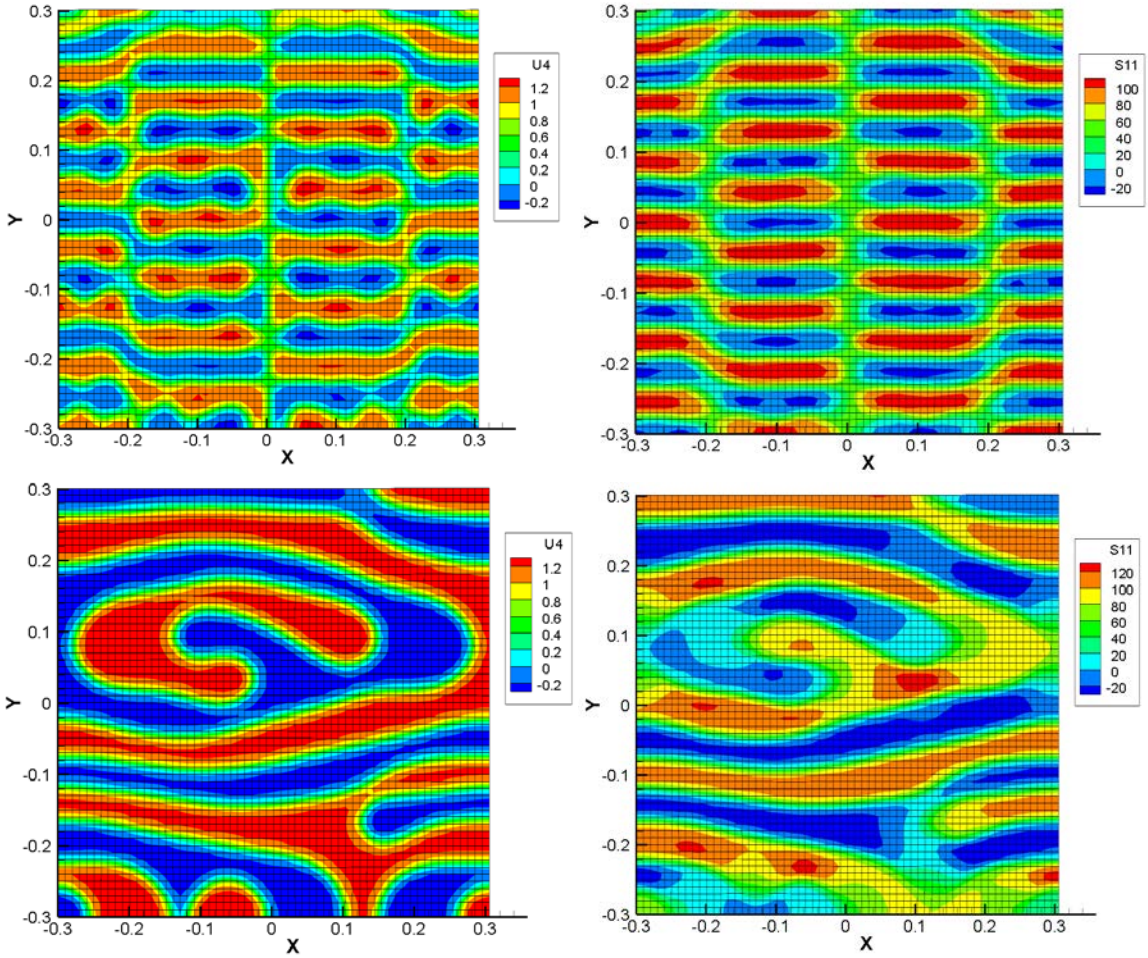
School of Engineering
Brown University

EN234: Computational methods in Structural and Solid Mechanics

Homework 8: Time dependent problems: phase field simulations
Due Fri Nov 10, 2017



In this homework you will develop a code to predict how the stress and concentration evolves in a binary solution of two atomic species A and B, which diffuse by mutual exchange on an elastically deforming lattice. We describe the composition of a point in the solid using the fraction c of B atoms: $c=0$ corresponds to pure A, while $c=1$ corresponds to pure B. We take the Gibbs free energy of the solution to have the form

$$F(c)=Wc^2(c-1)^2+\frac{1}{2}\kappa\left|\nabla c\right|^2+\frac{1}{2}\left(\varepsilon_{ij}-\frac{\Omega}{3}c\delta_{ij}\right)C_{ijkl}\left(\varepsilon_{kl}-\frac{\Omega}{3}c\delta_{kl}\right)$$

where W and κ are material properties (W quantifies the energy cost of deviating from a composition of pure A or pure B, while κ determines the energy per unit area of an interface between A and B); C_{ijkl} are the elastic constants (which we assume to be independent of composition, for simplicity), ε_{ij} is the strain (a lattice occupied by pure A is taken to be the zero strain state), and Ω is the ratio of the volume of an atom of

B to that of A. A stress free solid has minima at $c=0,\ c=1$. It is therefore energetically favorable for the solid solution to phase separate into A- and B-rich regions. Moreover, it is energetically favorable for the system to minimize concentration gradients. As a result, a material that starts with *c* close to zero phase separates into regions of A and B, which then gradually coarsen, as shown in the figure. Externally applied forces, or self-stress caused by changes in composition, will also influence the process.

The evolution of concentration is governed (approximately – we have neglected a small contribution from the elastic strain energy to the chemical potential μ) by the Cahn-Hilliard equation

$$\frac{\partial c}{\partial t}=\nabla\cdot D\nabla\mu \qquad \mu=\frac{\delta G}{\delta c}=2c(c-1)(2c-1)-\kappa\nabla^2 c-\frac{\Omega}{3}\sigma_{kk}$$

where *D* is a diffusion coefficient (which we will assume is constant, but could depend on *c*). The stress and strain fields satisfy the usual linear elastic field equations.

Our goal is to solve this system of equations for concentration *c(t)* and displacement **u**(t), given some initial conditions and boundary conditions. To keep things simple, we will consider a 2D rectangular region of material (shown in the figure), with symmetry boundary conditions (so $\nabla c\cdot\mathbf{n}=\nabla\mu\cdot\mathbf{n}=0$ on all boundaries).

The first step is to set up a finite element approximation to the PDEs. The displacement, strain and stress fields satisfy the usual finite element equations

$$\int_V C_{ijkl}\left(\frac{\partial u_k}{\partial x_l}-\frac{\Omega}{3}c\delta_{kl}\right)\frac{\partial\delta u_i}{\partial x_j}dV-\int_V t_i\delta u_i dV=0 \qquad \forall\{\delta u_i\}$$

We also need to solve the Cahn-Hilliard equation. This is usually done by solving simultaneously for μ and *c* (this avoids having to solve a fourth-order PDE). Introducing variations of $\delta\mu,\delta c$, you should be able to show that the weak form of the governing equations is

$$\int_V\frac{\partial c}{\partial t}\delta c dV-\int_V D\frac{\partial\mu}{\partial x_i}\frac{\partial\delta c}{\partial x_i}dV=0$$

$$\int_V\mu\delta\mu dV-\int_V\left(2c(c-1)(2c-1)\delta\mu-\frac{\Omega}{3}\sigma_{kk}\delta\mu+\kappa\frac{\partial c}{\partial x_i}\frac{\partial\delta\mu}{\partial x_i}\right)dV=0$$

$$\forall\{\delta c,\delta\mu\}$$

Introducing finite element interpolation functions for μ and *c* in the usual way

$$\mu=N^a\mu^a \qquad c=N^a c^a \qquad\qquad \mu=N^b\delta\mu^b \qquad c=N^b\delta c^b$$

then yields the discrete system of equations

$$M_{ab}\frac{dc^b}{dt}+DK_{ab}\mu^b=0 \qquad\qquad M_{ab}\mu^b-H^a(c^b)+\kappa P_{ab}c^b=0$$

where

$$M_{ab}=\int_V N^a N^b dV \qquad P_{ab}=\int_V\frac{\partial N^a}{\partial x_i}\frac{N^b}{\partial x_i}dV \qquad H^b=\int_V 2c(c-1)(2c-1)-\frac{\Omega}{3}\sigma_{kk}N^b dV$$

Finally, we need a way to integrate this discrete system of equations with respect to time. As in all FEA problems, we use a time-marching scheme: given values μ^a,c^a at time *t*, we find the increments $\Delta\mu^a,\Delta c^a$ during the next time interval Δt , and then update the solution. A backward-Euler integration is used for μ

$$M_{ab}\left(\mu^b + \Delta\mu^b\right) - H^a - \kappa P_{ab}(c^b + \Delta c^b) = 0$$

while a generalized mid-point time integration scheme is used to integrate the equation for the concentration

$$M_{ab}\frac{\Delta c^b}{\Delta t} + DP_{ab}\left[(1-\theta)\mu^b(t) + \theta(\mu^b(t) + \Delta\mu^b)\right] = 0$$

where $0 < \theta < 1$ is a numerical parameter. Choosing $\theta = 0$ gives a forward-Euler scheme; choosing $\theta = 1$ gives a backward-Euler scheme, and $\theta = 0.5$ (the usual choice) gives a mid-point scheme.

We now have a system of nonlinear equations to solve for $\Delta u,\ \Delta\mu^a, \Delta c^a$ and are on familiar territory.

Some care is required to implement the procedure, however. We have already seen that standard linear elastic elements are not able to accommodate an arbitrary volume change at all integration points. This means that changes in concentration at the integration points can generate large spurious stresses. We could use any of the various approaches discussed in class to avoid this kind of locking, but (for 2D simulations) the easiest one to implement in practice is to interpolate the displacement fields using 8 noded quadratic elements, and the concentration field using linear interpolation between the 4 nodes at the corners of the element. The stiffness and right hand side vectors should be assembled using a 4 point integration scheme.

- Note that each node in the finite element mesh will have two degrees of freedom: the value of μ and the value of *c*. At a generic time-step, we will be solving for $\Delta\mu^a, \Delta c^a$ at each node.
- Instead of the usual B matrix that maps displacements to strains, we can introduce a modified B matrix that maps nodal values of $u_i^a \mu^a, c^a$ to $\varepsilon_{ij}\mu, c, \partial\mu/\partial x_i, \partial c/\partial x_i$. Thus

$$\begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ 2\varepsilon_{12} \\ \mu \\ c \\ \partial\mu/\partial x_1 \\ \partial\mu/\partial x_2 \\ \partial c/\partial x_1 \\ \partial c/\partial x_2 \end{bmatrix} = [\mathbf{B}] \begin{bmatrix} u_1^1 \\ u_2^1 \\ \mu^1 \\ c^1 \\ u_1^2 \\ u_2^2 \\ \mu^2 \\ c^2 \\ \vdots \\ u_2^7 \\ u_1^8 \\ u_2^8 \end{bmatrix}$$

$$[\mathbf{B}] = \begin{bmatrix} \partial N^1/\partial x_1 & 0 & 0 & 0 & & \partial N^5/\partial x_1 & & \\ 0 & \partial N^1/\partial x_2 & 0 & 0 & & & \partial N^5/\partial x_2 & \\ \partial N^1/\partial x_2 & \partial N^1/\partial x_1 & 0 & 0 & & \partial N^5/\partial x_2 & \partial N^5/\partial x_1 & \\ 0 & 0 & \bar{N}^1 & 0 & & 0 & 0 & \\ 0 & 0 & 0 & \bar{N}^1 & \cdots & 0 & 0 & \cdots \\ & & \partial \bar{N}^1/\partial x_1 & & & 0 & 0 & \\ & & \partial \bar{N}^1/\partial x_2 & & & 0 & 0 & \\ & & & \partial \bar{N}^1/\partial x_1 & & 0 & 0 & \\ & & & \partial \bar{N}^1/\partial x_2 & & 0 & 0 & \end{bmatrix}$$

Here, N^a are the quadratic interpolation functions for an 8 noded element, and $\bar{N}^a$ are the linear interpolation functions for a 4 noded element.

- The finite element stiffness matrix and residual vector can then be expressed as

$$[k^{el}] = \int_V [\mathbf{B}]^T [\mathbf{D}][\mathbf{B}] dV \qquad \underline{r^{el}} = -\int_V [\mathbf{B}]^T \underline{q} dV$$

Where

$$\underline{q} = \begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{12} \\ \mu + \Delta\mu - f(c+\Delta c) - \Omega\sigma_{kk}/3 \\ \Delta c/\Delta t \\ -\kappa\partial(c+\Delta c)/\partial x_1 \\ -\kappa\partial(c+\Delta c)/\partial x_2 \\ D\partial(\mu+\theta\Delta\mu)/\partial x_1 \\ D\partial(\mu+\theta\Delta\mu)/\partial x_2 \end{bmatrix} \qquad f(c) = 2Wc(c-1)(2c-1)$$

$$[\mathbf{D}] = \begin{bmatrix} \ddots & & & & 0 & -\Omega(D^e_{11}+D^e_{12}+D^e_{13})/3 & 0 & 0 & 0 & 0 \\ & \mathbf{D}^e & & & 0 & -\Omega(D^e_{21}+D^e_{22}+D^e_{23})/3 & 0 & 0 & 0 & 0 \\ & & & \ddots & 0 & 0 & 0 & 0 & 0 & 0 \\ -\Omega(D^e_{11}+D^e_{12}+D^e_{13})/3 & -\Omega(D^e_{21}+D^e_{22}+D^e_{23})/3 & 0 & 1 & -\dfrac{df}{dc} - \Omega^2 \sum_{k=1}^{3}\sum_{l=1}^{3} D^e_{kl}/9 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/\Delta t & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\kappa & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\kappa \\ 0 & 0 & 0 & 0 & 0 & \theta D & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \theta D & 0 & 0 \end{bmatrix}$$

$$df/dc = W\left(12(c+\Delta c)^2 - 12(c+\Delta c) + 2\right)$$

Your goal is to implement this as an ABAQUS UEL, and run it in EN234FEA. Some guidelines:

(1) You will use 8 noded planar quadrilateral elements with straight sides. Nodes 1-4 will have four DOF (displacements, chemical potential, and concentration); nodes 5-8 will have two DOF (displacements only)
(2) Use 4 integration points.
(3) Assume isotropic elastic constants and plane strain deformation
(4) Three sample input files are provided for you in EN234FEA to run your code. These assume that the element properties are stored in the following order: $E, \nu, \Omega, \mathrm{W}, \kappa, \mathrm{D}, \theta$, where E, ν are Young's modulus and Poisson's ratio.
(5) Remember that an ABAQUS UEL (and EN234FEA) provides the degrees of freedom at the *end* of the step in the variable U. You will have to take this into account when computing the residual and stiffness.
(6) Store the stresses at each integration point $\sigma_{11}, \sigma_{22}, \sigma_{33}, \sigma_{12}$ as state variables (in the SVARS vector), so EN234FEA can plot stress distributions for you.
(7) You will find that you can solve the problem with rather minor changes to the 2D elasticity code you wrote for Homework 3 – you merely need to re-define the **B** matrix and **D** matrix (note that **D** depends on concentration, and so must be evaluated inside the integration loop), and implement a procedure to calculate the vector $\underline{q}$.
(8) You will need to define an initial value for the concentration. The solution shown in the figure was generated with

$$c(t=0) = 0.5 + 0.01\sin(15x_1)\sin(15x_2)$$

EN234FEA has a user-subroutine that can be used to define initial values of degrees of freedom, and this function has already been coded for you. Feel free to change it – the pattern you get is determined by the initial conditions.

To save you some time, three input files setting up this problem has been provided for you:

- Abaqus_uel_phasefield_1el.in runs a simple problem with one element with zero initial concentration, and stretched horizontally
- Abaqus_uel_phasefield_coarse.in runs a simulation showing spinodal decomposition in a crystal stretched horizontally with a coarse mesh (this simulation runs quickly
- Abaqus_uel_phasefield_fine.in runs the same simulation with a finer mesh (this has 30000 DOF so takes a few minutes to run all 100 steps in debug mode. It will run much faster in release mode, particularly with Parallel Studio)

You can change these files, or generate your own, to test your code and to explore how the system behaves (you could try repeating the simulation with $\Omega = 0$, in which case there is no interaction between the mechanics (stress) and chemistry (diffusion)

As a solution to this homework:

(1) Upload a description of tests you have run to check your code on CANVAS. Please include a link to your Github fork of EN234FEA
(2) Push your code to Github