8.0 Solving Time dependent problems

8.1) First order differential eqs : "Cahn - Hilliard equation"

- Goal: model "spinodal decomposition" of a solid solution of A & B

Let: ρ_A, ρ_B denote concentrations of A, B

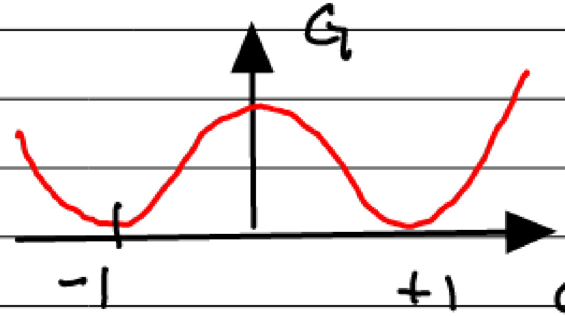
Let $c = \dfrac{\rho_A - \rho_B}{\rho_A + \rho_B}$ $\qquad -1 < c < 1$

$c = 1 \Rightarrow$ pure A

$c = -1 \Rightarrow$ pure B

Let free energy be $G(c) = \underbrace{\frac{1}{4}(c^2-1)^2}_{\text{Bulk}} + \underbrace{K\left[\frac{\partial c}{\partial x_i}\frac{\partial c}{\partial x_i}\right]}_{\text{Interface energy}}$

Free energy has minima @ $c = \pm 1$

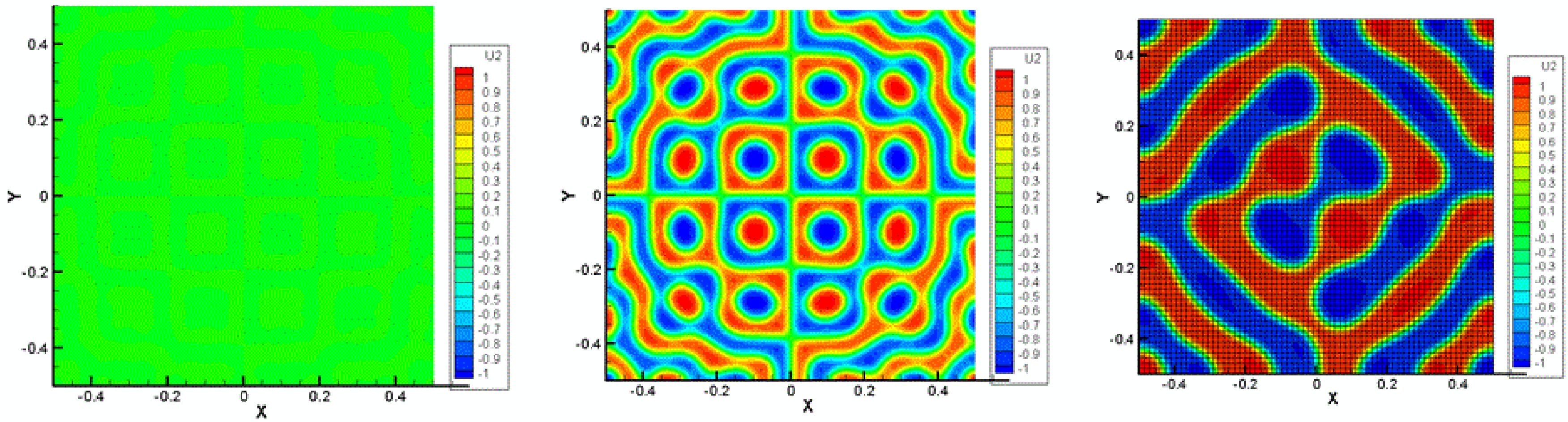


- Evolution equations for c

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x_i} D \frac{\partial \mu}{\partial x_i}$$

$$\mu = \frac{\delta G}{\delta c} = \underbrace{c(c^2-1)}_{f(c)} - \kappa \frac{\partial^2 c}{\partial x_i \partial x_i}$$

"Chemical Potential"



$t=0$ $c \approx 0$ → Phase separation → Coarsening

- Initial conditions $c(t=0, \underline{x}) = A \sin k x_1 \sin k x_2$
- Boundary conditions (symmetry) $\frac{\partial c}{\partial x_i} n_i \quad \frac{\partial \mu}{\partial x_i} n_i = 0$ on all 4 boundaries

Goal: Solve for $\mu(t)$, $c(t)$

Weak Form : Let $\delta\mu$, δc be two differentiable test functions

$$\int_R \left\{ \mu - f'(c) + k \frac{\partial^2 c}{\partial x_i \partial x_i} \right\} \delta\mu \, dV \Rightarrow \int_R \left\{ [\mu - f'(c)]\delta\mu - k \frac{\partial c}{\partial x_i} \frac{\partial \delta\mu}{\partial x_i} \right\} dV = 0$$

$$\int_R \left\{ \frac{\partial c}{\partial t} - \frac{\partial}{\partial x_i} D \frac{\partial \mu}{\partial x_i} \right\} \delta c \, dV \Rightarrow \int_R \left\{ \frac{\partial c}{\partial t} \delta c + D \frac{\partial c}{\partial x_i} \frac{\partial \delta c}{\partial x_i} \right\} dV = 0$$

$\forall \; \delta c, \; \delta\mu$

Introduce FE interpolations

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

} Usual N^a

Discrete system

$$M_{ab}\,\mu^b(t) - F^a(c^b) - k\,K_{ab}\,c^b(t) = 0 \qquad (1)$$

$$M_{ab}\frac{dc^b(t)}{dt} - D\,K_{ab}\,\mu^b(t) = 0 \qquad (2)$$

$$M_{ab} = \int_{\mathbb{R}} N^a N^b \, dV \qquad K_{ab} = \int_{\mathbb{R}} \frac{\partial N^a}{\partial x_i}\frac{\partial N^b}{\partial x_i}\, dV$$

$$F^a = \int_{\mathbb{R}} N^a f(c)\, dV \qquad c = \sum N^a c^a$$

Time Integration

FEA nearly always uses simple Euler scheme
- Estimate time derivatives; multiply by Δt

Assume μ^a c^a known @ time t
Calculate $\Delta\mu^a$ Δc^a during Δt
Update, repeat.

We need to find $\frac{dc^a}{dt}$: Could use

(1) Use μ^a @ time t ("Explicit")
(2) " " " " $t+\Delta t$ ("implicit")
(3) Combination

We can set up a general scheme

(2) in discrete form

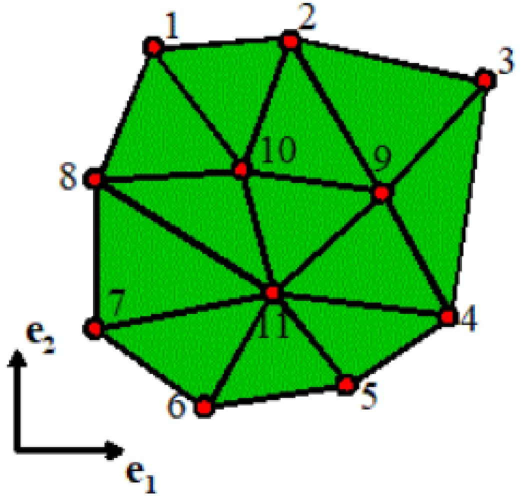
$$M_{ab}\frac{\Delta c^b}{\Delta t} - D K_{ab}\left\{(1-\theta)\mu^b + \theta(\mu^b + \Delta\mu^b)\right\}$$

$$0 < \theta < 1$$

$\theta = 0 \Rightarrow$ Explicit
$\theta = 1 \Rightarrow$ Implicit
$\theta = \frac{1}{2} \Rightarrow$ midpoint

(1) $\Rightarrow M_{ab}(\mu^b + \Delta\mu^b) - F^a(c^b + \Delta c^b) - \kappa K_{ab}(c^b + \Delta c^b) = 0$

Implementation



Goal: re-write in a form best suited for UEL

Note that our global equation system has same general structure as for mechanics

$$R_{ai}\,[\Delta u_{bk}\,,\Delta t] = 0$$

$\underline{u}$ – vector of unknowns $[\mu^1\ c^1,\ \mu^2\ c^2,\ \mu^3,\ c^3]$

$\Delta\underline{u}$ vector of increments

R_{ai} is i^{th} equation for a^{th} node

Rearrange in usual form

Note equations contain μ, c, $\frac{\partial \mu}{\partial x_i}$ $\frac{\partial c}{\partial x_i}$

Hence define $\underline{p} = [\mu, c, \frac{\partial \mu}{\partial x_1} \; \frac{\partial \mu}{\partial x_2} \; \frac{\partial c}{\partial x_1} \; \frac{\partial c}{\partial x_2}]$

Define [B] such that $\underline{p} = [B]\,\underline{u}^{el}$

$$[\mathbf{B}] = \begin{bmatrix} N^1 & 0 & N^2 & \\ 0 & N^1 & 0 & \\ \partial N^1/\partial x_1 & 0 & \partial N^2/\partial x_1 & \cdots\cdots \\ \partial N^1/\partial x_2 & 0 & \partial N^2/\partial x_2 & \\ 0 & \partial N^1/\partial x_1 & 0 & \\ 0 & \partial N^1/\partial x_2 & 0 & \end{bmatrix}$$

Now note that our equation system can be expressed as

$$\delta \underline{p}^T \underline{q} = 0$$

where $\underline{q}$ is (Get from weak form)

$$\underline{q} = \begin{bmatrix} \mu + \Delta\mu - f(c) \\ \dfrac{\Delta c}{\Delta t} \\ -k\dfrac{\partial(c+\Delta c)}{\partial x_1} \\ -k\dfrac{\partial(c+\Delta c)}{\partial x_2} \\ D\dfrac{\partial(\mu+\theta\Delta\mu)}{\partial x_1} \\ D\dfrac{\partial(\mu+\theta\Delta\mu)}{\partial x_2} \end{bmatrix}$$

Recall also

$$\delta\underline{p} = [B]\,\delta\underline{u}$$

Hence $\underline{R}^{el} = \int_{\Omega_{el}} [B]^T \underline{q}\, dV$

This is identical to stress analysis with $\underline{q}$ replacing $\underline{\sigma}$

Nonlinear system $R[\underline{u}] = \underline{0}$

Solve with Newton - Raphson

Guess $\underline{u} = \underline{w}$

Correct $[K]\, d\underline{w} = -R[\underline{w}]$

Where $$[K] = \frac{\partial \underline{R}}{\partial \Delta \underline{u}} = \int_{\Omega_{el}} [B]^T \underbrace{\frac{\partial \underline{q}}{\partial \underline{p}}}_{[D]} \overbrace{\frac{\partial \underline{p}}{\partial \Delta \underline{u}}}^{[B]} dV$$

Here $[D] = \begin{bmatrix} \partial q_1/\partial p_1 & \partial q_1/\partial p_2 & \partial q_1/\partial p_3 \\ \partial q_2/\partial p_1 & & \\ \partial q_3/\partial p_3 & & \end{bmatrix}$

$$[\mathbf{D}] = \begin{bmatrix} 1 & -df/dc & 0 & 0 & 0 & 0 \\ 0 & 1/\Delta t & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\kappa & 0 \\ 0 & 0 & 0 & 0 & 0 & -\kappa \\ 0 & 0 & \theta D & 0 & 0 & 0 \\ 0 & 0 & 0 & \theta D & 0 & 0 \end{bmatrix} \qquad df/dc = 3(c+\Delta c)^2 - 1$$

Summary: UEL computes $-\int_{\Omega_{el}} [B]^T \underline{q} = -\underline{R}$

$[K] = \int_{\Omega_{el}} [B]^T [D][B]\, dV$