CMSE821 FS23 Final exam

Date: 12/11/2023 (Mon) due on 12/14/2023 (Thu); You need to submit executable files so that we can test your code. You can either embed text, formulas, and figures to the same file, or submit the text files separately.

In this exam, you are asked to reproduce phase field simulations in a published paper. Particularly, we will simulate snowflake formation (six-fold solidification in materials science terminology). The example results are provided at the two links below.

- solid growth: https://youtu.be/VpP-nweuPCk
- temperature: https://youtu.be/HqFnUwgMkpY

Not only in snowflake formation, dendritic growth is also generic for all solidification processes; see the video clip linked.

The original paper of dendritic growth modeling is here:

Ryo Kobayashi, Modeling and numerical simulations of dendritic crystal growth, *Physica D*, **63** (1993) 410-423. https://doi.org/10.1016/0167-2789(93)90120-P

This is a widely used solidification model, which couples two governing equations. The first is the Allen-Cahn (or Ginzburg-Landau) equation, which describes the solid growth process. The second is the heat equation, which describes the temperature evolution around the growing solid. They are given as

$$\frac{\partial \phi}{\partial t} = -M\left(\frac{\partial f}{\partial \phi} - \nabla \cdot \varepsilon^2 \nabla \phi + m(T)\right) \tag{1}$$

$$\frac{\partial T}{\partial t} = \nabla^2 T + K\frac{\partial \phi}{\partial t}, \tag{2}$$

where

$$\frac{\partial f}{\partial \phi} = \frac{1}{2}\phi\big(1-\phi\big)\big(1-2\phi\big) \tag{3}$$

$$m(T) = \frac{\alpha}{\pi}\phi\big(1-\phi\big)\tan^{-1}\big[\gamma\big(T-T_m\big)\big]. \tag{4}$$

ϕ in Eq. (1) indicates the solid region and T in Eq. (2) indicates temperature. Here, let's set up the simulation parameters as $M = 3000$, $\alpha = 0.9$, $\gamma = 10$, $T_m = 1$, and $K = 1.6$. This set of equations are derived from thermodynamics, but we are not going to walk through that. We can simply think $m(T)$ is the formation enthalpy due to temperature deviation away from equilibrium point (melting/solidification point). The term of $K(\partial\phi/\partial t)$ accounts for the transfer between formation energy and thermal energy, *i.e.,* the latent heat. Note that the molecules in the vapor phase have a higher energy than those in solid. Thus, when they transform to solid, the energy is released by increasing the temperature. The solid temperature increases (observed in the video clip).

Task 1. (10 pt) Discretization and initial conditions. The 2D domain is shown in Fig. 1(a), where $L_x = L_y = 9$. No-gradient Neumann boundary conditions (for both ϕ and T) are imposed on the four sides. Discretize the 2D domain with grid spacing $h = 0.03$, such that we have 301×301 grid points over the 2D domain. The initial condition of ϕ is a loose nucleus. Let's define it by

$$\phi_0 = \frac{1}{2}\left[1 - \tanh\left(\frac{r-0.25}{0.015}\right)\right]\eta, \tag{5}$$

where η is a random noise (between 0 and 1 at each grid point within the region of ϕ_0). The radius is defined by

$$r = \sqrt{(x-4.5)^2 + (y-4.5)^2}. \tag{6}$$

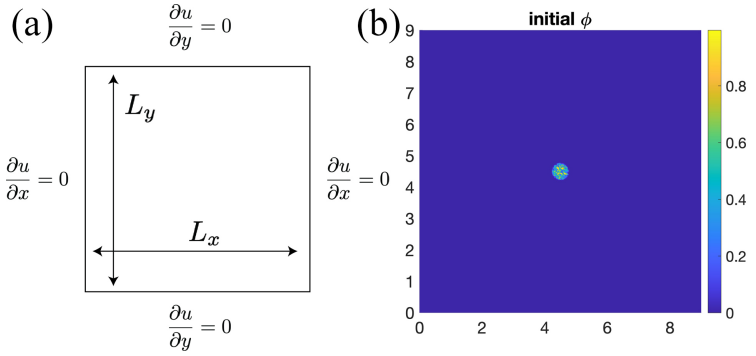

Figure 1: (a) 2D domain and boundary conditions in the problem set. (b) Initial condition of ϕ.

The initial temperature is uniformly zero throughout the domain, *i.e.*, $T_0 = 0$. Plot the initial conditions of ϕ and T. You should get something like Fig. 1(b).

Task 2. (30 pt) Isotropic growth. Let's use simplest methods first. Assume ε is a constant and $\varepsilon = 0.01$. Use **Euler method** in time and **5-point stencil** for the Laplacians in Eqs. (1) and (2). In each time step, you can update ϕ by

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = -M\left(\frac{\partial f}{\partial \phi} - \varepsilon^2 \nabla^2 \phi + m(T)\right)^n \tag{7}$$

and then update T by

$$\frac{T^{n+1} - T^n}{\Delta t} = \nabla^2 T^n + K\frac{\phi^{n+1} - \phi^n}{\Delta t}. \tag{8}$$

Simulate the growth of the solid phase for a duration of 4.5 with $\Delta t = 0.0001$. Grab snapshots of both ϕ and T every 0.5 time period. An example result of so-called kelp growth is linked.

Task 3. (10 pt) Surface orientation. You may observe that the order parameter, ϕ, is uniformly one in the solid region and is uniformly zero outside. Consequently, the solid surface is indicated by where ϕ value transitions between one and zero; namely where $|\nabla\phi| > 0$. $\nabla\phi$ is a vector:

$$\nabla\phi = \left(\frac{\partial \phi}{\partial x}, \frac{\partial \phi}{\partial y}\right) \tag{9}$$

at each grid point and its magnitude is a scalar quantity:

$$|\nabla\phi| = \sqrt{\left(\frac{\partial \phi}{\partial x}\right)^2 + \left(\frac{\partial \phi}{\partial y}\right)^2}. \tag{10}$$

Use **first-order central difference** to calculate the gradients. Since the value of $|\nabla\phi|$ is very small in either the solid region or vapor region, for convenience, let's set up a cutoff value to ignore $|\nabla\phi|$ in the bulk of solid and vapor by

$$\text{if} \quad |\nabla\phi| < 0.01 \cdot h, \quad |\nabla\phi| = 0. \tag{11}$$

Plot $|\nabla\phi|$ from your final result in Task 2. See an example linked. The inward-pointing unit vector of the solid surface is defined as

$$\vec{n} = \frac{\nabla\phi}{|\nabla\phi|} = (n_x, n_y). \tag{12}$$

Set $\vec{n} = 0$ where $|\nabla\phi| = 0$. Make a **quiver plot** to illustrate $\vec{n}$. Lastly, the surface orientation with respect to the coordinate system is defined as

$$\theta = \tan^{-1}\left(\frac{n_y}{n_x}\right). \tag{13}$$

Set $\theta = 0$ where $|\nabla\phi| = 0$. **Plot** θ.

Task 4. (30 pt) Anisotropic growth. In phase field models, the $\nabla \cdot \left(\varepsilon^2 \nabla\phi\right)$ term accounts for the interfacial/surface energy. In Task 2, a constant ε indicates a scenario that the surface energy is isotropic, *i.e.*, independent of orientations. For crystalline solids, surface energy is anisotropic (depending on the directions). The surface orientations, θ, is calculated using the method in Task 3. Here, we set

$$\varepsilon(\theta) = \bar{\varepsilon}\big[1 + \delta \cos\big(s \cdot (\theta - \theta_0)\big)\big], \tag{14}$$

such that

$$\varepsilon(\theta)' = -\bar{\varepsilon}\delta \sin\big(s \cdot (\theta - \theta_0)\big). \tag{15}$$

With a nonconstant ε, Eq. (1) using chain rule becomes

$$\frac{\partial\phi}{\partial t} = -M\left[\frac{\partial f}{\partial\phi} - \left(\nabla \cdot \varepsilon(\theta)^2 \nabla\phi - \frac{\partial \varepsilon\varepsilon'}{\partial x} \cdot \frac{\partial\phi}{\partial y} + \frac{\partial \varepsilon\varepsilon'}{\partial y} \cdot \frac{\partial\phi}{\partial x}\right) + m(T)\right]. \tag{16}$$

Recall that, for variant coefficient, the 5-point stencil of Laplacian is

$$\begin{aligned}\big(\nabla \cdot \kappa \nabla u\big)_{5p} = \frac{1}{h^2}\Bigg[&\left(\frac{\kappa_{i,j+1} + \kappa_{i,j}}{2}\right)\big(U_{i,j+1} - U_{i,j}\big) - \left(\frac{\kappa_{i,j} + \kappa_{i,j-1}}{2}\right)\big(U_{i,j} - U_{i,j-1}\big) + \\ &\left(\frac{\kappa_{i+1,j} + \kappa_{i,j}}{2}\right)\big(U_{i+1,j} - U_{i,j}\big) - \left(\frac{\kappa_{i,j} + \kappa_{i-1,j}}{2}\right)\big(U_{i,j} - U_{i-1,j}\big)\Bigg].\end{aligned} \tag{17}$$

The temperature field is still governed by Eq. (2) **as in Task 2.** Now let's set $s = 6$ in Eqs. (14) and (15) for a six-fold symmetry, $\delta = 0.04$, and $\bar{\varepsilon} = 0.01$. Assume the crystalline orientation intersects the coordinate axis system at $\theta_0 = 0.5$. Use the same initial condition, time step size, and Euler method in time as in Task 2. Simulate the growth for a duration of 0.4. Grab snapshots of ϕ and T every 0.5 time period.

Task 5. (5 pt) Play with the code. Here, let's change the initial temperature field to

$$T_0 = \frac{x}{L_x} - 0.3. \tag{18}$$

The growth will be affected by the temperature gradient. Set $\theta_0 = 0.15$, run the code of Task 4 for a duration of 0.3, and grab snapshots every 0.5 period. The low temperature side should grow fast. See the linked.

$$\nabla^2_{9p} = \frac{2}{3}\left(\begin{array}{ccc} & 1 & \\ 1 & -4 & 1 \\ & 1 & \end{array}\right) + \frac{1}{3}\left(\begin{array}{ccc} 1 & & 1 \\ & -4 & \\ 1 & & 1 \end{array}\right)$$

Figure 2: Simple representation of 9-point stencil.

Task 6. (15 pt) Increase Accuracy. Recall that using 9-point stencil increases the accuracy. Use the 9-point stencil in Eq. (20) for $\nabla^2 T$ in Eq. (2) and the stencil in Eq. (22) for $\nabla \cdot \varepsilon\nabla\phi$ in Eq. (16). Use 6-point stencils in Eqs. (23) and (24) for the gradients in Eq. (16). Set $s = 4$ for four-fold symmetry that is commonly seen in metal crystals. Redo Task 4 and Task 5. Example result.

The stencils are described below. For constant coefficient, the stencil is

$$\big(\nabla^2 u\big)_{9p} = \frac{2}{3}\big(\nabla^2 u\big)_{5p} + \frac{1}{3}\big(\nabla^2 u\big)_{off-diag}, \tag{19}$$

i.e.,

$$\begin{aligned}\left(\nabla^2 u\right)_{9p} &= \frac{2}{3}\cdot\frac{1}{h^2}\Big[\left(U_{i,j+1}-U_{i,j}\right)-\left(U_{i,j}-U_{i,j-1}\right)+\left(U_{i+1,j}-U_{i,j}\right)-\left(U_{i,j}-U_{i-1,j}\right)\Big]+\\ &\frac{1}{3}\cdot\frac{1}{2h^2}\Big[\left(U_{i+1,j+1}-U_{i,j}\right)-\left(U_{i,j}-U_{i-1,j-1}\right)+\left(U_{i+1,j-1}-U_{i,j}\right)-\left(U_{i,j}-U_{i-1,j+1}\right)\Big]\\ &= \frac{1}{6h^2}\Big[4U_{i,j+1}+4U_{i,j-1}+4U_{i+1,j}+4U_{i-1,j}+\\ &\qquad U_{i+1,j+1}+U_{i-1,j-1}+U_{i+1,j-1}+U_{i-1,j+1}-20U_{i,j}\Big].\end{aligned} \tag{20}$$

See Fig. 2 for an illustration. For variant coefficients, the stencil is

$$\left(\nabla\cdot\kappa\nabla u\right)_{9p} = \frac{2}{3}\left(\nabla\cdot\kappa\nabla u\right)_{5p} + \frac{1}{3}\left(\nabla\cdot\kappa\nabla u\right)_{off-diag}, \tag{21}$$

i.e.,

$$\begin{aligned}\left(\nabla\cdot\kappa\nabla u\right)_{9p} = \frac{2}{3}\cdot\frac{1}{h^2}\Bigg[&\left(\frac{\kappa_{i,j+1}+\kappa_{i,j}}{2}\right)\left(U_{i,j+1}-U_{i,j}\right)-\left(\frac{\kappa_{i,j}+\kappa_{i,j-1}}{2}\right)\left(U_{i,j}-U_{i,j-1}\right)+\\ &\left(\frac{\kappa_{i+1,j}+\kappa_{i,j}}{2}\right)\left(U_{i+1,j}-U_{i,j}\right)-\left(\frac{\kappa_{i,j}+\kappa_{i-1,j}}{2}\right)\left(U_{i,j}-U_{i-1,j}\right)\Bigg]+\\ \frac{1}{3}\cdot\frac{1}{2h^2}\Bigg[&\left(\frac{\kappa_{i+1,j+1}+\kappa_{i,j}}{2}\right)\left(U_{i+1,j+1}-U_{i,j}\right)-\left(\frac{\kappa_{i,j}+\kappa_{i-1,j-1}}{2}\right)\left(U_{i,j}-U_{i-1,j-1}\right)+\\ &\left(\frac{\kappa_{i+1,j-1}+\kappa_{i,j}}{2}\right)\left(U_{i+1,j-1}-U_{i,j}\right)-\left(\frac{\kappa_{i,j}+\kappa_{i-1,j+1}}{2}\right)\left(U_{i,j}-U_{i-1,j+1}\right)\Bigg].\end{aligned} \tag{22}$$

See the visual representation in Fig. 3 for a 6-point stencil of gradient in the x direction:

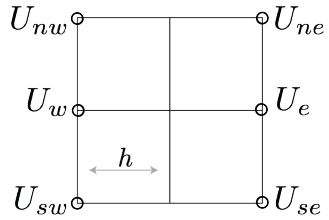

Figure 3: Simple representation of 6-point stencil for gradient in the horizontal direction.

$$\begin{aligned}\left(\frac{\partial u}{\partial x}\right)_{6p} &= \frac{1}{2}\cdot\frac{U_e-U_w}{2h}+\frac{1}{4}\cdot\frac{U_{ne}-U_{nw}}{2h}+\frac{1}{4}\cdot\frac{U_{se}-U_{sw}}{2h}\\ &= \frac{1}{2}\cdot\frac{U_{i,j+1}-U_{i,j-1}}{2h}+\frac{1}{4}\cdot\frac{U_{i+1,j+1}-U_{i+1,j-1}}{2h}+\frac{1}{4}\cdot\frac{U_{i-1,j+1}-U_{i-1,j-1}}{2h}\\ &= \frac{1}{8h}\Big(2U_{i,j+1}-2U_{i,j-1}+U_{i+1,j+1}-U_{i+1,j-1}+U_{i-1,j+1}-U_{i-1,j-1}\Big).\end{aligned} \tag{23}$$

In the y direction,

$$\left(\frac{\partial u}{\partial y}\right)_{6p} = \frac{1}{8h}\Big(2U_{i+1,j}-2U_{i-1,j}+U_{i+1,j+1}-U_{i-1,j+1}+U_{i+1,j-1}-U_{i-1,j-1}\Big). \tag{24}$$