Prof. Mark D Shattuck
Physics 39907 Computational Physics
December 22, 2023

Final Exam

Question 1. *Finite Element Method (FEM):* FEM can be used to find the solution $u(x)$ to differential equations like those based on:

$$u(x) \xrightarrow{A=\frac{d}{dx}} e(x) = \frac{d}{dx}u(x) \xrightarrow{C(x)} w(x) = C(x)e(x) \xrightarrow{A^T=-\frac{d}{dx}} -\frac{d}{dx}w(x) = f(x),$$

which gives a strong form:

$$-\frac{d}{dx}w(x) = f(x) \qquad [1]$$

$$-\frac{d}{dx}\left(C(x)e(x)\right) = f(x) \qquad [2]$$

$$-\frac{d}{dx}\left(C(x)\frac{d}{dx}u(x)\right) = f(x) \quad \text{plus B.C.} \qquad [3]$$

For FEM convert the strong form [[3] to the weak form by taking the inner product of the strong form with a test function $v(x)$ and applying integration by parts:

$$\int_a^b \frac{du(x)}{dx}v(x)\,dx = [u(x)v(x)]_a^b - \int_a^b u(x)\frac{dv(x)}{dx}\,dx$$

The inner product on the range $[a, b]$ of $u(x)$ and $v(x)$ is

$$(u(x), v(x)) = \int_a^b u(x)v(x)\,dx.$$

Then the weak form of [3] is:

$$\left(-\frac{d}{dx}\left(C(x)\frac{d}{dx}u(x)\right), v(x)\right) = (f(x), v(x)), \qquad [4]$$

$$\int_a^b -\frac{d}{dx}\left(C(x)\frac{du(x)}{dx}\right)v(x)\,dx = \int_a^b f(x)v(x)\,dx, \qquad [5]$$

$$\int_a^b C(x)\frac{du(x)}{dx}\frac{dv(x)}{dx}\,dx - \left[C(x)\frac{u(x)}{dx}v(x)\right]_a^b = \int_a^b f(x)v(x)\,dx, \qquad [6]$$

$$\int_a^b C(x)u'(x)v'(x)\,dx - [C(x)u'(x)v(x)]_a^b = \int_a^b f(x)v(x)\,dx. \qquad [7]$$

(1) Given the strong form:

$$-u''(x) = \delta(x-a) \quad \text{with } u'(0) = 0,\ u(1) = 0,\ 0 < a < 1,$$

show that the weak form is:

$$\int_0^1 u'(x)v'(x)\,dx = v(a). \qquad [8]$$

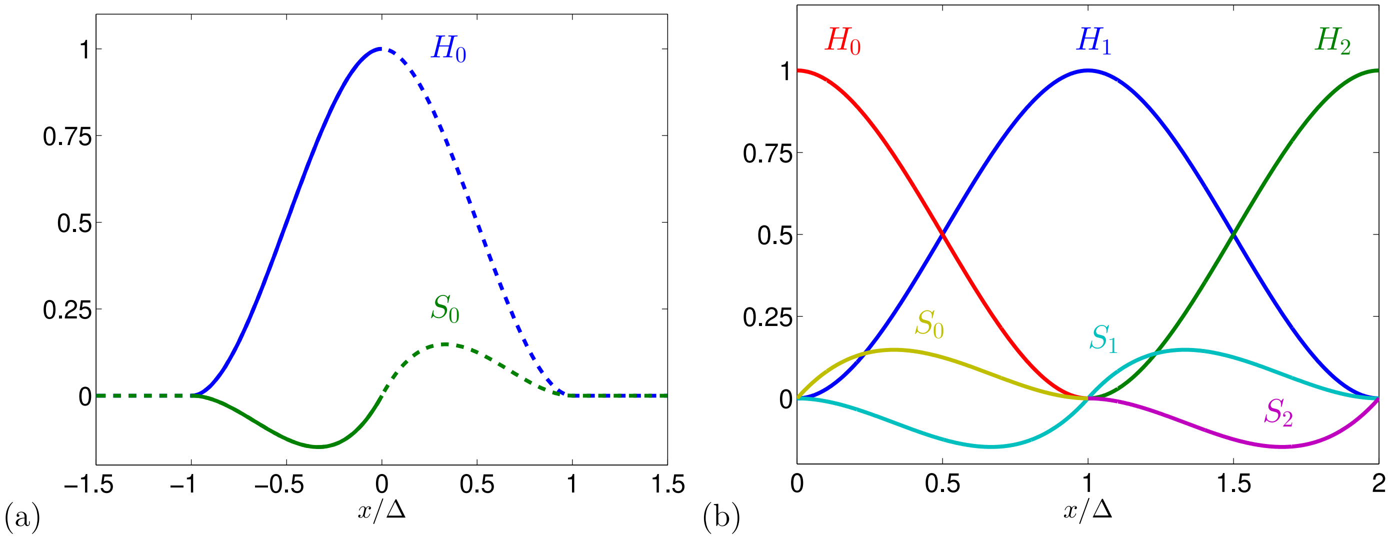

FIGURE 1. Piece-wise Cubic functions (a) at node 0 and (b) all functions that overlap H_1.

(2) In FEM, the solution $u(x)$ is approximated by:

$$u(x) = \sum_{k=0}^{K} u_k \phi_k(x). \qquad [9]$$

For this problem we will use two piece-wise cubic functions centered at each node located at $x_n = n\Delta$: a (H)eight function $H_n(x)$ and a (S)lope function $S_n(x)$ and corresponding coefficients u_n^H and u_n^S. Figure 1(a) shows $H_0(x)$ and $S_0(x)$ centered at node 0. The functions are zero and have zero slope at and beyond adjacent nodes at ± 1. At the central node 0, $H_0(0)$ has height 1 and slope 0, but $S_0(0)$ has slope 1 and height 0, so that $u_n^H H_n(x) + u_n^S S_n(x)$ has height u_n^H and slope u_n^S at node n. Using the symmetries, $H_0(x) = H_0(-x)$ and $S_0(x) = -S_0(-x)$, we can define them in terms local functions $H(x/\Delta)$ and $S(x/\Delta)$ on the interval $[-\Delta/\Delta, 0] = [-1, 0]$, shown as the solid lines in figure 1(a) as follows:

$$H_0(x) = H_0(x;\Delta) = \begin{cases} 0 & x/\Delta \leq -1 \\ H(x/\Delta) & -1 \leq x/\Delta \leq 0 \\ H(-x/\Delta) & 0 \leq x/\Delta \leq 1 \\ 0 & x/\Delta \geq 1 \end{cases} \qquad [10]$$

and

$$S_0(x) = S_0(x;\Delta) = \begin{cases} 0 & x/\Delta \leq -1 \\ S(x/\Delta) & -1 \leq x/\Delta \leq 0 \\ -S(-x/\Delta) & 0 \leq x/\Delta \leq 1 \\ 0 & x/\Delta \geq 1 \end{cases} \qquad [11]$$

H and S are defined in local grid coordinates x/Δ. These functions can be shifted to other nodes as shown in figure 1(b) using this equation $H_n(x) = H_0((x/\Delta - n)\Delta)$ and $S_n(x) = S_0((x/\Delta - n)\Delta)$. All of the functions $H_n(x)$ and $S_n(x)$ are shown in figure 1(b) for the interval $[0, 2\Delta]$. This represents all of the functions that overlap $H_1(x)$ and $S_1(x)$.

Find a cubic function $H(x)$ with the following properties:
(a) $H(x)$ is a cubic. For example, $H(x) = s(x-a)(x-b)(x-c)$.
(b) The derivative $H'(-1) = 0$ and $H'(0) = 0$.
(c) $H(-1) = 0$ and $H(0) = 1$.
Show that the cubic function $S(x) = x(x+1)^2$ has the following properties:
(a) $S(x)$ is a cubic.
(b) The derivative $S'(-1) = 0$ and $S'(0) = 1$.
(c) $S(-1) = 0$ and $S(0) = 0$.

(3) Using the approximation above, the solution for nodes 0-N is

$$u(x) = \sum_{n=0}^{N} u_n^S S_n(x) + u_n^H H_n(x), \tag{12}$$

and

$$u'(x) = \sum_{n=0}^{N} u_n^S S_n'(x) + u_n^H H_n'(x). \tag{13}$$

From this equation or figure 1 find the value of $u(\Delta)$, $u(\Delta/2)$, and $u'(\Delta)$ in terms of u_n^S and u_n^H.

(4) Show that [12] can be written in matrix form:

$$u(x) = \begin{bmatrix} u_0^S & u_0^H & \dots & u_N^S & u_N^H \end{bmatrix} \begin{bmatrix} S_0(x) \\ H_0(x) \\ \vdots \\ S_N(x) \\ H_N(x) \end{bmatrix} = u^T \phi(x)$$

and find a similar equation for $u'(x)$ from [13]. What is the shape (size) of u and ϕ?

(5) Plug [12] into the weak form [8] for

$$v_k(x) = \begin{bmatrix} v_0(x) \\ \vdots \\ v_{2N+1}(x) \end{bmatrix} = \begin{bmatrix} S_0(x) \\ H_0(x) \\ \vdots \\ S_N(x) \\ H_N(x) \end{bmatrix} = \phi(x)$$

to show that

$$\sum_{n=0}^{N} \int_0^1 (u_n^S S_n'(x) + u_n^H H_n'(x)) v_k'(x)\, dx = v_k(a) \tag{14}$$

$$\left(\int_0^1 \phi'(x) \phi'(x)^T\, dx \right) u = \phi(a) \tag{15}$$

$$K u = f. \tag{16}$$

What is the shape of K? Is K symmetric? Why? Why not?

(6) Set up [16] to solve [3] with $a = 3/8$, on a grid with 5 nodes and 4 intervals $x = \begin{bmatrix} 0 & 1 & 2 & 3 & 4 \end{bmatrix}^T \Delta$, $\Delta = 1/4$ by follow these steps:

(a) Fill in the missing elements in f for $N = 5$:

$$f = \begin{bmatrix} S_0(3/8) \\ H_0(3/8) \\ S_1(3/8) \\ H_1(3/8) \\ S_2(3/8) \\ H_2(3/8) \\ S_3(3/8) \\ H_3(3/8) \\ S_4(3/8) \\ H_4(3/8) \end{bmatrix} = \begin{bmatrix} 0 \\ ??? \\ S_0((3/8/\Delta - 1)\Delta) = S_0(1/2\Delta) = -S(-1/2) = -(-1/2)(-1/2+1)^2 = 1/8 \\ ??? \\ ??? \\ 1/2 \\ 0 \\ ??? \\ 0 \\ 0 \end{bmatrix}$$

(b) Find the functions S_0', H_0', S_1', H_1' in the interval $[0,1]$. From figure 1(b) notice that interval from $[0,1]$ is repeated in the interval $[1,2]$, but with $H_0 \to H_1$, $H_1 \to H_2$, $S_0 \to S_1$, $S_1 \to S_2$. Therefore all of the terms in K can be constructed from just the overlaps in the interval $[0,1]$. Fill in the missing function in this vector:

$$\phi_{loc} = \begin{bmatrix} S_0'(x) \\ H_0'(x) \\ S_1'(x) \\ H_1'(x) \end{bmatrix} = \begin{bmatrix} 3x^2 - 4x + 1 \\ 6x(x-1) \\ x(3x-2) \\ ??? \end{bmatrix}$$

(c) Evaluate [15] using the local ϕ_{loc}. There are 4 local function in each unit interval. Fill in the missing integrals in

$$K_{loc} = \int_0^1 \phi_{loc}\phi_{loc}^T \, dx = \int_0^1 \begin{bmatrix} S_0'(x) \\ H_0'(x) \\ S_1'(x) \\ H_1'(x) \end{bmatrix} \begin{bmatrix} S_0'(x) & H_0'(x) & S_1'(x) & H_1'(x) \end{bmatrix} dx$$

$$= \begin{bmatrix} \int_0^1 S_0'(x)S_0'(x)\,dx & \int_0^1 S_0'(x)H_0'(x)\,dx & ??? & ??? \\ \int_0^1 H_0'(x)S_0'(x)\,dx & \int_0^1 H_0'(x)H_0'(x)\,dx & ??? & ??? \\ ??? & ??? & ??? & ??? \\ ??? & ??? & ??? & ??? \end{bmatrix}$$

$$= \frac{1}{30} \begin{bmatrix} 30\int_0^1 (3x-1)^2(x-1)^2\,dx = 4 & ??? & ??? & ??? \\ 30\int_0^1 6x(3x-1)(x-1)^2\,dx = 3 & ??? & ??? & ??? \\ -1 & 3 & ??? & ??? \\ -3 & -36 & -3 & ??? \end{bmatrix}$$

$$= \frac{1}{30} \begin{bmatrix} 4 & ??? & ??? & ??? \\ 3 & ??? & ??? & ??? \\ -1 & 3 & ??? & ??? \\ -3 & -36 & -3 & ??? \end{bmatrix}$$

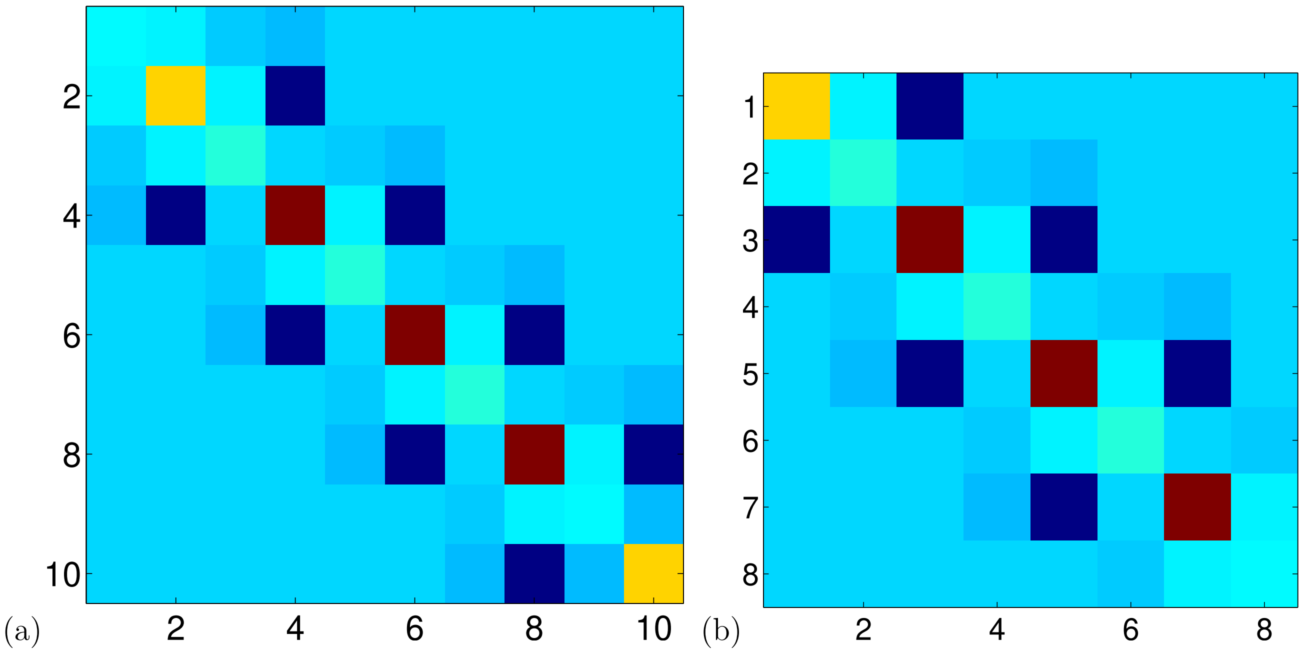

FIGURE 2. Global K.

(d) Use the following equation to build the global K from K_{loc}. The local matrix is shifted by 2 in each direction, then all of them are added for each unit in the grid.

$$K = \begin{bmatrix} k_{11} & k_{12} & k_{13} & k_{14} & 0 & 0 & 0 & \dots & 0 \\ k_{21} & k_{22} & k_{23} & k_{24} & 0 & 0 & 0 & \dots & 0 \\ k_{31} & k_{32} & k_{33} & k_{34} & 0 & 0 & 0 & \dots & 0 \\ k_{41} & k_{42} & k_{43} & k_{44} & 0 & 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 \\ 0 & 0 & k_{11} & k_{12} & k_{13} & k_{14} & 0 & \dots & 0 \\ 0 & 0 & k_{21} & k_{22} & k_{23} & k_{24} & 0 & \dots & 0 \\ 0 & 0 & k_{31} & k_{32} & k_{33} & k_{34} & 0 & \dots & 0 \\ 0 & 0 & k_{41} & k_{42} & k_{43} & k_{44} & 0 & \dots & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 \end{bmatrix} + \dots$$

$$+ \begin{bmatrix} 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \dots & 0 & 0 & 0 & k_{11} & k_{12} & k_{13} & k_{14} \\ 0 & \dots & 0 & 0 & 0 & k_{21} & k_{22} & k_{23} & k_{24} \\ 0 & \dots & 0 & 0 & 0 & k_{31} & k_{32} & k_{33} & k_{34} \\ 0 & \dots & 0 & 0 & 0 & k_{41} & k_{42} & k_{43} & k_{44} \end{bmatrix}$$

The properly assembled K is shown in figure 2(a). The figure was made using the following MATLAB command:

```
imagesc(K); axis('image'); colormap(jet(256));
```

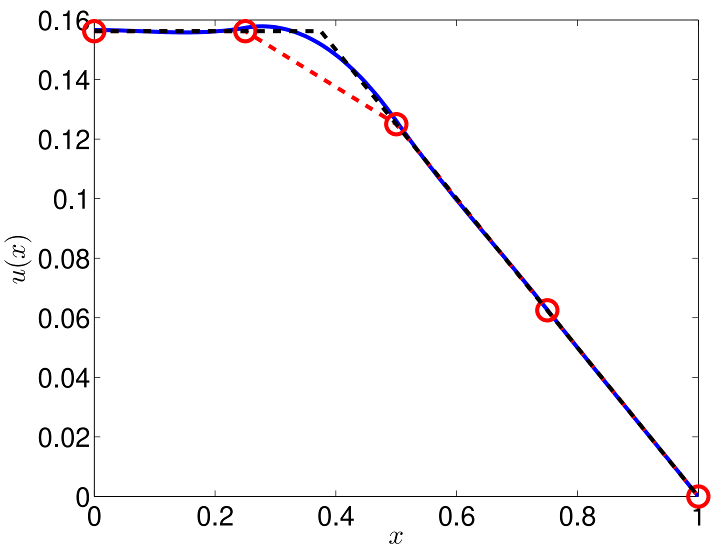

FIGURE 3. Comparison of FEM, finite differences, and exact result.

(e) Apply the boundary conditions. Eliminate any S_n or H_n that are determined by the boundary conditions and trim the global K. The final K is shown in figure 2(b).

(7) Use the K and f defined above to solve for u and report the values.

(8) Use the following MATLAB script to plot the results:

```
N=5;       % Number of nodes
a=3/8;     % Location of forcing delta function

dx=1/(N-1);  % grid spacing \Delta
K=???; % fill in the values for K
f=???; % fill in the values for f

u=???; % solve for u. note: include any boundary values as well.

u2=???; % solve the same problem using finite differences e.g., free-fixed (T)

x=0:dx/50:1;  % locations to find U(x)

U=evalFEM(x,u,dx); % calculate U(x) from x, u, and, dx

ue=((1-x).*(x>a)+(1-a).*(x<=a))/4;  % exact solution

% plot results
h=plot(x,U,(0:N-1)*dx,u2,'ro--',x,ue,'k--');

% make it pretty
set(h,'linewidth',3,'markersize',15);
set(gca,'fontsize',20);
xlabel('$x$','interp','latex');
ylabel('$u(x)$','interp','latex');
```

In the script you will need to provide K and f, and code to calculate the resulting coefficients u. The MATLAB function `evalFEM()` used to evaluate equation [12] is here `evalFEM.m` and listed below. It uses absolute values to express 10 and 11 more compactly in local coordinates $\nu = x/\Delta$:

$$S_0(\nu) = \begin{cases} \nu(|\nu|-1)^2 & |\nu| < 1 \\ 0 & else \end{cases}$$

$$H_0(\nu) = \begin{cases} (2|\nu|+1)(|\nu|-1)^2 & |\nu| < 1 \\ 0 & else \end{cases}$$

You will need to supply code to calculate the same solution using 5-point finite differences. The exact solution:

$$u_e(x) = \begin{cases} (1-x)/4 & a \geq x \leq 1 \\ (1-a)/4 & 0 \geq x \leq a \end{cases}$$

Use the code above or your own code to plot the FEM, FD, and exact solution.

```
function [U,S,H]=evalFEM(x,u,dx,H,S)
% evalFEM <Find value of C1 cubic FEM>
% Usage:: [U,S,H]=evalFEM(x,u,dx[1],...
%   H[@(x) (2*abs(x)+1).*(abs(x)-1).^2.*(abs(x)<1)],...
%   S[@(x) x.*(abs(x)-1).^2.*(abs(x)<1)])
%

% revision history:
% 12/10/2023 Mark D. Shattuck <mds> evalFEM.m

%% Parse Input
if(~exist('dx','var') || isempty(dx))
    dx=1;
end

if(~exist('H','var') || isempty(H))
    H=@(x) (2*abs(x)+1).*(abs(x)-1).^2.*(abs(x)<1);
end

if(~exist('S','var') || isempty(S))
    S=@(x) x.*(abs(x)-1).^2.*(abs(x)<1);
end

%% Main
N=length(u)/2;
U=0;
for n=0:N-1;
  U=U+u(2*n+1)*S(x/dx-n)+u(2*n+2)*H(x/dx-n);
end;
```

Question 2. *Partial Differential Equation PDE:* A PDE is a differential equation which depends on derivatives of more than one variable. In this problem, we will solve a modified 2D Cahn–Hilliard equation on periodic boundary conditions:

$$\frac{\partial c}{\partial t} = \nabla^2 \mu \tag{[1]}$$

$$\mu = W(c) - \gamma \nabla^2 c \tag{[2]}$$

$$W(c) = (c-1)c(c-1/2) \tag{[3]}$$

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \tag{[4]}$$

and $c = c(x, y, t)$ is a function of space and time. This equation determines the concentration $c(x, y, t)$ of one fluid mixed with another immiscible fluid, like oil and water. A concentration of 1 at position (x, y) and time t means all of one fluid. The concentration of the second fluid is $1 - c(x, y, t)$. If the fluids start mixed, they will demix over time.

(1) Convert the equations to 1 dimension, by eliminating y. To get an equation of the form:

$$\frac{\partial c(x,t)}{\partial t} = A(c(x,t)).$$

The function A will depend on c and its x-derivatives.

(2) Create a MATLAB script to begin solving these equation. You will need the constant `gam=3e-5`, the grid size `Nx=128`, a domain of size `Lx=1;`, and a time step of `dt=1e-6`. From these calculate the grid spacing `dx=???`.

(3) We will use first-order forward Euler integration to solve the equation in time. Discretize the equation in time and write the first order approximation for

$$\frac{\partial c(x,t)}{\partial t} \approx \frac{c_{n+1}(x) - c_n(x)}{\Delta t} = A(c_n(x)),$$

and solve for $c_{n+1}(x)$. This represents our update rule. What is $c_n(x)$ in terms of $c(x, t)$?

(4) To update $c_n(x)$ we need an initial condition. Add a variable `c` to your code to represent $c_n(x)$ and set the initial condition to get a random 0 or 1 at each location. A good way to get random 1's and 0's is with `rand(3,1)>1/2`. This will give a 3×1 column vector of random 1's and 0's. `c` should be a column vector of size `[Nx,1]`.

(5) To evaluate $A(c(x))$ second derivatives are needed. If we use a discrete representation of $c_k = c(k\Delta x)$, the second derivative is:

$$c''(k\Delta x) \approx \frac{c_{k-1} - 2c_k + c_{k+1}}{(\Delta x)^2}$$

With periodic boundary conditions the matrix version is `Dxx*c`, where

```
Dxx=toeplitz([-2 1 0 ??? 0 1])/dx/dx;.
```

Add this to your code and replace the `0 ??? 0` so that `Dxx*c` works for any size `Nx` vector `c`.

(6) Test `Dxx` on `sin(2*pi*x)`, where `x` is size `[Nx,1]` and goes from `0` to `1-1/Nx`. When it is working `Dxx*sin(2*pi*x)` should be approximately `-(2*pi)^2*sin(2*pi*x)`, since $(\sin(ax))'' = -a^2 \sin(x)$.

(7) Putting it all together. Add a loop to your code that will use the update rule above to move forward by steps of `dt`. The code will calculate $A(c)$ then update c then repeat. Add an integration total time `TT=.05;` to your code. Calculate the integer number of time steps `Nt` needed to reach `TT`

i.e., `Nt*dt` is approximately `TT`. Here is my version with some blanks. It includes code to plot the solution, comments, and code to save the result which you should add to your code.

```
%% 1D Cahn-Hillard Simulator
% <CH1d.m> Mark D. Shattuck 12/10/2023

% revision history:
% 12/10/2023 Mark D. Shattuck <mds> CH1d.m
%
% 12/10/2023 mds set up for PHYS 339 final
%
%% Experimental Parameters
gam=.00003;  % control parameter

Nx=128;      % Number of grid points on
Lx=1;        % Size of container

TT=.05;      % Total simulation time

%% Simulation parameters
dt=1e-6;

%% Calculated parameters
Nt=???;    % number of Time steps
dx=???;    % grid spacing
x=(0:Nx-1)'*dx;  % x-grid for plotting and testing

% 2nd derivative of a column vector
Dxx=toeplitz([-2 1 ???? 1])/dx/dx;
Dxx=sparse(Dxx);  % convert to sparse for speed

%% initial conditions
c=rand(Nx,1)>1/2;  % random initial condition

%% Save State
cs=zeros(Nx,Nt);  % save every time step

%% Main loop

for nt=1:Nt
  mu=???;    % mu is function of c, Dxx, and gam
  dc=Dxx*mu; % from equation [1]
  c=c+???;   % update rule

  % give feedback by plotting
  if(rem(nt,fix(Nt/100))==0)
    plot(x,c)
    drawnow;
    disp([nt/100 mean(c(:))]);
  end

  cs(:,nt)=c;  % save results
end
```

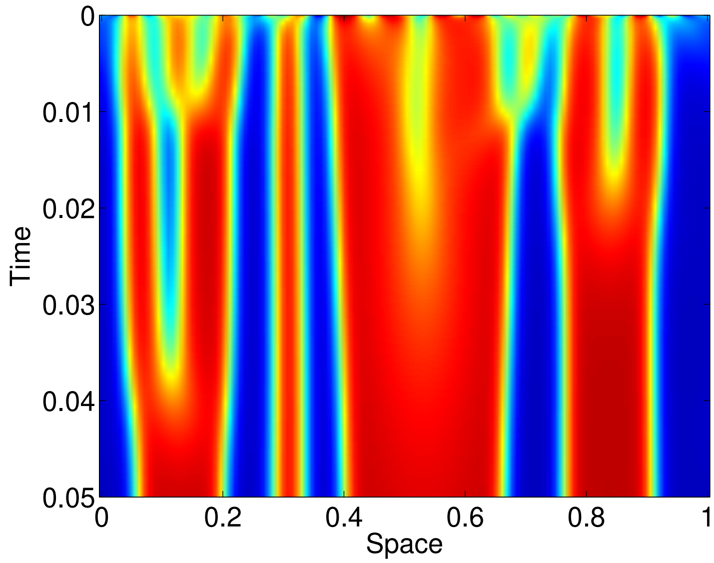

FIGURE 4. Space-time plot of 1D Cahn-Hillard equation.

When it is working use:

```
imagesc([0 Lx],[0 TT],cs');
xlabel('Space');
ylabel('Time');
colormap(jet(256));
```

to get a plot like figure 4. The red is one fluid and the blue is the second fluid. The red regions separate from the blue.

(8) Copy your 1D code to a new script and convert to 2D. There is not a lot to change. The main issue is the derivatives in y. If you convert `c` from a `[Nx,1]` matrix to a `[Nx,Ny]` matrix, then it turns out that multiplying `c*Dyy'` from the right by the transpose will take the derivative in the other direction, where `Dyy` is defined in analogy to `Dxx`. Second derivatives are symmetric `Dyy=Dyy'` so the transpose is not needed. Here is my version with missing parts:

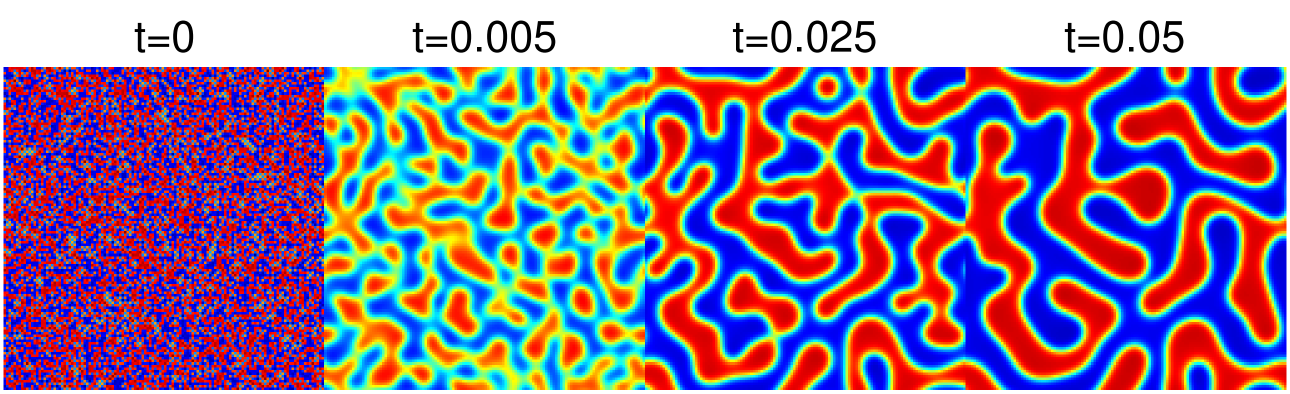

FIGURE 5. 2D evolution of Cahn-Hillard equation

```
%% 2D Cahn-Hillard Simulator
% <CH1d.m> Mark D. Shattuck 12/10/2023

% revision history:
% 12/10/2023 Mark D. Shattuck <mds> CH1d.m
%
% 12/10/2023 mds set up for PHYS 339 final
% 12/14/2023 mds conver to 2D CH2d.m

%% Experimental Parameters
gam=.00003;  % control parameter

Nx=128;      % Number of grid points in x
Ny=128;      % Number of grid points in y
Lx=1;        % Size of container in x
Ly=1;        % Size of container in y

TT=.05;      % Total simulation time

%% Simulation parameters
dt=1e-6;

%% Calculated parameters
Nt=???;   % number of Time steps
dx=???;        % x-grid spacing
dy=???;        % y-grid spacing

% 2nd derivative of a matrix
Dxx=toeplitz([-2 1 ???? 1]/dx/dx);
Dxx=sparse(Dxx);  % convert to sparse for speed

Dyy=toeplitz([-2 1 ????? 1]/dy/dy);
Dyy=sparse(Dyy);  % convert to sparse for speed

%% initial conditions
c=????;  % random initial condition now (Nx,Ny)

%% Main loop
for nt=1:Nt
  mu=????;              % mu is function of c, Dxx, and gam
  dc=Dxx*mu+mu*Dyy;     % from equation [1]
  c=c+???;              % update rule

  % give feedback by plotting
  if(rem(nt,fix(Nt/200))==0)
    imagesc([0 Ly],[0 Lx],c);  % now display current image
    axis('image');
    drawnow;
    disp([nt/100 mean(c(:))]);
  end
end
```

When it is working it will look like figure 5.

(9) Try changing some things a see what happens. Some examples:
  (a) Make `Ly` and/or `Ny` bigger or smaller.
  (b) Change the initial condition so that there are more or less 1's.
  (c) Changing the 1/2 in $W(c)$ is interesting, 1/4 or 3/4.
  (d) What happens if `dt` is too big? How big can it be? Is the maximum `dt` effected by other parameters.
  (e) What does `gam` do?