 12). This should be sufficient, since the error E_{fixed} very crudely satisfies

$$\begin{aligned}
|E_{fixed}| &= \left| \sum_{n \geq 26} \frac{1}{n} \sin(n\pi X) e^{-n^2 \pi^2 T} \right| \\
&\leq \sum_{n \geq 26} \left| \frac{1}{n} \sin(n\pi X) e^{-n^2 \pi^2 T} \right| \\
&\leq \sum_{n \geq 26} e^{-n^2 \pi^2 T} \\
&\leq \sum_{n \geq 26} e^{-n \pi^2 T} \\
&= e^{-26 \pi^2 T} \frac{1}{1 - e^{-\pi^2 T}} \\
&\leq 2.36 \times 10^{-7} \quad \text{for } T \geq 0.0625
\end{aligned}$$

Similarly, we get the same bound for $E_{insulated}$, and for the derivatives. This error should be sufficiently small, since we are considering a function varying between 0 and 1. We will confirm whether this accuracy is suitable when doing Q3.

```
>> evaluateanalytic.m %with T=0.25
```

X	U_{fixed}	$U_{insulated}$	$U_{semi-inf}$
0.000	1.000	1.000	1.000
0.125	0.854	0.865	0.860
0.250	0.712	0.736	0.724
0.375	0.575	0.617	0.596
0.500	0.446	0.513	0.480
0.625	0.325	0.428	0.377
0.750	0.212	0.366	0.289
0.875	0.104	0.327	0.216
1.000	-6.61E-18	0.315	0.157

Table 1: Analytical Solutions at T=0.25

```
>> evaluateanalyticflux
```

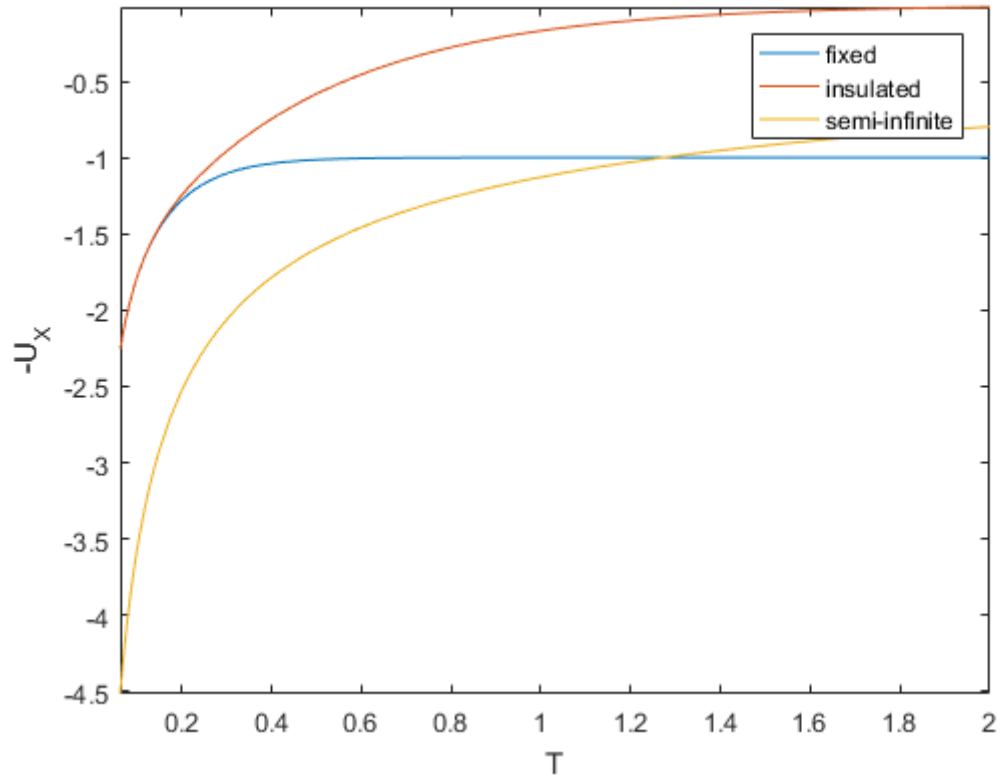


Figure 1: Flux at $X = 0$

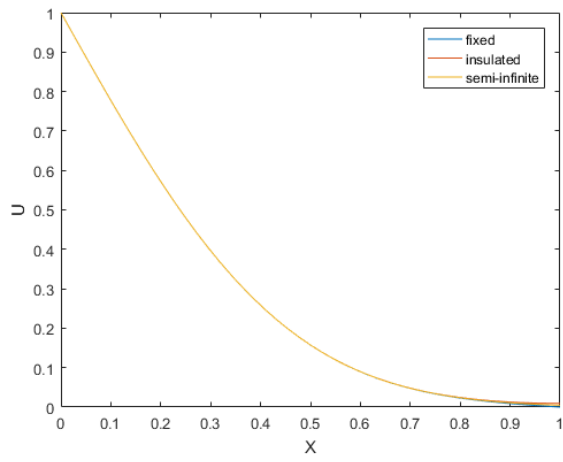


Figure 2: Output of with $T = 0.0625$

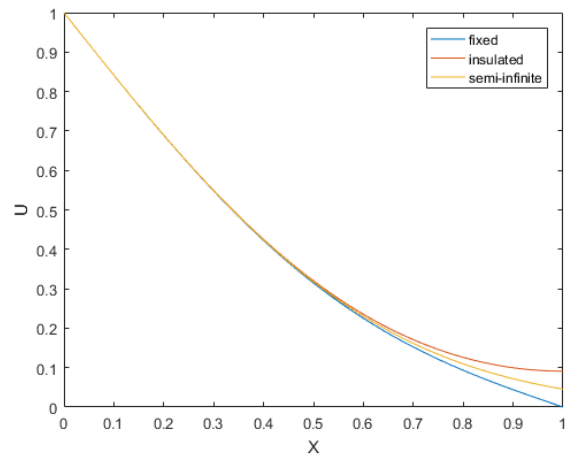


Figure 3: Output with $T = 0.125$

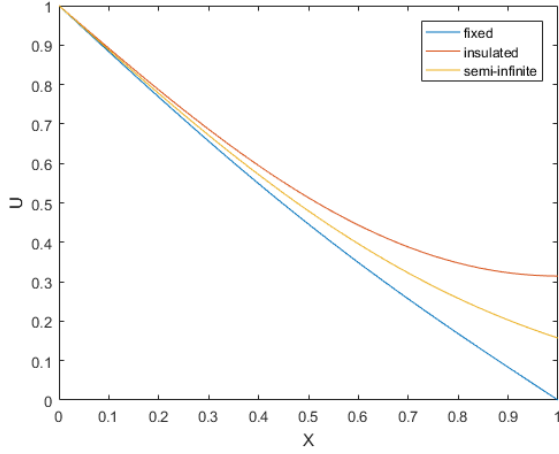


Figure 4: Output with $T = 0.25$

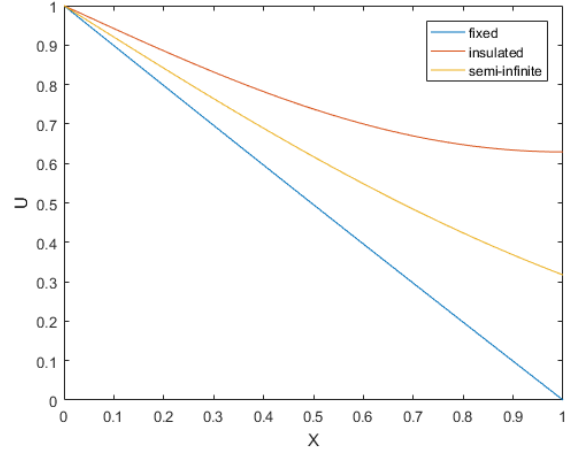


Figure 5: Output with $T = 0.5$

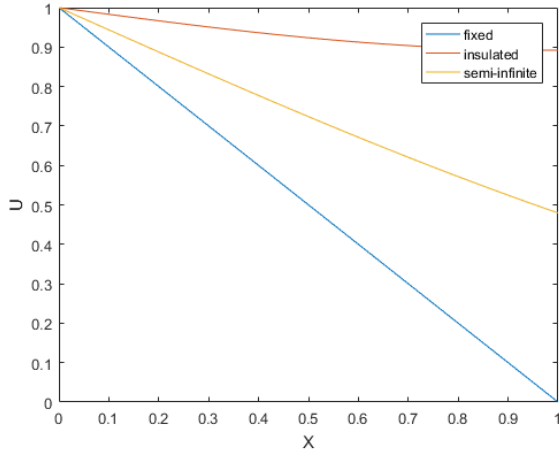


Figure 6: Output with $T = 1$

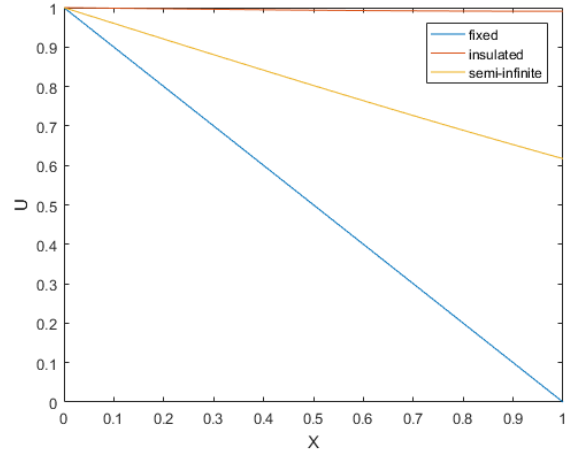


Figure 7: Output with $T = 2$

For all 3 solutions, the $U(X, 0) = 0$ for $0 < X < 1$ and $U(0, T) = 1$ initial and boundary conditions define the behaviour for small time; we get a sharp continuous drop functions value over a small change in X . This can be seen in figure 1, the magnitude of flux grows as $T \rightarrow 0$ in all 3 cases.

The long term behaviour is determined by the boundary conditions at $X = 1$ or as $X \rightarrow \infty$. The fixed boundary condition solution converges quite quickly to its "steady state" solution $1 - X$, since the infinite sum $\rightarrow 0$ as $T \rightarrow \infty$ due to the negative exponentials. The insulated boundary condition solution is similar, converging to its steady state solution 1. However, it converges slower to 1, possibly due to the $n - 1/2$ (as opposed to n) eigenvalue factor in the exponential.

The semi-infinite solution does not have any significant behaviour at $X=1$, but rather is controlled as $X \rightarrow \infty$, and shares properties of both other solutions at ∞ in that both U and U_X tend to 0 there. As T increases, the graph shifts up, since the argument $\varepsilon/2$, of erfc , is inversely proportional to \sqrt{T} , with the solution tending to 1 for fixed X as $T \rightarrow \infty$.

Physically, the initial high flux makes sense, since we have a very high temperature at one end, adjacent to 0K. The evolution in time can be thought of as heat "travelling down the bar", until the bar eventually reaches its long term behaviour. In the fixed case, we have some "hot" end, and some "cold" end and one would expect a linear decrease in temperature along the rod, as we observe. For the insulated case, since we have no heat flux out of the system, we would expect the whole rod to eventually become the same temperature, 1. This intuition is easily extended to the infinite case.

Question 3

The script *NumericalScheme.m*, found on page 13 runs the given numerical scheme, by calculating all U_n^m for fixed m , before moving onto the next m . Note

$$U(X, 0) = 0 \quad \text{for } 0 < X < 1 \quad \Rightarrow \quad U_n^0 = 0 \quad \text{for } n \neq 0$$

$$U(0, T) = 1 \quad \text{for } T > 0 \quad \Rightarrow \quad U_0^m = 1 \quad \text{for } m \neq 0$$

and combining these conditions at $X = T = 0$ gives a best approximation $U_0^0 = 0.5$. To implement the derivative boundary condition, consider the symmetric central difference in space at $X=1$. Note the function is only defined on $0 \leq X \leq 1$, but by uniqueness of solution, we can extend this domain and retain the same solution on $0 \leq X \leq 1 + \varepsilon$.

$$U_X(1, T) = \frac{U(1 + \delta X, T) - U(1 - \delta X, T)}{2\delta X} + O(\delta X) = 0$$

Hence, as $\delta X \rightarrow 0$

$$U(1 + \delta X, T) = U(1 - \delta X, T) \quad \text{for } T > 0 \quad \Rightarrow \quad U_{N+1}^m = U_{N-1}^m$$

(i) The script *q3i.m*, found on page 13, produces the following output for varying T . Note we define the error $E = U_{\text{numerical}} - U_{\text{analytic}}$

X	$U_{\text{numerical}}$	U_{analytic}	E
0.000	1.000	1.000	0.000E+00
0.125	0.804	0.803	9.071E-04
0.250	0.618	0.618	7.831E-04
0.375	0.455	0.454	6.104E-04
0.500	0.319	0.320	-1.315E-03
0.625	0.214	0.217	-2.964E-03
0.750	0.141	0.146	-5.012E-03
0.875	0.098	0.105	-6.484E-03
1.000	0.084	0.091	-6.803E-03

Table 2: Output with $T = 0.125$

X	$U_{\text{numerical}}$	U_{analytic}	E
0.000	1.000	1.000	0.000E+00
0.125	0.865	0.865	-9.164E-05
0.250	0.735	0.736	-3.187E-04
0.375	0.616	0.617	-5.147E-04
0.500	0.512	0.513	-9.898E-04
0.625	0.427	0.428	-1.307E-03
0.750	0.364	0.366	-1.817E-03
0.875	0.325	0.327	-1.989E-03
1.000	0.312	0.315	-2.201E-03

Table 3: Output with $T = 0.25$

X	$U_{\text{numerical}}$	U_{analytic}	E
0.000	1.000	1.000	0.000E+00
0.125	0.928	0.928	1.156E-04
0.250	0.858	0.858	1.995E-04
0.375	0.794	0.794	3.274E-04
0.500	0.738	0.738	3.657E-04
0.625	0.692	0.692	4.860E-04
0.750	0.658	0.657	4.739E-04
0.875	0.637	0.636	5.701E-04
1.000	0.630	0.629	5.112E-04

Table 4: Output with $T = 0.5$

X	$U_{\text{numerical}}$	U_{analytic}	E
0.000	1.000	1.000	0.000E+00
0.125	0.979	0.979	2.010E-04
0.250	0.959	0.959	3.865E-04
0.375	0.941	0.940	5.723E-04
0.500	0.924	0.924	7.141E-04
0.625	0.911	0.910	8.565E-04
0.750	0.901	0.900	9.331E-04
0.875	0.895	0.894	1.010E-03
1.000	0.893	0.892	1.010E-03

Table 5: Output with $T = 1$

(ii) The script *q3ii.m*, found on page 14, produces the following figures when run with different T , $N=8$, $C=1/2$. Note the scale on the y axis changes, so the graphs are in fact shifting up.

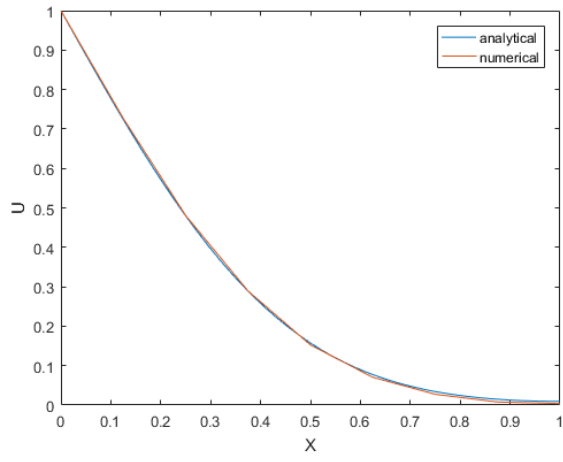


Figure 8: Output with $T = 0.0625$

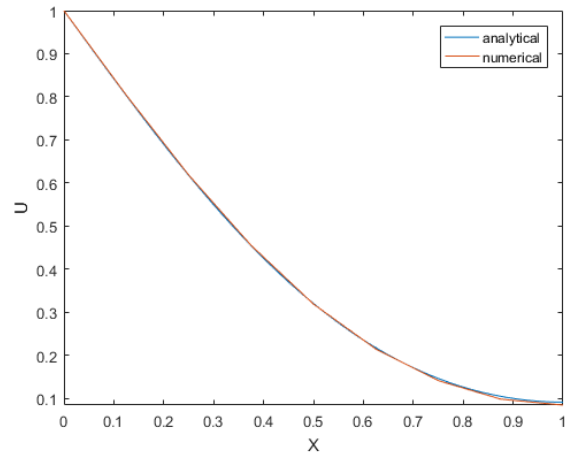


Figure 9: Output with $T = 0.125$

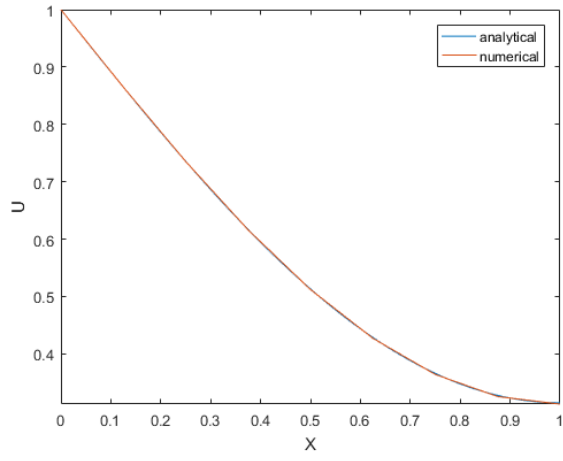


Figure 10: Output with $T = 0.25$

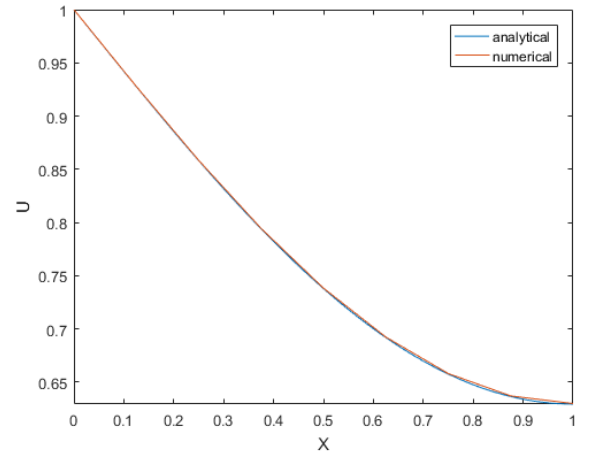


Figure 11: Output with $T = 0.5$

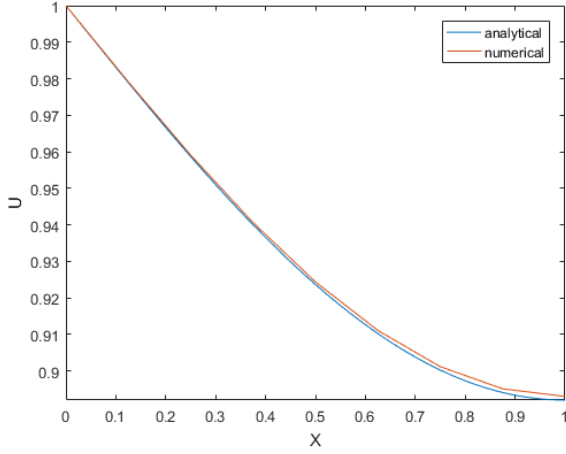


Figure 12: Output with $T = 1$

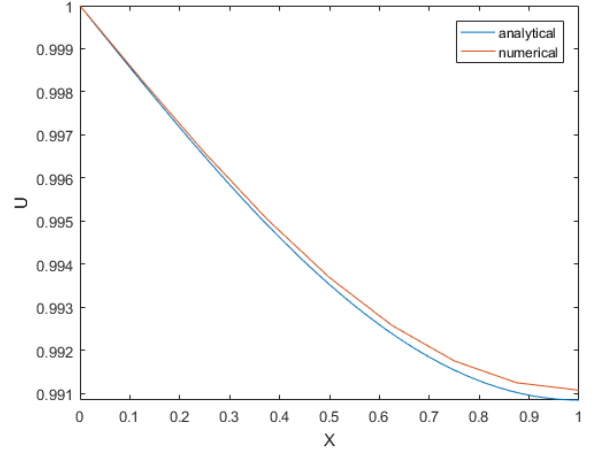


Figure 13: Output with $T = 2$

Stability

We run the script *NumericalScheme.m* for $N = 8, 16, 32$, $C = \frac{1}{12}, \frac{1}{6}, \frac{1}{3}, \frac{1}{2}, \frac{2}{3}$ and 1, and observe stability in all cases but $C = \frac{2}{3}$ or 1. An example can be seen in figure 14. The instability manifests as oscillations growing in magnitude rapidly.

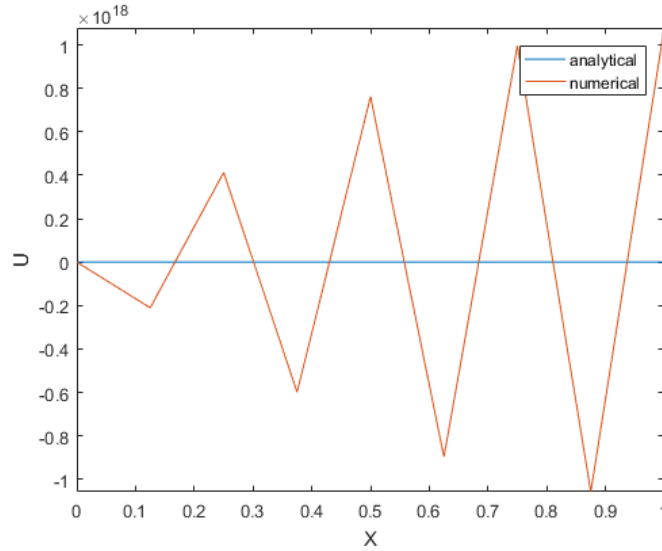


Figure 14: Output of *q3ii.m* with $N=8$, $C=2/3$, $T=1$

The data seems to suggest the scheme is stable for $C \leq \frac{1}{2}$ and unstable otherwise. This is in fact true, and can be shown by "Von Neumann Stability Analysis" ¹ ; a method involving taking the fourier series of the round off errors, defined as $\epsilon_n^m = N_n^m - U_n^m$ where N_n^m is the exact solution to the difference equation (21) and U_n^m is the computed solution (with errors) . We then bound the amplification factor G by 1 for stability:

$$|G| \equiv \left| \frac{\epsilon_n^{m+1}}{\epsilon_n^m} \right| \leq 1$$

This condition turns out to be equivalent to, for fixed δX , a sufficiently small δT is needed for stability; in particular δT must satisfy

$$\delta T \leq \frac{1}{2}(\delta X)^2$$

¹ See https://en.wikipedia.org/wiki/Von-Neumann_stability_analysis, in particular, subsection "Illustration of the Method". Date Accessed 30/12/18

Accuracy

We can see from figures 8-13 that when the numerical scheme is stable it seems to be a good approximation to the solution at all times, with error maximised at $T=2$. We therefore consider errors at $T=2$ within this section. Note that at this time, the calculation for the error in the analytical solution through summing finite terms is at most order 10^{-223} by the previous calculation so we need not consider it.

To determine the theoretical accuracy of the scheme, we have;

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

$$(20) \Rightarrow U_{XX}(X, T) + O((\delta X)^2) = \frac{U(X + \delta X, T) - 2U(X, T) + U(X - \delta X, T)}{(\delta X)^2}$$

and equating gives an error $E_n^m = O(\delta T) + O((\delta X)^2)$, and hence for small δX and δT , $E_n^m \approx A(\delta X)^2 + B(\delta T)$ for some constants A and B depending on various other factors (including the time we take the error at). We can test whether this is the case in our implementation by fixing say δT , and checking whether the differences between errors for changing δX are quadratic. A similar approach can be applied to check the errors for fixed δX and changing δT are linear. Note the error itself for fixed δX will not tend to 0, and will rather tend to a non zero limit as δT tends to 0 due to the other terms depending on δX in E_n^m . The same occurs for δX tending to 0 with δT fixed.

N	C	δX	δT	E
8	1/15625	1/8	10^{-6}	-1.162E-04
16	4/15625	1/16	10^{-6}	-2.893E-05
32	16/15625	1/32	10^{-6}	-7.19E-06
64	64/15625	1/64	10^{-6}	-1.76E-06

Table 6: Errors for varying δX and fixed δT at $T=2$

N	C	δX	δT	E
256	1/2	1/128	2^{-21}	9.04E-07
256	1/4	1/128	2^{-22}	2.26E-07
256	1/8	1/128	2^{-23}	-1.13E-07
256	1/16	1/128	2^{-24}	-2.83E-07

Table 7: Errors for varying δT and fixed δX at $T=2$

Table 6 and 7 are created using data from *q3i.m* run with different values of C and N. In Table 6 the errors appear to behave quadratically; halving δX quarters the error. This is since we have sufficiently small δT such that $B\delta T$ is negligible and $E_n^m \approx A(\delta X)^2$. In table 7 however, we have that $A(\delta X)^2$ (and possibly higher terms in δX) are not small, so the errors don't appear linear. However, considering the differences in the errors (which only depend on δT), show they are in fact linear with respect to δT , with differences $\approx 6.67, 3.39$, and 1.7×10^{-7} with halving δT . From this, we can calculate the values of A and B, from tables 6 and 7 respectively. We get

$$A \approx -7.30 \times 10^{-3}$$

$$B \approx 2.84$$

noting the approximation $E_n^m \approx A(\delta X)^2 + B(\delta T)$ is only valid for sufficiently small δX and δT . To calculate A more accurately, it would have been better to take δX even smaller in Table 6, to ensure higher order terms are negligible, but this forces δT smaller too, taking up far too much memory to compute.

Thus, as long as we are careful to ensure $C \leq \frac{1}{2}$, and both δT and $\delta X \rightarrow 0$, we can make the error arbitrarily small. However, the amount of computation required to make δT small enough for stability with δX increases rapidly. For computation up to some fixed time T for instance, the algorithm is $O(\delta T \delta X) = O(\delta X^3)$.

Programs

Analytic Solutions

(i) *Ufixedfunc.m*

```
function [ f ] = Ufixedfunc( )
f=@(X,T) 1-X
for n = 1:25
    fn=@(X,T) 2*sin(n*pi*X)*exp(-n^2*pi^2*T)/(pi*n);
    f=@(X,T) f(X,T)-fn(X,T);
end
end
```

(ii) *Uinsulfunc.m*

```
function [ f ] = Uinsulfunc()
f=@(X,T) 1
for n = 1:25
    fn=@(X,T) 2*sin((n-1/2)*pi*X)*exp(-(n-1/2)^2*pi^2*T)/(pi*(n-1/2));
    f=@(X,T) f(X,T)-fn(X,T);
end
end
```

(iii) *Usemiinfunc.m*

```
function [ f ] = Usemiinfunc()
%K=1
f=@(X,T) erfc(X/(2*sqrt(T)));
end
```

(iv) *evaluateanalytic*

T=0.25 %this value must be changed

```
Ufix=Ufixedfunc
Ufix=@(X)Ufix(X,T)
Uins=Uinsulfunc
Uins=@(X)Uins(X,T)
Usemi=Usemiinfunc
Usemi=@(X)Usemi(X,T)
```

```
Ufixtabulate=[]
Uinstabulate=[]
Usemิตabulate=[]
```

```
x=[]
```

```
for n=1:9
    x(n)=(n-1)*0.125
    Ufixtabulate=[Ufixtabulate; Ufix(x(n))]
    Usemิตabulate=[Usemิตabulate; Usemi(x(n))]
    Uinstabulate=[Uinstabulate; Uins(x(n))]
end
```

```
fplot(Ufix,[0,1])
hold on
```

```

fplot(Uins,[0,1])
hold on
fplot(Usemi,[0,1])
legend('fixed','insulated','semi-infinite')
xlabel('X')
ylabel('U')

(v) evaluateanalyticflux.m

X=0;

Ufixflux=@(X,T) 1;
for n = 1:25
    Ufixflux=@(X,T)Ufixflux(X,T)+2*cos(n*pi*X)*exp(-n^2*pi^2*T);
end

Uinsflux=@(X,T)0
for n = 1:25
    Uinsflux=@(X,T)Uinsflux(X,T)+2*cos((n-1/2)*pi*X)*exp(-(n-1/2)^2*pi^2*T);
end

epsilon= @(X,T) X/sqrt(T);
Usemiflux=@(X,T) 2*exp(-(epsilon(X,T)/2)^2)/(sqrt(pi*T));

Ufixflux=@(T)-Ufixflux(0,T)
Uinsflux=@(T)-Uinsflux(0,T)
Usemiflux=@(T)-Usemiflux(0,T)

fplot(Ufixflux,[0.0625,2])
hold on
fplot(Uinsflux,[0.0625,2])
hold on
fplot(Usemiflux,[0.0625,2])
legend('fixed','insulated','semi-infinite')
xlabel('T')
ylabel('U_X')

```

Numerical Integration

(i) *NumericalScheme.m*

```
N=32;
C=16/15625;

dx=1/N;
dt=C*(dx)^2;

%we have to go up to t=2 maximum, hence we run the numerical scheme up to
%t=2

rows=2/dt +1;
columns=N+1; %+1's required as we have a 0 entry

%we set up a matrix of the required size who's elements will be the various
%X(m+1,n+1)=U_n^m (as in the project) (see project for description)

X=zeros(rows,columns);

%Initial and boundary data tells us U_n^0=0 and U_0^m=1 m/=0, with
%U_0^0=0.5. Hence first column is all 1's, bar the first element.

X(:,1)=zeros(rows,1)+1;
X(1,1)=0.5;

%Now we loop through the rows, applying the numerical scheme.

for m=0:rows-1 %this is the actual value of m, hence we need to offset by 1 in matrix indexing
    % loop at m calculates the U_*^m+1

    for n=1:columns-2 %the case for U_N^* is slightly different, due to the boundary condition

        X(m+2,n+1)=X(m+1,n+1)+C*(X(m+1,n+2)-2*X(m+1,n+1)+X(m+1,n));

    end

    %U_N^*

    X(m+2,columns)=X(m+1,columns)+C*(2*X(m+1,columns-1)-2*X(m+1,columns));
end
```

(ii) *q3i.m*

```
T=2

%Note must set N and C beforehand in NumericalScheme.m
NumericalScheme

m=T/dt

Uins=Uinsulfunc
Uins=@(X)Uins(X,T)

V=[] %X, but variable X is in use.
U_anal=[]
for i=1:N+1
    V(i)=(i-1)*dx
```

```

        U_anal=[U_anal; Uins(V(i))]  

    end  
  

    U_numerical=transpose(X(m+1,:))  
  

    E=U_numerical-U_anal  
  

    (iii) q3ii.m  
  

    T=1  

    %must set values of N and C in NumericalScheme  

    NumericalScheme  
  

    m=T/dt  
  

    V=[] %again, X in use, so use V to store x values  

    for i=1:N+1  

        V(i)=(i-1)*dx  

    end  

    U_numerical=transpose(X(m+1,:))  
  

    Uins=Uinsulfunc  

    Uins=@(X)Uins(X,T)  
  

    fplot(Uins,[0,1])  

    hold on  

    plot(V,U_numerical)  

    legend('analytical','numerical')  

    xlabel('X')  

    ylabel('U')

```