Prof. Mark D Shattuck Physics 39907 Computational Physics November 26, 2024

## 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:

$$-\frac{d}{dx}w(x) = f(x) \tag{1}$$

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

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

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

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:

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

$$\int_{a}^{b} -\frac{d}{dx} \left( C(x) \frac{du(x)}{dx} \right) v(x) \ dx = \int_{a}^{b} f(x) v(x) \ dx, \tag{5}$$

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

$$\int_{a}^{b} C(x)u'(x)v'(x) dx - \left[C(x)u'(x)v(x)\right]_{a}^{b} = \int_{a}^{b} f(x)v(x) dx.$$
 [7]

(1) Given the strong form:

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

show that the weak form is:

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

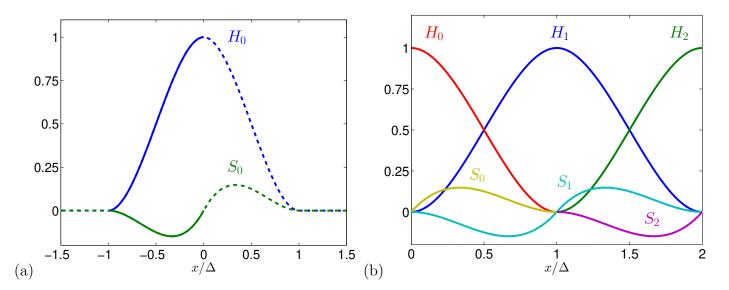


FIGURE 1. Piece-wise Cubic functions (a) at node 0 and (b) all functions that overlap  $H_1$ .

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

$$u(x) = \sum_{k=0}^{K} u_k \phi_k(x).$$
 [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  $\pm 1$ . 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  $u_n^S$  at node

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

and

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

H and S are defined in local grid coordinates  $x/\Delta$ . These functions can be shifted to other nodes as shown in figure  $\mathbf{1}(b)$  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  $\mathbf{1}(b)$  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

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

and

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

(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

$$\sum_{n=0}^{N} \int_{0}^{1} (u_{n}^{S} S_{n}'(x) + u_{n}^{H} H_{n}'(x)) v_{k}'(x) dx = v_{k}(a)$$
 [14]

$$\left(\int_0^1 \phi'(x)\phi'(x)^T dx\right) u = \phi(a)$$
 [15]

$$Ku = f. [16]$$

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:

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

(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  $\phi_{loc}$ . There are 4 local function in each unit interval. Fill in the missing integrals in

$$K_{loc} = \int_{0}^{1} \phi_{loc} \phi_{loc}^{T} dx = \int_{0}^{1} \begin{bmatrix} S_{0}'(x) \\ H_{0}'(x) \\ S_{1}'(x) \\ H_{1}'(x) \end{bmatrix} \begin{bmatrix} S_{0}'(x) & H_{0}'(x) & S_{1}'(x) & H_{1}'(x) \end{bmatrix} dx$$

$$= \begin{bmatrix} \int_{0}^{1} S_{0}'(x) S_{0}'(x) dx & \int_{0}^{1} S_{0}'(x) H_{0}'(x) dx & ???? & ??? \\ \int_{0}^{1} H_{0}'(x) S_{0}'(x) dx & \int_{0}^{1} H_{0}'(x) H_{0}'(x) dx & ???? & ??? \\ ??? & ??? & ???? & ???? & ???? & ???? \\ ??? & ??? & ???? & ???? & ???? & ???? \\ 30 \int_{0}^{1} (3x - 1)^{2} (x - 1)^{2} dx = 4 & ??? & ???? & ??? \\ & & -1 & 3 & ???? & ??? \\ & & -3 & -36 & -3 & ??? \end{bmatrix}$$

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

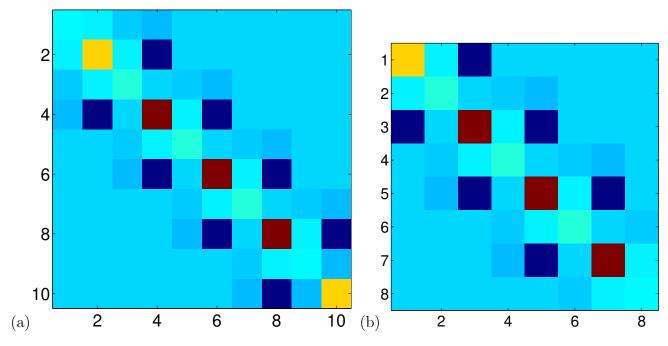


FIGURE 2. Global K.

(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.

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));
```

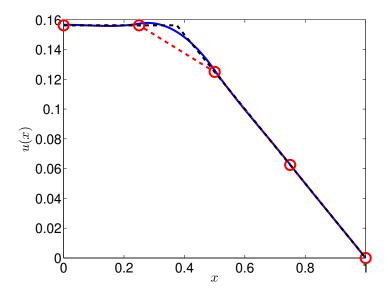


FIGURE 3. Comparison of FEM, finite differences, and exact result.

- (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 (FEMOOO.m) to plot the results:

```
1 N=5;
             % Number of nodes
             % Location of forcing delta function
  a=3/8;
  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)
10
11
  x=0:dx/50:1; % locations to find U(x)
12
13
  U=evalFEM(x,u,dx); % calculate U(x) from x, u, and, dx
14
15
16
  ue=((1-x).*(x>a)+(1-a).*(x<=a))/4; % exact solution
17
  % plot results
  h=plot(x,U,(0:N-1)*dx,u2,'ro--',x,ue,'k--');
20
  % make it pretty
  set(h,'linewidth',3,'markersize',15);
23 set(gca,'fontsize',20);
24 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:

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

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

```
1 function [U,S,H]=evalFEM(x,u,dx,H,S)
2 % 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)])
6
7
  % revision history:
  % 12/10/2023 \text{ Mark D. Shattuck } < mds > evalFEM.m
10
  %% Parse Input
11
  if(~exist('dx','var') || isempty(dx))
13
       dx=1;
14
  end
15
  if(~exist('H','var') || isempty(H))
16
       H=@(x) (2*abs(x)+1).*(abs(x)-1).^2.*(abs(x)<1);
17
18
  end
19
  if(~exist('S','var') || isempty(S))
20
       S=@(x) x.*(abs(x)-1).^2.*(abs(x)<1);
21
22
  end
23
24 %% Main
25 N=length(u)/2;
26 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);
28
29 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:

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

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

$$W(c) = (c-1)c(c-1/2)$$
 [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 (outlined below) 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.

```
1 %% 1D Cahn-Hillard Simulator
2 % <CHld.m> Mark D. Shattuck 12/10/2023
4 % revision history:
5 \% 12/10/2023 Mark D. Shattuck <mds> CHld.m
7 \% 12/10/2023 mds set up for PHYS 339 final
9 %% Experimental Parameters
10 gam=.00003; % control parameter
11
12 \text{ Nx}=128;
                % Number of grid points on
13 Lx=1;
                % Size of container
14
                % Total simulation time
15 TT=.05;
16
17 %% Simulation parameters
18 dt=1e-6;
19
20 %% Calculated parameters
           % number of Time steps
21 Nt=???;
  dx = ???;
             % grid spacing
23
  x=(0:Nx-1)'*dx; % x-grid for plotting and testing
24
25 % 2nd derivative of a column vector
26 Dxx=toeplitz([-2 1 ???? 1])/dx/dx;
27 Dxx=sparse(Dxx); % convert to sparse for speed
28
29 %% initial conditions
30 c=rand(Nx,1)>1/2; % random initial condition
31
32 %% Save State
33 cs=zeros(Nx,Nt); % save every time step
34
35 %% Main loop
36
  for nt=1:Nt
37
38
    mu=???;
                % mu is function of c, Dxx, and gam
    dc=Dxx*mu; % from equation [1]
39
     c=c+???;
              % update rule
40
41
     % give feedback by plotting
42
43
    if(rem(nt, fix(Nt/100)) == 0)
44
      plot(x,c)
45
       drawnow;
46
       disp([nt/100 mean(c(:))]);
47
    end
48
    cs(:,nt)=c; % save results
49
50 end
```

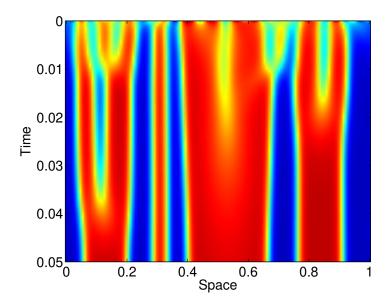


FIGURE 4. Space-time plot of 1D Cahn-Hillard equation.

When it is working use:

```
1 imagesc([0 Lx],[0 TT],cs');
2 xlabel('Space');
3 ylabel('Time');
4 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:

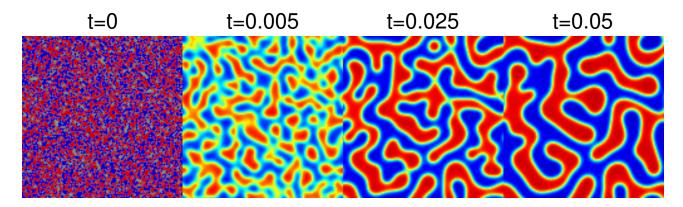


Figure 5. 2D evolution of Cahn-Hillard equation

```
1 %% 2D Cahn-Hillard Simulator
2 % <CHld.m> Mark D. Shattuck 12/10/2023
4 % revision history:
5 % 12/10/2023 Mark D. Shattuck <mds> CHld.m
  % 12/10/2023 mds set up for PHYS 339 final
7
  % 12/14/2023 mds conver to 2D CH2d.m
10 %% Experimental Parameters
11 gam=.00003; % control parameter
12
                % Number of grid points in x
13 Nx=128;
14 Ny=128;
                % Number of grid points in y
15 Lx=1;
                % Size of container in x
                % Size of container in y
16 Ly=1;
17
18 TT=.05;
             % Total simulation time
19
20 %% Simulation parameters
21 dt = 1e - 6;
22
23 %% Calculated parameters
24 Nt=???; % number of Time steps
25 dx=???;
                  % x-grid spacing
                  % y-grid spacing
26 dy=???;
27
28 % 2nd derivative of a matrix
29 Dxx=toeplitz([-2 1 ???? 1]/dx/dx);
30 Dxx=sparse(Dxx); % convert to sparse for speed
31
32 Dyy=toeplitz([-2 1 ????? 1]/dy/dy);
33 Dyy=sparse(Dyy); % convert to sparse for speed
34
35 %% initial conditions
36 c=????; % random initial condition now (Nx, Ny)
37
38 %% Main loop
39 for nt=1:Nt
40
    mu=????;
                         % mu is function of c, Dxx, Dyy, and gam
    dc=Dxx*mu+mu*Dyy;
41
                         % from equation [1]
42
    c=c+???;
                         % update rule
43
44
     % give feedback by plotting
    if(rem(nt, fix(Nt/200)) == 0)
45
46
       imagesc([0 Ly],[0 Lx],c); % now display current image
47
       axis('image');
       drawnow;
48
       disp([nt/100 mean(c(:))]);
49
    end
51 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?