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PDE Project Proposal

Parabolic PDE's are approximated numerically by discretizing and replacing the derivatives with respect to space by numerical approximations. The most common use is the three point central difference formulas for the first and second derivatives:

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + O(h^2)$$

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + O(h^2)$$

The derivatives are described in terms of the original functions and the spacing between sampling of the function. The final term describes the error in the approximations. In the case of the three point formulas, the error is on the order of the square of the discretization spacing. In order to achieve sufficient accuracy, the discretization may be required to be very small and thus increases the computation time and memory requirements. There are five point formulas for example the central difference first derivative:

$$f'(x) = \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h} + O(h^4)$$

These five-point formulas have error on the order of the fourth power of h. These formulas can be used to achieve greater accuracy for the same discretization step size, or can be used to increase the discretization step size and achieve the same accuracy level. Often, the increased computation required to calculate the five point derivatives can be offset by the decrease in discrete steps.

Project Tasks

1 – Outline the method for deriving the differential approximations using the Taylor Series expansion and matrix algebra to solve a system of algebraic equations for the discrete difference formulas.

2 – Use the above method to derive the 2-point, 3-point, 4-point, and 5-point formulas for the first and second derivatives in all forms (forward difference, backward difference, and central difference). Include the first term in the error of the formula to determine the order of the accuracy.

3 – Use the three point and five point formulas to solve a parabolic PDE with a known analytical solution.

4 – Determine the levels of discretization necessary to achieve to same accuracy using the three point formulas versus the five point formulas. Is there a computational or memory improvement to using the five-point formula over the three-point formula?

The first few terms of the Taylor Series expansion of a function f(x) are expressed as:

$$f(x)=\frac{f(x_0)}{0!}(x-x_0)^0+\frac{f'(x_0)}{1!}(x-x_0)^1+\frac{f''(x_0)}{2!}(x-x_0)^2+\frac{f'''(x_0)}{3!}(x-x_0)^3+\frac{f^{[4]}(x_0)}{4!}(x-x_0)^4+\frac{f^{[5]}(x_0)}{5!}(x-x_0)^5+\ldots$$

Therefore substitution reveals:

$$f(x_0+h)=f(x_0)+\frac{f'(x_0)}{1!}h+\frac{f''(x_0)}{2!}h^2+\frac{f'''(x_0)}{3!}h^3+\frac{f^{[4]}(x_0)}{4!}h^4+\frac{f^{[5]}(x_0)}{5!}h^5+\ldots$$

$$f(x_0+2h)=f(x_0)+\frac{f'(x_0)}{1!}2h+\frac{f''(x_0)}{2!}4h^2+\frac{f'''(x_0)}{3!}8h^3+\frac{f^{[4]}(x_0)}{4!}16h^4+\frac{f^{[5]}(x_0)}{5!}32h^5+\ldots$$

The goal is to add these two equations using linear operators to solve for f'(x_0) or f''(x_0) and eliminate the lowest order term. Rearranging and adding linear multipliers:

$$a\left[f(x_0+h)-f(x_0)\right]\approx a\left[\frac{f'(x_0)}{1!}h+\frac{f''(x_0)}{2!}h^2\right]$$

$$b\left[f(x_0+2h)-f(x_0)\right]\approx b\left[\frac{f'(x_0)}{1!}2h+\frac{f''(x_0)}{2!}4h^2\right]$$

In order to eliminate the second derivative and solve for the first derivative, the right hand side columns can be written in the form:

$$ax+2bx=1$$

$$ay+4by=0$$

Solving for a and b using matrix algebra:

$$\begin{bmatrix}1 & 2\\ 1 & 4\end{bmatrix}\begin{bmatrix}a\\ b\end{bmatrix}=\begin{bmatrix}1\\ 0\end{bmatrix}$$

$$\begin{bmatrix}a\\ b\end{bmatrix}=\begin{bmatrix}2\\ -0.5\end{bmatrix}$$

Now, using the solved values of a and b, look at the sum of the above equations:

$$2\left[f(x_0+h)-f(x_0)\right]-0.5\left[f(x_0+2h)-f(x_0)\right]\approx 2\left[\frac{f'(x_0)}{1!}h+\frac{f''(x_0)}{2!}h^2\right]-0.5\left[\frac{f'(x_0)}{1!}2h+\frac{f''(x_0)}{2!}4h^2\right]$$

Rearranging and isolating f'(x_0):

$$\frac{-1.5f(x_0)+2f(x_0+h)-0.5f(x_0+2h)}{h}\approx f'(x_0)$$

Multiplying by 2 in numerator and denominator to get integer coefficients gives the final form:

$$f'(x_0)\approx\frac{-3f(x_0)+4f(x_0+h)-f(x_0+2h)}{2h}$$

This is the three-point forward difference algorithm for the first derivative. If the next higher order term is included:

$$f'(x_0)\approx\frac{-3f(x_0)+4f(x_0+h)-f(x_0+2h)}{2h}+h^2\frac{f'''(x_0)}{3}$$

The error in using this formula scales with the square of h and the third derivative. The same method can be used to calculate the central difference and backward difference formulas:

$$f'(x_0) \approx \frac{f(x_0+h) - f(x_0-h)}{2h} - h^2 \frac{f'''(x_0)}{6}$$

$$f'(x_0) \approx \frac{f(x_0-2h) - 4f(x_0-h) + 3f(x_0)}{2h} + h^2 \frac{f'''(x_0)}{3}$$

In a similar fashion, the five point formulas can be calculated by using the first through fourth order terms of the Taylor expansion and four equations. The example of the five-point center difference equation for the second derivative is below:

$$\begin{bmatrix} -2 & -1 & 1 & 2 \\ 4 & 1 & 1 & 4 \\ -8 & -1 & 1 & 8 \\ 16 & 1 & 1 & 16 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = \begin{bmatrix} -1/24 \\ 2/3 \\ 2/3 \\ -1/24 \end{bmatrix}$$

$$24 \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = \begin{bmatrix} -1 \\ 16 \\ 16 \\ -1 \end{bmatrix}$$

$$f''(x_0) \approx \frac{-f(x_0-2h) + 16f(x_0-h) - 30f(x_0) + 16f(x_0+h) - f(x_0+2h)}{12h^2} + h^4 \frac{f^{[6]}(x_0)}{120}$$

Note that the five-point formula has error with h^4 and the 6^{th} derivative. Using this method, all the possible combinations of 2, 3, 4, and 5 point methods are listed below for the first and second derivative as well as the first error term.

2-point Formulas

$$f'(x_0) \approx \frac{-f(x_0) + f(x_0+h)}{h} - h \frac{f''(x_0)}{2}$$

$$f'(x_0) \approx \frac{-f(x_0-h) + f(x_0)}{h} + h \frac{f''(x_0)}{2}$$

3-point Formulas

$$f'(x_0) \approx \frac{f(x_0-2h)-4f(x_0-h)+3f(x_0)}{2h} + h^2\,\frac{f'''(x_0)}{3}$$

$$f'(x_0) \approx \frac{-f(x_0-h)+f(x_0+h)}{2h} - h^2\,\frac{f'''(x_0)}{6}$$

$$f'(x_0) \approx \frac{-3f(x_0)+4f(x_0+h)-f(x_0+2h)}{2h} + h^2\,\frac{f'''(x_0)}{3}$$

$$f''(x_0) \approx \frac{f(x_0-2h)-2f(x_0-h)+f(x_0)}{h^2} - hf'''(x_0)$$

$$f''(x_0) \approx \frac{f(x_0-h)-2f(x_0)+f(x_0+h)}{h^2} - h^2\,\frac{f^{[4]}(x_0)}{12}$$

$$f''(x_0) \approx \frac{f(x_0)-2f(x_0+h)+f(x_0+2h)}{h^2} - hf'''(x_0)$$

4-point Formulas

$$f'(x_0) \approx \frac{-2f(x_0-3h)+9f(x_0-2h)-18f(x_0-h)+11f(x_0)}{6h} + h^3\,\frac{f^{[4]}(x_0)}{72}$$

$$f'(x_0) \approx \frac{f(x_0-2h)-6f(x_0-h)+3f(x_0)+2f(x_0+h)}{6h} - h^3\,\frac{f^{[4]}(x_0)}{12}$$

$$f'(x_0) \approx \frac{-2f(x_0-h)-3f(x_0)+6f(x_0+h)-f(x_0+2h)}{6h} + h^3\,\frac{f^{[4]}(x_0)}{12}$$

$$f'(x_0) \approx \frac{-11f(x_0)+18f(x_0+h)-9f(x_0+2h)+2f(x_0+3h)}{6h} - h^3\,\frac{f^{[4]}(x_0)}{72}$$

$$f''(x_0) \approx \frac{f(x_0-3h)-4f(x_0-2h)+5f(x_0-h)-2f(x_0)}{h^2} + h^2\,\frac{5f^{[4]}(x_0)}{24}$$

$$f''(x_0) \approx \frac{2f(x_0)-5f(x_0+h)+4f(x_0+2h)-f(x_0+3h)}{h^2} - h^2\,\frac{5f^{[4]}(x_0)}{24}$$

Note: The other two 4-point formulas for the second derivative are identical to the 3-point center difference formula.

5-point Formulas

$$f'(x_0) \approx \frac{-25f(x_0)+48f(x_0+h)-36f(x_0+2h)+16f(x_0+3h)-3f(x_0+4h)}{12h} + h^4\frac{f^{[5]}(x_0)}{5}$$

$$f'(x_0) \approx \frac{-3f(x_0-h)-10f(x_0)+18f(x_0+h)-6f(x_0+2h)+f(x_0+3h)}{12h} - h^4\frac{f^{[5]}(x_0)}{20}$$

$$f'(x_0) \approx \frac{f(x_0-2h)-8f(x_0-h)+8f(x_0+h)-f(x_0+2h)}{12h} + h^4\frac{f^{[5]}(x_0)}{30}$$

$$f'(x_0) \approx \frac{-f(x_0-3h)+6f(x_0-2h)-18f(x_0-h)+10f(x_0)+3f(x_0+h)}{12h} + h^4\frac{f^{[5]}(x_0)}{20}$$

$$f'(x_0) \approx \frac{3f(x_0-4h)-16f(x_0-3h)+36f(x_0-2h)-48f(x_0-h)+25f(x_0)}{12h} - h^4\frac{f^{[5]}(x_0)}{5}$$

$$f''(x_0) \approx \frac{35f(x_0)-104f(x_0+h)+114f(x_0+2h)-56f(x_0+3h)+11f(x_0+4h)}{12h^2} - h^3\frac{5f^{[5]}(x_0)}{6}$$

$$f''(x_0) \approx \frac{11f(x_0-h)-20f(x_0)+6f(x_0+h)+4f(x_0+2h)-f(x_0+3h)}{12h^2} - h^3\frac{f^{[5]}(x_0)}{24}$$

$$f''(x_0) \approx \frac{-f(x_0-2h)+16f(x_0-h)-30f(x_0)+16f(x_0+h)-f(x_0+2h)}{12h^2} + h^4\frac{f^{[6]}(x_0)}{90}$$

$$f''(x_0) \approx \frac{-f(x_0-3h)+4f(x_0-2h)+6f(x_0-h)-20f(x_0)+11f(x_0+h)}{12h^2} - h^3\frac{f^{[5]}(x_0)}{24}$$

$$f''(x_0) \approx \frac{11f(x_0-4h)-56f(x_0-3h)+114f(x_0-2h)-104f(x_0-h)+35f(x_0)}{12h^2} - h^3\frac{5f^{[5]}(x_0)}{6}$$

Note: The error term is smallest for the centered difference approximations. If fact, symmetry allows the error in the second derivative to be on the order of h^4 versus h^3 for the other second derivative terms.

As an example, let's compare the use of the 3-point central difference versus the 5-point central difference to estimate the value of the second derivative of f(x)=cos(x) at x=0. Since the analytical solution is known f''(x=0) = -cos(0) = -1, then the accuracy can be compare for various values of h. The table below summarizes the results.

h	3-point	5-point
1.0000	-0.9193953883	-0.9898360449
0.1000	-0.9991669444	-0.9999988899
0.0100	-0.9999916667	-0.9999999999
0.0010	-0.9999999167	-0.9999999999
0.0001	-0.9999999939	-0.9999999939

The accuracy increases with decreasing h for both methods, but the 5-point method is more accurate for all h above 10^{-3}. Below this value of h and the formula error is no longer the dominant error as the computer precision begins to add errors.

Application to PDE Numerical Solutions

The 3-point center finite difference formulas are commonly used to approximate the first and second derivatives in numerical solutions to partial differential equations. If the 5-point finite difference formulas are used, then the accuracy could be improved or the number of discrete steps in the spatial dimensions can be reduced without sacrificing the accuracy of the solution. In order to investigate the usefulness of using the 5-point formulas over the 3-point formulas, a PDE with a known analytical solution will be solved using both 5-point and 3-point formulas. The parabolic PDE:

$$\frac{\partial c}{\partial t} = \frac{1}{\pi^2}\frac{\partial^2 c}{\partial x^2}$$

$$c(0,t) = 0$$

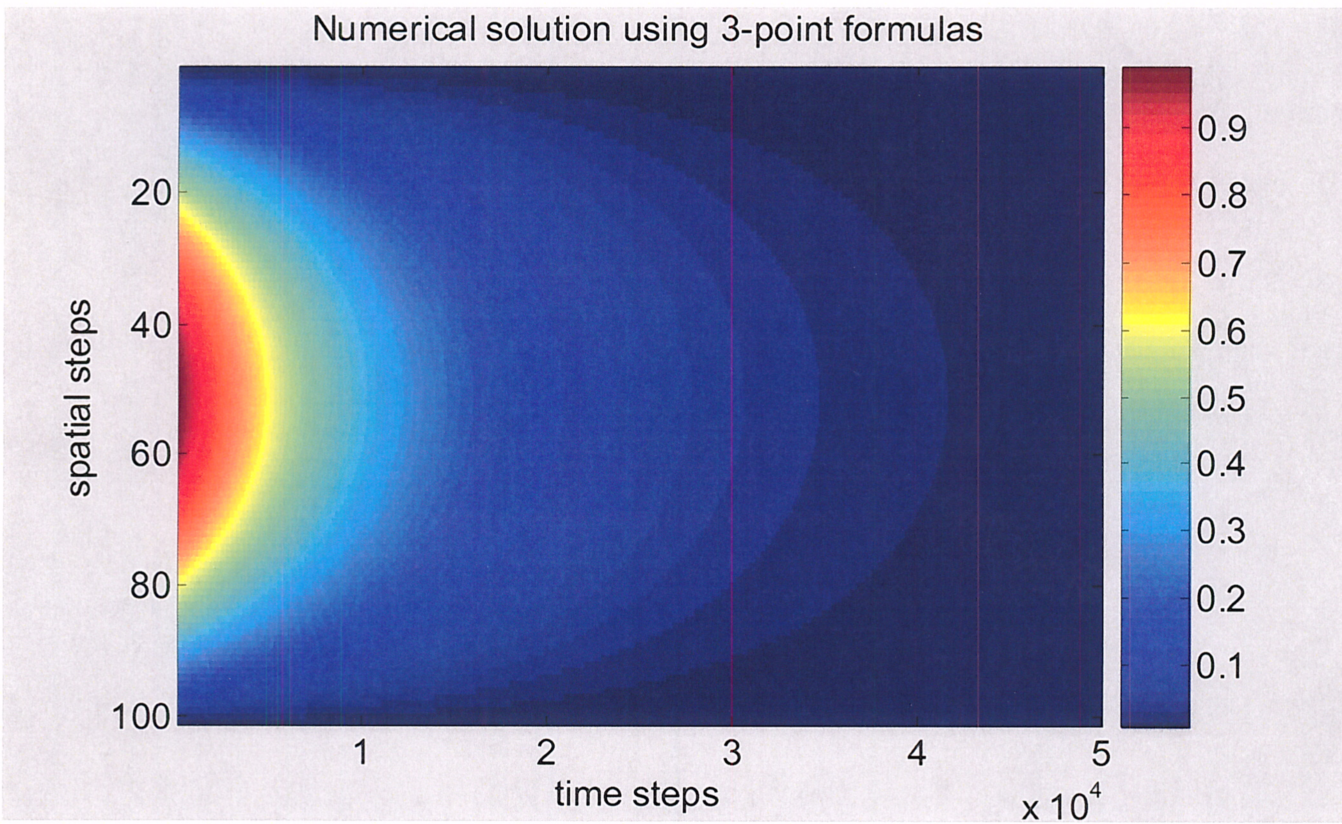
$$c(1,t) = 0$$

$$c(x,0) = \sin(\pi x)$$

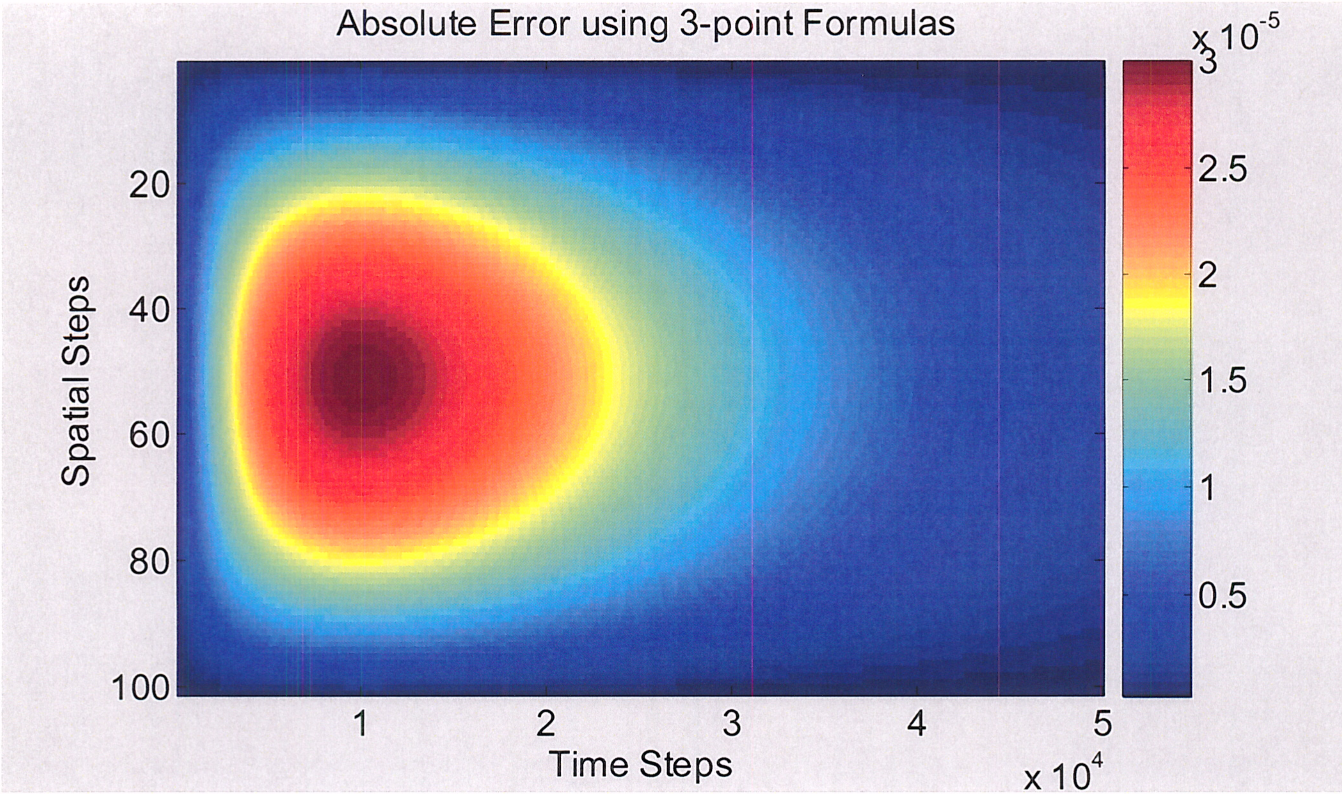
has the analytical solution:

$$c(x,t) = \sin(\pi x)e^{-t}$$

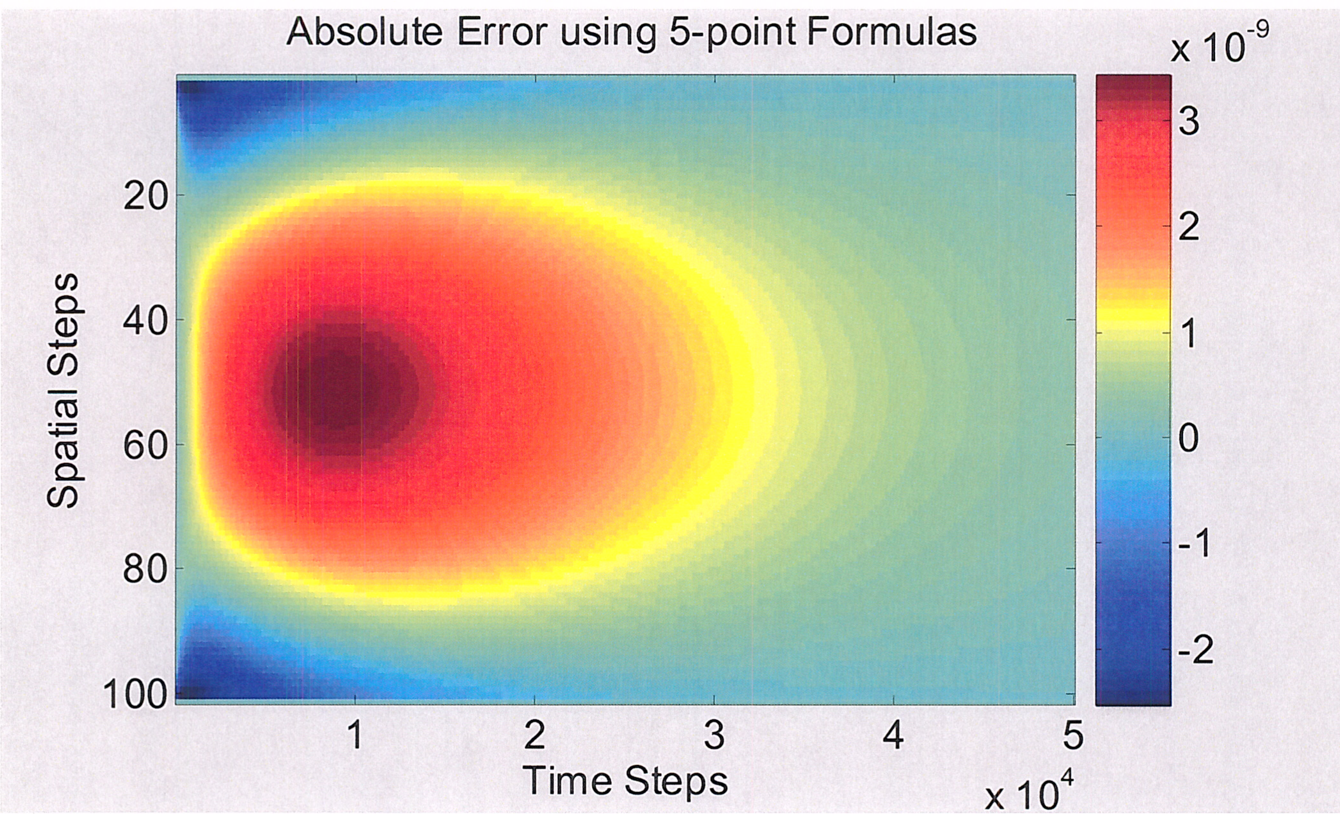
Using the 3-point formulas and dt=10^{-4}sec and dl=0.01, the numerical solution is plotted below:



The absolute error from the analytical solution is plotted below:



The maximum error is 3.03×10^{-5}. If the 5-point method is used for the same spatial and temporal resolution, the maximum error is 3.49×10^{-9}. A plot of absolute error is included below:



The spatial step size using 5-point formulas can be increased to 1/15 and still have comparable absolute error ($<2.2 \times 10^{-5}$) to the 1/100 step size using 3-point formulas. The code for the two methods is attached below as addendum.

```
%MSE 505 Project 2 3-point formula method for PDE approximation
% Solve dc/dt=1/pi^2*(d2c/dx2) 1-D PDE
clear;

%Simulation Parameters
L=1; %[m]
dl=0.01; %[m]
TotalTime=5; %[s]
dt=1e-4; %[s]
Cboundary=0.0;

%Initialize Arrays
x=[0:dl:L]';
C=zeros(floor(L/dl+1),floor(TotalTime/dt+1));
C(:,1)=sin(pi*x);
C(1,:)=Cboundary;
C(size(x),:)=Cboundary;
temp1=zeros(floor(L/dl+1),1);
temp2=zeros(floor(L/dl+1),1);

%2nd order Predictor-Corrector integration solver with 3-point
%approximations for spatial derivatives
TimeSteps=floor(TotalTime/dt);
LengthSteps=floor(L/dl);
for j=1:TimeSteps;
    for i=2:LengthSteps;
        temp1(i)=dt*(1/pi^2)*((C(i-1,j)-2*C(i,j)+C(i+1,j))/dl^2);
    end;
    for i=2:LengthSteps;
        temp2(i)=dt*(1/pi^2)*(((C(i-1,j)+temp1(i-1))-
2*(C(i,j)+temp1(i))+(C(i+1,j)+temp1(i+1)))/(dl^2));
    end;
    for i=2:LengthSteps;
        C(i,j+1)=C(i,j)+(temp1(i)+temp2(i))/2;
    end;
end;

%calculate analytical solution
A=zeros(floor(L/dl+1),floor(TotalTime/dt+1));
for i=1:(LengthSteps+1);
    for j=1:(TimeSteps+1);
        A(i,j)=sin(pi*(i-1)*dl)*exp(-1*(j-1)*dt);
    end;
end;
```

```
%MSE 505 Project 2 5-point formula method for PDE approximation
% Solve dc/dt=1/pi^2*(d2c/dx2) 1-D PDE
clear;

%Simulation Parameters
L=1; %[m]
dl=0.06666666666; %[m]
TotalTime=5; %[s]
dt=1e-4; %[s]
Cboundary=0.0;

%Initialize Arrays
x=[0:dl:L]';
C=zeros(floor(L/dl+1),floor(TotalTime/dt+1));
C(:,1)=sin(pi*x);
C(1,:)=Cboundary;
C(size(x),:)=Cboundary;
temp1=zeros(floor(L/dl+1),1);
temp2=zeros(floor(L/dl+1),1);

%2nd order Predictor-Corrector integration solver with 5-point
%approximations for spatial derivatives
TimeSteps=floor(TotalTime/dt);
LengthSteps=floor(L/dl);
for j=1:TimeSteps;
    temp1(2)=dt*(1/pi^2)*((11*C(1,j)-20*C(2,j)+6*C(3,j)+4*C(4,j)-
C(5,j))/(12*dl^2));
    for i=3:(LengthSteps-1);
        temp1(i)=dt*(1/pi^2)*((-1*C(i-2,j)+16*C(i-1,j)-
30*C(i,j)+16*C(i+1,j)-C(i+2,j))/(12*dl^2));
    end;
    temp1(LengthSteps)=dt*(1/pi^2)*((-1*C(LengthSteps-
3,j)+4*C(LengthSteps-2,j)+6*C(LengthSteps-1,j)-
20*C(LengthSteps,j)+11*C(LengthSteps+1,j))/(12*dl^2));
    temp2(2)=dt*(1/pi^2)*((11*(C(1,j)+temp1(1))-
20*(C(2,j)+temp1(2))+6*(C(3,j)+temp1(3))+4*(C(4,j)+temp1(4))-
(C(5,j)+temp1(5)))/(12*dl^2));
    for i=3:(LengthSteps-1);
        temp2(i)=dt*(1/pi^2)*((-1*(C(i-2,j)+temp1(i-2))+16*(C(i-
1,j)+temp1(i-1))-30*(C(i,j)+temp1(i))+16*(C(i+1,j)+temp1(i+1))-
(C(i+2,j)+temp1(i+2)))/(12*dl^2));
    end;
    temp2(LengthSteps)=dt*(1/pi^2)*((-1*(C(LengthSteps-
3,j)+temp1(LengthSteps-3))+4*(C(LengthSteps-2,j)+temp1(LengthSteps-
2))+6*(C(LengthSteps-1,j)+temp1(LengthSteps-1))-
20*(C(LengthSteps,j)+temp1(LengthSteps))+11*(C(LengthSteps+1,j)+temp1(L
engthSteps+1)))/(12*dl^2));
    for i=2:LengthSteps;
        C(i,j+1)=C(i,j)+(temp1(i)+temp2(i))/2;
    end;
end;

%calculate analytical solution
A=zeros(floor(L/dl+1),floor(TotalTime/dt+1));
for i=1:(LengthSteps+1);
    for j=1:(TimeSteps+1);
```

```
        A(i,j)=sin(pi*(i-1)*dl)*exp(-1*(j-1)*dt);
    end;
end;
```