2.4

2.1 The Diffusion Equation

All programs are attached at the end of the report.

Question 1:
Consider the equation

$$\frac{\partial F}{\partial t}(x,t) = K\frac{\partial^2 F}{\partial x^2}(x,t), F(x,0) = 0, F(0,t) = 1 \tag{1}$$

For simplicity, instead of (x,t), we want to use one non-dimensional variable ξ that is a combination of quantities concerned in the equation (x, t, and K) to rewrite our equation as a single variable ODE. Let $\xi = x^a t^b K^c$. Since $[X] = M$, $[t] = S$ and $[K] = M^2S^{-1}$, [1]by comparing indices we have $a + 2c = b - c = 0$. A reasonable choice is $a = 1, b = c = -\frac{1}{2}$, with $\xi = \dfrac{x}{(kt)^{1/2}}$.

Now with $F(x,t) = f(\xi) = f(\dfrac{x}{(Kt)^{1/2}})$, we use the chain rule to obtain:

$$\frac{\partial f}{\partial t} = \frac{\partial \xi}{\partial t}\frac{\partial f}{\partial \xi} = -\frac{x}{2(Kt^3)^{1/2}}\frac{\partial f}{\partial \xi} = -\frac{\xi}{2t}\frac{\partial f}{\partial \xi}$$

$$\frac{\partial f}{\partial x} = \frac{\partial \xi}{\partial x}\frac{\partial f}{\partial \xi} = \frac{1}{(kt)^{1/2}}\frac{\partial^2 f}{\partial \xi^2}$$

$$\frac{\partial^2 f}{\partial x^2} = \frac{1}{Kt}\frac{\partial^2 f}{\partial \xi^2}$$

Eequation (1) becomes

$$-\frac{\xi}{2}\frac{\partial f}{\partial \xi} = \frac{\partial^2 f}{\partial \xi^2} \tag{2}$$

Hence

$$\frac{\partial f}{\partial \xi} = Ae^{-\xi^2/4}$$

$$f(\xi) = \int_{t_0}^{\xi} Ae^{-x^2/4}\,dx \overset{u=\frac{x}{2}}{=\!=\!=} \int_{t}^{\xi/2} Ce^{-u^2}\,du,$$

where C and t are determined by initial and boundary conditions.

[1]Here square brackets denote dimension of a quantity

In terms of ξ, the initial and boundary conditions are $f(\infty) = 0$ and $f(0) = 1$, which gives $t = \infty$ and $C = -\frac{2}{\sqrt{\pi}}$. Therefore

$$f(\xi) = \frac{2}{\sqrt{\pi}} \int_{\xi/2}^{\infty} e^{-u^2}\, du = \mathrm{erfc}(\frac{1}{2}\xi) \tag{3}$$

Question 2:
Analytic Solutions:

Now consider the equation

$$U_T = U_{XX}, T > 0, 0 < X < 1 \tag{4}$$

with

$$U(X, 0) = 0 \text{ for } 0 < X < 1; U(0, T) = 1, U(1, T) = 0 \text{ for } T > 0$$

Note that boundary condition is not homogeneous. We identify a steady solution $U_s(X)$ and write $U(X, T) = U_s(X) + U_t(X, T)$ to settle the problem: The appropriate steady solution is $U_s(X) = 1 - X$.

Substitute $U(X, T) = U_s(X) + U_t(X, T)$ in (4) we find that

$$(U_t)_T = (U_t)_{XX}, T > 0, 0 < X < 1 \tag{5}$$

with initial and boundary conditions

$$U_t(X, 0) = X - 1 \text{ for } 0 < X < 1; U_t(0, T) = 0, U_t(1, T) = 0 \text{ for } T > 0 \tag{6}$$

Write $U_t(X, T) = F(X)G(T)$ we have

$$\frac{G'}{G} = \frac{F''}{F} = -\lambda, \text{for some positive } \lambda \tag{7}$$

Hence

$$F(X) = A\cos(\sqrt{\lambda}X) + B\sin(\sqrt{\lambda}X).$$

Using the boundary condition $F(0) = F(1) = 0$ we have

$$A = 0, \lambda = n^2\pi^2$$

Thus

$$G(T) = e^{-\pi^2 n^2 T}, F(X) = B\sin(n\pi X) \tag{8}$$

The general solution is

$$U_t(X,T) = \sum_1^\infty B_n \sin(n\pi X) e^{-\pi^2 n^2 T}, \text{for some } B_n \text{ to be determined.}$$

Using the initial condition and orthogonality of sine,

$$B_m = 2\int_0^1 (x-1)\sin(m\pi x)\,dx = -\frac{2}{m\pi} \tag{9}$$

$$U = 1 - X - \frac{2}{\pi}\sum_1^\infty \frac{1}{n} e^{-\pi^2 n^2 T}\sin(n\pi X) \tag{10}$$

Now consider (5) with initial and boundary conditions

$$U_t(X,0) = -1 \text{ for } 0 < X < 1; U_t(0,T) = 0, (U_t)_X(1,T) = 0 \text{ for } T > 0 \tag{11}$$

Following the same procedure as above we find that

$$U_t = \sum_1^\infty C_n \sin((n-\frac{1}{2})\pi X) e^{-\pi^2 (n-\frac{1}{2})^2 T}$$

Note that

$$\int_0^1 \sin((n-\frac{1}{2})\pi x)\sin((m-\frac{1}{2})\pi x)\,dx = \int_0^1 \frac{1}{2}(\cos((n-m)\pi x)) - \cos((m+n-1)\pi x))\,dx$$

$= \begin{cases} \frac{1}{2} & m = n \\ 0 & m \neq n \end{cases}$. Exploiting this orthogonality relation we have

$$C_m = -2\int_0^1 \sin((m-\frac{1}{2})\pi x)\,dx = -\frac{4}{(2m-1)\pi}$$

$$U(X,T) = 1 - \frac{4}{\pi}\sum_1^\infty \frac{1}{(2n-1)} e^{-\pi^2(n-\frac{1}{2})^2 T}\sin((n-\frac{1}{2})\pi X) \tag{12}$$

Truncation error:
The truncation error in (10) is

$$E_N = -\frac{2}{\pi}\sum_{n=N}^\infty \frac{1}{n} e^{-\pi^2 n^2 T}\sin(n\pi X)$$

We have the inequality

$$|E_N| = |\frac{2}{\pi}\sum_{n=N}^\infty \frac{1}{n} e^{-\pi^2 n^2 T}\sin(n\pi X)| \leqslant \frac{2}{\pi}\sum_{n=N}^\infty |\frac{1}{n} e^{-\pi^2 n^2 T}\sin(n\pi X)| \leqslant \frac{2}{\pi}\sum_{n=N}^\infty |e^{-\pi^2 n^2 T}|$$

$$= \frac{2}{\pi}\sum_{n=0}^{\infty} e^{-\pi^2(N+n)^2T} \leqslant \frac{2}{\pi}\sum_{0}^{\infty} e^{-\pi^2(N^2+nN)T} = \frac{2e^{-\pi^2N^2T}}{\pi(1-e^{-\pi^2NT})} \tag{13}$$

The truncation error in (12) is

$$E_N = -\frac{4}{\pi}\sum_{n=N}^{\infty}\frac{1}{2n-1}e^{-\pi^2(n-\frac{1}{2})^2T}\sin((n-\frac{1}{2})\pi X)$$

We have the inequality

$$|E_N| =\leqslant \frac{4}{\pi}\sum_{n=N}^{\infty}|\frac{1}{2n-1}e^{-\pi^2(n-\frac{1}{2})^2T}\sin((n-\frac{1}{2})\pi X)| \leqslant \frac{4}{\pi}\sum_{n=N}^{\infty}|e^{-\pi^2(n-\frac{1}{2})^2T}|$$

$$\leqslant \frac{4}{\pi}\sum_{0}^{\infty} e^{-\pi^2(N^2+nN)T} = \frac{4e^{-\pi^2N^2T}}{\pi(1-e^{-\pi^2NT})} \tag{14}$$

For $N = 4$, the above estimation gives $|E_N| \leqslant 10^{-5}$ for all values of T concerned in the question.

Table 1: Values of U with Different Values of X

Values of X	0.1250	0.2500	0.3750	0.5000	0.6250	0.7500	0.8750	1.0000
Value of U in (10)	0.8543	0.7118	0.5751	0.4460	0.3251	0.2118	0.1044	0.0000
Value of U in (12)	0.8650	0.7355	0.6167	0.5130	0.4284	0.3658	0.3275	0.3146
Semi-infinite Solution	0.8597	0.7237	0.5959	0.4795	0.3768	0.2888	0.2159	0.1573

Graphs:
Now we plot U against X for different values of T:

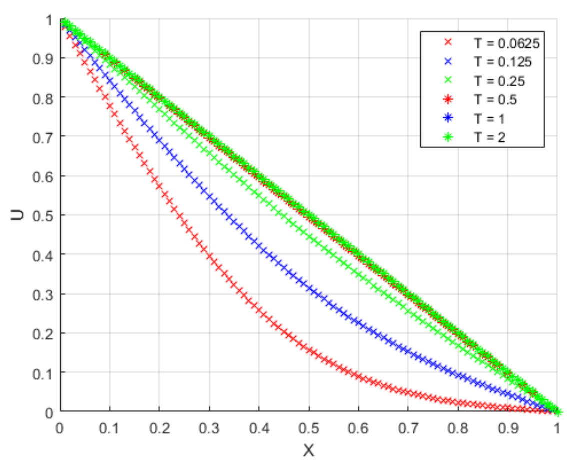

Figure 1: U against X for (10)

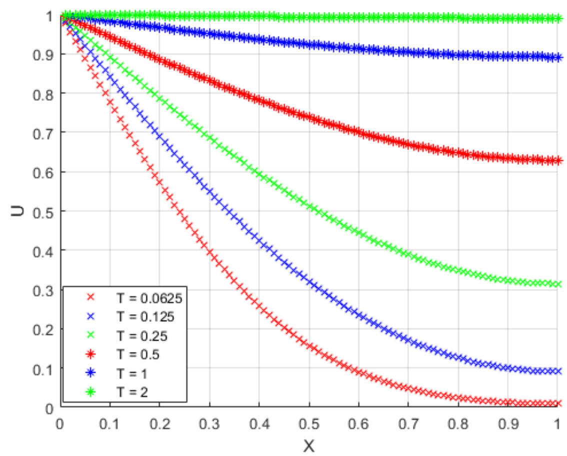

Figure 2: U against X for (12)

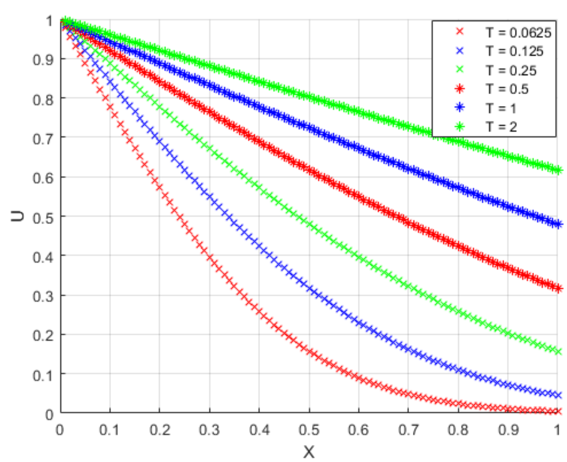

Figure 3: U against X for (3)

From Figure 1 we deduce that with initial condition (6) the solution converges rapidly to the line $U(X,T) = 1 - X$ as T becomes large. This is expected: From (10) and (13) with $N = 1$ we see that as T gets large the series tend to $1 - X$.

From Figure 2 we see that with initial condition (11) the solution converges to the line $U(X,T) = 1$ as T gets large but with a slower rate of convergence than Figure 1. This is expected: From (12) and (14) with $N = 1$ we see that as T gets large the series tend to 1. Also from (12) we see that the exponent of e is proportional to $(n - \frac{1}{2})^2$, smaller then n^2, leading to a slower rate of convergence.

From Figure 3 we see that, for selected range of T, the graph moves upwards as T becomes large(but rather slowly). This is expected: $f(\xi)$ increases much slower since any increment in T will only result in a decrement proportional to $\dfrac{1}{\sqrt{T}}$ in the lower limit of the integral. Also, from (3) we deduce that in the limit as T tends to infinity the graph will converge to the line $U(X,T) = 1$. Note also that the analytic solution(3) is a very good approximation to (10).

X**-Derivatives**:
Differentiate (3) with respect to X:

$$-\frac{\partial f}{\partial X} = -\frac{2}{\sqrt{\pi}}\frac{\partial}{\partial \frac{\xi}{2}}\int_{\xi/2}^{\infty} e^{-u^2}\,du\frac{\partial \frac{\xi}{2}}{\partial \xi}\frac{\partial \xi}{\partial x} = \frac{1}{\sqrt{\pi T}}e^{-\dfrac{X^2}{4T}}$$

Substitute $X = 0$,

$$-U_X(0,T) = \frac{1}{\sqrt{\pi T}} \tag{15}$$

Differentiate (term-by-term) (10) with respect to X:

$$-U_X = 1 + 2\sum_{1}^{\infty} e^{-\pi^2 n^2 T}\cos(n\pi X)$$

Substitute $X = 0$,

$$-U_X(0,T) = 1 + 2\sum_{1}^{\infty} e^{-\pi^2 n^2 T} \tag{16}$$

Consider the truncation error $E_N = 2\sum_{n=N}^{\infty} e^{-\pi^2 n^2 T}$:

Similar to the above we have

$$|E_N| \leqslant \frac{2e^{-\pi^2 N^2 T}}{1 - e^{-\pi^2 N T}}$$

Differentiate (term-by-term) (12) with respect to X:

$$-U_X = 2\sum_{1}^{\infty} e^{-\pi^2 n^2 T}\cos((n - \frac{1}{2})\pi X)$$

Substitute $X = 0$,

$$-U_X(0,T) = 2\sum_{1}^{\infty} e^{-\pi^2 n^2 T} \tag{17}$$

The truncation error also satisfies the inequality

$$|E_N| \leqslant \frac{2e^{-\pi^2 N^2 T}}{1 - e^{-\pi^2 N T}}$$

Based on previous calculation we see that $N = 4$ will suffice for all values of $T \geqslant 0.0625$, since $\dfrac{2e^{-\pi^2 N^2 T}}{1-e^{-\pi^2 NT}}$ is decreasing in T.

We use the first 4 terms in series (13) and (14) to produce the following graphs of $-U_X$ against T in [0.0625,1]:

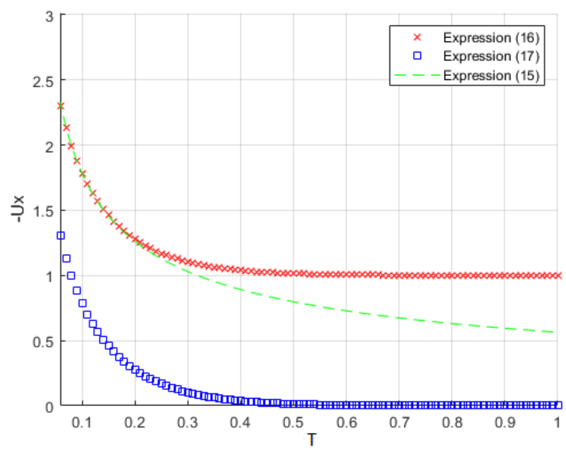

Figure 4: $-U_X(0,T)$ against T for (15), (16), and (17).

From the graph we see that $-U_X(0,T)$ tends to 1, 0, and 0 for (16),(17),and (15) with a descending rate of convergence. This is consistent with the discussion we have for Figure 1, 2, and 3.

Question 3:
Let X-derivative be approximated by central difference quotients[2]

$$U_X(X,T) = \frac{U(X+\delta X,T) - U(X-\delta X,T)}{2\delta X} = \frac{U^m_{n+1} - U^m_{n-1}}{2\delta X} \tag{18}$$

Substitute $n = N$ in (18). We see that $U_X(1,T) = \dfrac{U^m_{N+1} - U^m_{N-1}}{2\delta X} = 0$ by (6), which implies $U^m_{N+1} = U^m_{N-1}$.
Similarly we approximate U^0_0 by

$$U^0_0 = \frac{1}{2}(\lim_{X\to\ 0} U(X,0) + \lim_{T\to\ 0} U(0,T)) = 0.5 \tag{19}$$

Now we use the recurrence relation to find the numerical solution:
For the case $N = 8, C = 0.5$ the result for different values of T is tabulated below.

Table 2: The Numerical and Analytic Solutions at $T = 0.125, 0.25$

	$T = 0.125$			$T = 0.25$		
	Numerical	Analytic	Error	Numerical	Analytic	Error
$X = 0$	1.00000	1.00000	0.00000	1.00000	1.00000	0.00000
$X = 0.125$	0.80365	0.80274	0.00091	0.86495	0.86504	0.00009
$X = 0.25$	0.61832	0.61753	0.00079	0.73522	0.73554	0.00032
X= 0.375	0.45502	0.45441	0.00061	0.61614	0.61666	0.00052
$X = 0.5$	0.31870	0.32001	0.00131	0.51200	0.51299	0.00099
$X = 0.625$	0.21429	0.21726	0.00297	0.42707	0.42838	0.00131
$X = 0.75$	0.14102	0.14603	0.00501	0.36402	0.36584	0.00182
$X = 0.875$	0.09808	0.10457	0.00649	0.32549	0.32748	0.00199
$X = 1$	0.08420	0.09100	0.00680	0.31235	0.31455	0.00220

Table 3: The Numerical and Analytic Solutions at $T = 0.5, 1$

	$T = 0.5$			$T = 1$		
	Numerical	Analytic	Error	Numerical	Anallytic	Error
$X = 0$	1.00000	1.00000	0.00000	1.00000	1.00000	0.00000
$X = 0.125$	0.92778	0.92766	0.00012	0.97914	0.97893	0.00021
$X = 0.25$	0.85830	0.85810	0.00020	0.95907	0.95868	0.00039
$X = 0.375$	0.79432	0.79400	0.00032	0.94058	0.94001	0.00057
$X = 0.5$	0.73818	0.73781	0.00037	0.92436	0.92365	0.00071
$X = 0.625$	0.69219	0.69170	0.00049	0.91108	0.91022	0.00086
$X = 0.75$	0.65792	0.65744	0.00048	0.90118	0.90024	0.00094
$X = 0.875$	0.63692	0.63635	0.00057	0.89511	0.89410	0.00101
$X = 1$	0.62973	0.62922	0.00051	0.89303	0.89202	0.00101

The graphs of the analytic and numerical solutions for $T = 0.0625, 0.125, 0.25, 0.5, 1$, and 2 are plotted:

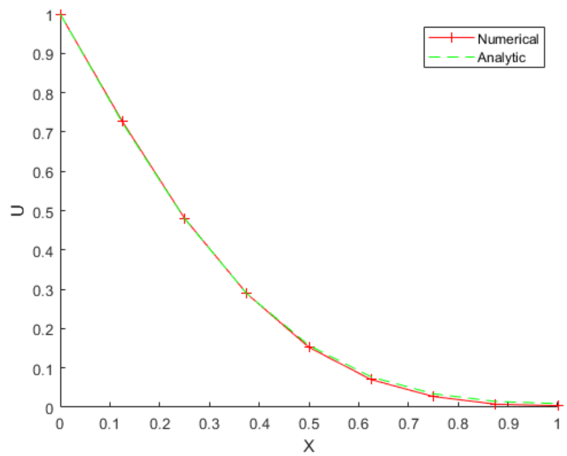

Figure 5: $T = 0.0625$.

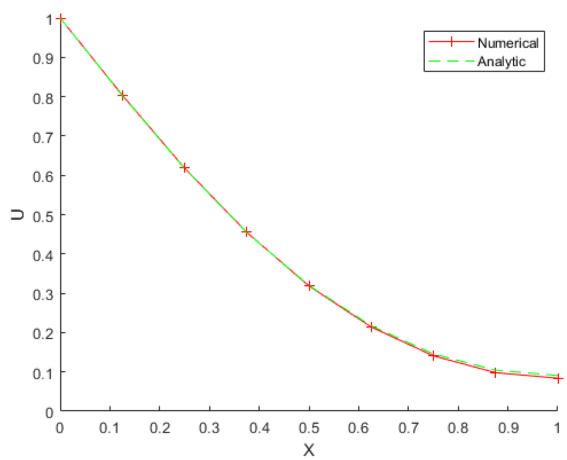

Figure 6: $T = 0.125$.

[2]MSc Course in Mathematics and Finance, Mark Davis `http://wwwf.imperial.ac.uk/~mdavis/FDM11/LECTURE_SLIDES2.PDF`

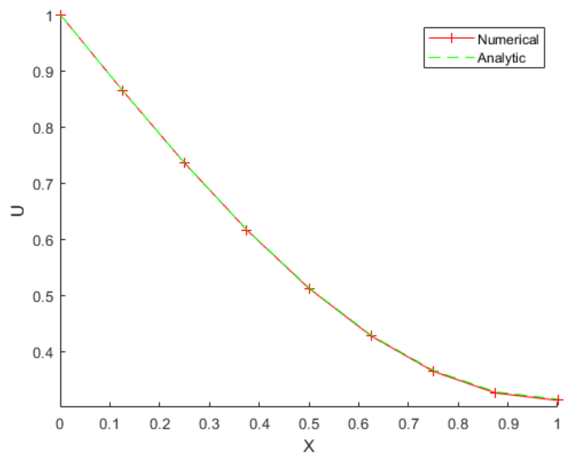

Figure 7: $T = 0.25$.

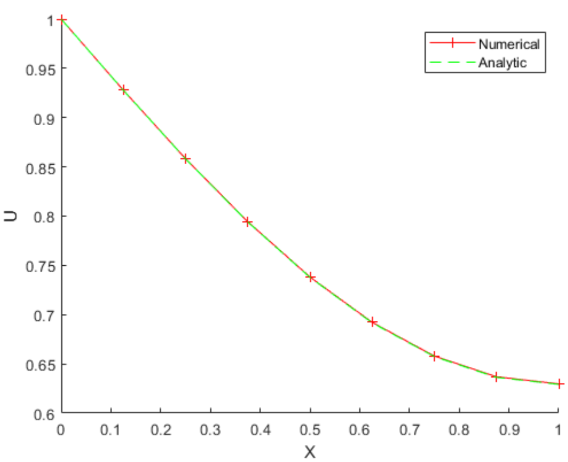

Figure85: $T = 0.5$.

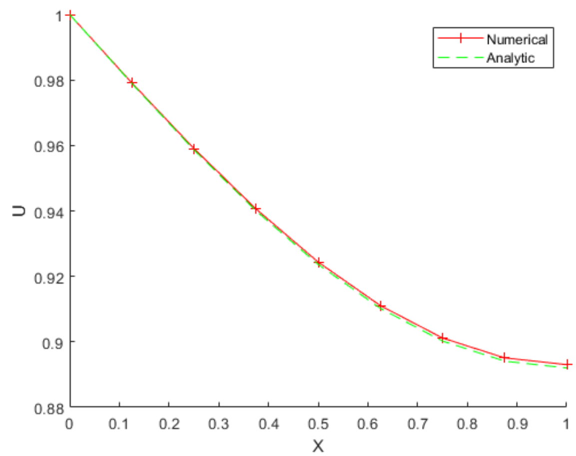

Figure 9: $T = 1$.

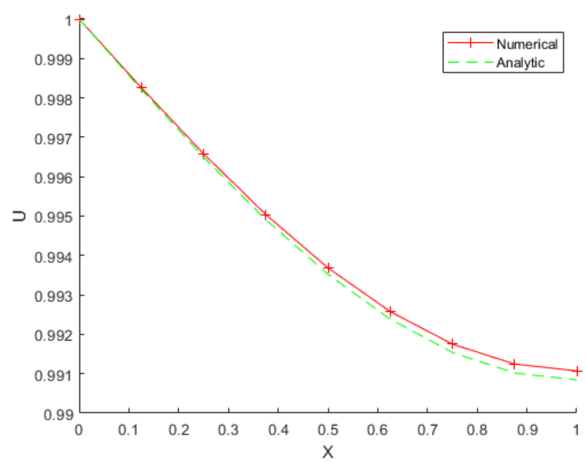

Figure 10: $T = 2$.

Stability of the Numerical Scheme:
Note that the error due to numerical approximation is accumulated at $X = 1$. We use the absolute difference between the analytic and numerical solution at $X = 1$ to give an estimation of error at a particular time.
We run our program for different values of N and C and observe that when $C = \frac{2}{3}$, the numerical scheme is unstable for all values of N(The iterated value of $U(1, 1)$ diverges in each case).
However, when the Finite Element Method does work, the result converges to the analytic solution.
The above phenomenon is expected: The theoretic order of accuracy of the

method is $O(\delta T^2)$.[3] When C becomes larger while δX is small, δT will become large, which leads to a significant $O(\delta^2)$ term.

Source Code

```
function y = FS1(n,x,t) %fourier series solution 1
y = 1-x;
s = 0;
for i = 1:n
s = s -(2/(i*pi))*exp(-pi^2*i^2*t)*sin(i*pi*x);
end
y = y+s;
end
```

```
function y = FS2(n,x,t) %fourier series solution 2
y = 1;
s = 0;
for i = 1:n
s = s -(4/((2*i-1)*pi))*exp(-pi^2*(i-1/2)^2*t)*sin((i-1/2)*pi*x);
end
y = y+s;
end
```

```
S1 = zeros(1,8);
S2 = zeros(1,8);
S3 = zeros(1,8);
for j = 1:8
format long
S1(j) = FS1(3,0.125*j,0.25);
S2(j) = FS2(3,0.125*j,0.25);
S3(j) = AS(0.125*j,0.25);
end
```

```
function y = AS(x,t)
p = x/sqrt(t);
y = erfc(p/2);
end
```

```
function y = DAS(t)
```

[3] Taylor expand U_n^{m+1} we see that $U_n^{m+1} = U_n^m + \delta T \frac{\partial U}{\partial T} + O(\delta T^2) = U_n^m + \delta T(\frac{U_n^{m+1} - U_n^m}{\delta T} + \delta T) = U_n^m + \delta T(\frac{U_n^{m+1} - U_n^m}{\delta T}) + O(\delta T^2)$.Use the numerical scheme ,$U_n^{m+1} = U_n^m + C(U_{n+1}^m - 2U_n^m + U_{n-1}^m) + O(\delta T^2)$

```
y = 1/sqrt(pi*t)
end
```

```
function y = DFS1(n,t)
y = 1;
s = 0;
for j=1:n
s = s + 2*exp(-pi^2*j^2*t);
end
y = y + s;
end
```

```
function y = DFS2(n,t)
y = 0;
s = 0;
for j=1:n
s = s + 2*exp(-pi^2*j^2*t);
end
y = y + s;
end
```

```
function [e] = Err(N,C,T)
[s,A] = FE(N,C,T);
X = listofAS(N,T);
e = A(s+1,N+1) - X(N+1);
end
```

```
function [s,A] = FE(N,C,T)
dx = 1/N
dt = C*(dx)^2
s = round(T/dt)
A = zeros(s+1,N+2);
A(1,1) = 0.5;
for i = 2:s+1
A(i,1) = 1;
for j = 2:N+1
A(i,j) = A(i-1,j)+C*(A(i-1,j+1) - 2*A(i-1,j) + A(i-1,j-1));
end
A(i,N+2) = A(i,N);
end
end
```

```
function [X] = listofAS(N,T)
X = zeros(1,N);
dx = 1/N;
for i = 1:N+1
X(i) = FS2(5,(i-1)*dx,T);
end
```

```
end
```

```
A = zeros(1,100);
B = zeros(1,100);
C = zeros(1,100);
D = zeros(1,100);
E = zeros(1,100);
F = zeros(1,100);
G = zeros(1,100);
for i = 1:100
A(i) = 0.01*i;
end
for j = 1:100
B(j) = FS1(4,A(j),0.0625);
C(j) = FS1(4,A(j),0.125);
D(j) = FS1(4,A(j),0.25);
E(j) = FS1(4,A(j),0.5);
F(j) = FS1(4,A(j),1);
G(j) = FS1(4,A(j),2);
end
hold on
xlabel('X');
ylabel('U')

hold on
plot(A,B,'rx')
plot(A,C,'bx')
plot(A,D,'gx')
plot(A,E,'r*')
plot(A,F,'b*')
plot(A,G,'g*')
hold off

grid on

%second sol
A = zeros(1,100);
B = zeros(1,100);
C = zeros(1,100);
D = zeros(1,100);
E = zeros(1,100);
F = zeros(1,100);
G = zeros(1,100);
for i = 1:100
A(i) = 0.01*i;
end
for j = 1:100
B(j) = FS2(4,A(j),0.0625);
C(j) = FS2(4,A(j),0.125);
D(j) = FS2(4,A(j),0.25);
E(j) = FS2(4,A(j),0.5);
F(j) = FS2(4,A(j),1);
G(j) = FS2(4,A(j),2);
end
hold on
xlabel('X');
```

```
ylabel('U')

hold on
plot(A,B,'rx')
plot(A,C,'bx')
plot(A,D,'gx')
plot(A,E,'r*')
plot(A,F,'b*')
plot(A,G,'g*')
hold off

grid on
%3rd sol
A = zeros(1,100);
B = zeros(1,100);
C = zeros(1,100);
D = zeros(1,100);
E = zeros(1,100);
F = zeros(1,100);
G = zeros(1,100);
for i = 1:100
A(i) = 0.01*i;
end
for j = 1:100
B(j) = AS(A(j),0.0625);
C(j) = AS(A(j),0.125);
D(j) = AS(A(j),0.25);
E(j) = AS(A(j),0.5);
F(j) = AS(A(j),1);
G(j) = AS(A(j),2);
end
hold on
xlabel('X');
ylabel('U')

hold on
plot(A,B,'rx')
plot(A,C,'bx')
plot(A,D,'gx')
plot(A,E,'r*')
plot(A,F,'b*')
plot(A,G,'g*')
hold off

grid on
```

```
A = zeros(1,100);
B = zeros(1,100);
C = zeros(1,100);
D = zeros(1,100);
for i = 1:100
A(i) = 0.01*i;
end
for j = 1:100
B(j) = DFS1(4,A(j));
C(j) = DFS2(4,A(j));
```

```
D(j) = DAS(A(j));
end
hold on
xlabel('X');
ylabel('-Ux')

hold on
plot(A,B,'rx')
plot(A,C,'bs')
plot(A,D,'g--')
hold off

grid on
```

```
[s,A] = FE(8,0.5,0.0625);%t=0.0625
for j = 1:9
K(j) = (j-1)*0.125;
end
X = A(s+1,:);
for i = 1:9
Y(i) = X(i);
end
Z = listofAS(8,0.0625);
hold on
xlabel('X')
ylabel('U')
plot(K,Y,'r-+')
plot(K,Z,'g--')
hold off
%t = 0.125
[s,A] = FE(8,0.5,0.125);
for j = 1:9
K(j) = (j-1)*0.125;
end
X = A(s+1,:);
for i = 1:9
Y(i) = X(i);
end
Z = listofAS(8,0.125);
hold on
xlabel('X')
ylabel('U')
plot(K,Y,'r-+')
plot(K,Z,'g--')
hold off
%t = 0.25
[s,A] = FE(8,0.5,0.25);
for j = 1:9
K(j) = (j-1)*0.125;
end
X = A(s+1,:);
for i = 1:9
Y(i) = X(i);
end
Z = listofAS(8,0.25);
hold on
```

```
xlabel('X')
ylabel('U')
plot(K,Y,'r-+')
plot(K,Z,'g--')
hold off
%T=0.5
[s,A] = FE(8,0.5,0.5);
for j = 1:9
K(j) = (j-1)*0.125;
end
X = A(s+1,:);
for i = 1:9
Y(i) = X(i);
end
Z = listofAS(8,0.5);
hold on
xlabel('X')
ylabel('U')
plot(K,Y,'r-+')
plot(K,Z,'g--')
hold off
%t=1
[s,A] = FE(8,0.5,1);
for j = 1:9
K(j) = (j-1)*0.125;
end
X = A(s+1,:);
for i = 1:9
Y(i) = X(i);
end
Z = listofAS(8,1);
hold on
xlabel('X')
ylabel('U')
plot(K,Y,'r-+')
plot(K,Z,'g--')
hold off
%t = 2
[s,A] = FE(8,0.5,2);
for j = 1:9
K(j) = (j-1)*0.125;
end
X = A(s+1,:);
for i = 1:9
Y(i) = X(i);
end
Z = listofAS(8,2);
hold on
xlabel('X')
ylabel('U')
plot(K,Y,'r-+')
plot(K,Z,'g--')
hold off
```