MSE 493/593
Fall 2011
Thornton

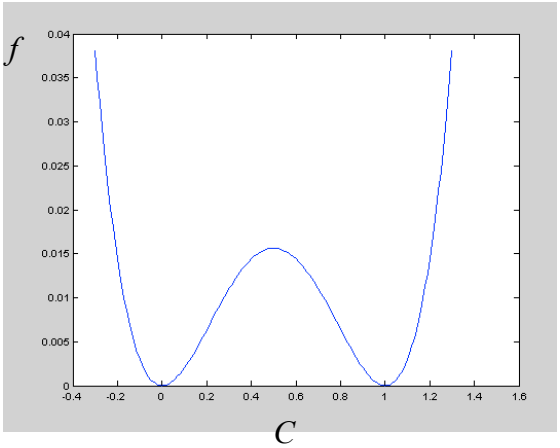
Homework #6/Lab6
November 21, 2011

MSE 493/593
Computational Approaches in Materials Science and Engineering
Homework #6
Due November 30, 2011

The purpose of this lab and assignment is to get hands-on experience in a phase-field model and use it to examine spinodal decomposition and nucleation and growth. This assignment is 60 points total.

As we discussed, the Cahn-Hilliard (CH) equation describes evolution of a conserved order parameter. In this lab, you will modify the program you wrote for Lab #3 (unless you want to start from scratch) to solve the equation with constant mobility M:

$$\frac{\partial c}{\partial t} = M\nabla^2 \frac{\delta \mathsf{F}}{\delta c} = M\nabla^2\left(\frac{df}{dc} - \varepsilon^2\nabla^2 c\right), \text{ where } \frac{df}{dc} = \frac{d}{dc}\left(\frac{W}{4}c^2(1-c)^2\right) = \frac{W}{2}c(1-c)(1-2c).$$



Double well potential, W=1

Use the first order explicit time stepping scheme (Euler's method) and the second order centered differencing for the Laplacians.

The parameters are:

$$W = 1 \quad dx = 0.1 \quad M = 1 \quad t_f = 50$$
$$\varepsilon = 0.1 \quad N = 200 \quad t_0 = 0 \quad dt = 0.001$$

1. [10 points] **Verify** the steady-state solution of the CH equation by substituting

$$\phi = \tanh\left(\frac{x - x_0}{2\ell}\right)$$

into the equation as was given in the lecture note (Lecture 11, page 16). **Derive** the relationship between ℓ, ε, and W.

2. [15 points] **Modify** the Matlab program used for the diffusion equation to solve the CH equation using the parameters above. You may use any reasonable initial conditions, but

the one specified for #3 below is a good place to start. **Plot the concentration profile** every 500 time steps (to view) so that you can observe the change in real time (for now, just set up to do this). Make sure you put a pause statement when you plot so you can stop the run when needed. Remember:

$$\nabla^2 f = \frac{f_{i+1} - 2f_i + f_{i-1}}{(\Delta x)^2}$$

$$C_i^{n+1} = C_i^n + \left.\frac{dC}{dt}\right|_i^n \Delta t \,.$$

3. [10 points] For this part, the initial condition should be set such that there is a random fluctuation around C_{ave} with maximum fluctuation of ±0.1. Set $C_{ave} = 0.5$ and **evolve** the concentration. **Describe** what happens. **Select three times to represent the evolution and capture the screen shots for submission.**

4. [10 points] Now, **set** the initial condition with $C_{ave} = 0.20$ (with the same fluctuation as above) and **evolve** the concentration. **Describe** what happens. (You may want to run this a few times with a different seed to make sure you get the same result, especially if you get an unexpected result.) **Select three times to represent the evolution and capture the screen shots for submission.**

5. [5 points] **Offer an explanation** between the difference between the results in #3 & #4.

6. [10 points] **Set** C at index range of 100 to 111 to 0.95, with the rest of concentration having $C_{ave} = 0.15$ with maximum fluctuation of ±0.1 (this will keep C_{ave} to be about 0.2, same as in #4). **Describe** the observation, and **explain** the physical/mathematical cause of the difference. **Select three times to represent the evolution and capture the screen shots for submission.**

7. (Optional; just for fun) The program can easily be extended to 2D. For this, remember that the Laplacian is given by

$$\nabla^2 f = \frac{f_{i,j+1} + f_{i,j-1} + f_{i+1,j} + f_{i-1,j} - 4f_{i,j}}{\Delta^2},$$

where $\Delta=\Delta x=\Delta y=0.1$. Matlab is slow so only early evolution can be observed, but you can obtain beautiful pictures describing phase separation nevertheless. Modify the 1D code to 2D (use the same parameters as before, except for the following: $N_x=N_y=100$, $\Delta t=0.0003$, $t_f=5$), and visualize the phase separation for $C_{ave} = 0.5$ (with ±0.1 fluctuation as before) every 100 time steps using

```
pcolor(C);
shading flat
axis equal
```

You should print out the maximum and minimum of C every time you plot so that you know what values the color range spans. Submit a picture if you like.