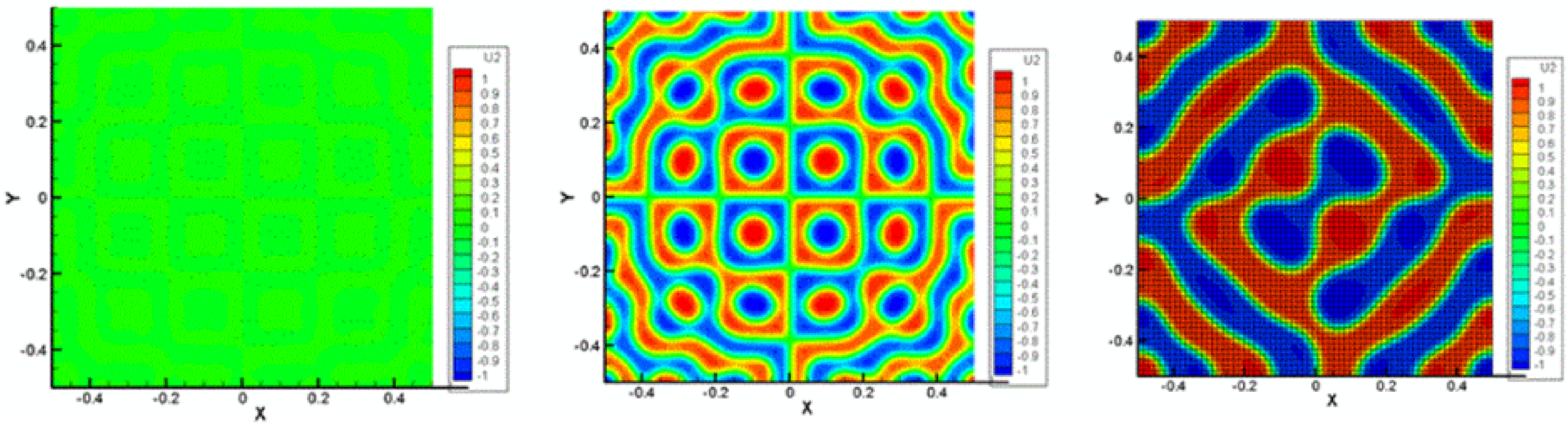
Review – Solving the Cahn-Hilliard Equation



Free energy: $G(c) = \frac{1}{4}(c^2 - 1)^2 + \frac{1}{2}\kappa|\nabla c|^2$

Evolution equation for concentration $\frac{\partial c}{\partial t} = \nabla \cdot D\nabla\mu$ $\qquad \mu = \frac{\delta G}{\delta c} = c(c^2 - 1) - \kappa\nabla^2 c$

Discrete weak form $M_{ab}\frac{dc^b}{dt} + DK_{ab}\mu^b = 0 \qquad M_{ab}\mu^b - F^a(c^b) + \kappa K_{ab}c^b = 0$

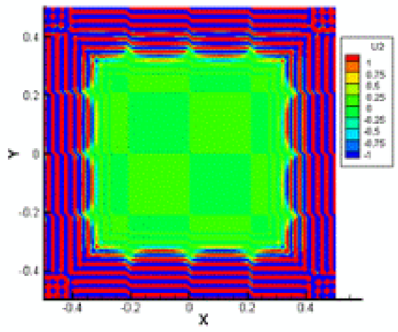
$$M_{ab} = \int_V N^a N^b dV \qquad K_{ab} = \int_V \frac{\partial N^a}{\partial x_i}\frac{N^b}{\partial x_i}dV \qquad F^b = \int_V c(c^2 - 1)N^b dV$$

Time integration $M_{ab}\left(\mu^b + \Delta\mu^b\right) - F^a(c^b + \Delta c^b) - \kappa K_{ab}(c^b + \Delta c^b) = 0$

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

Effects of θ:

Choosing $\theta = 0$ makes time stepping unstable

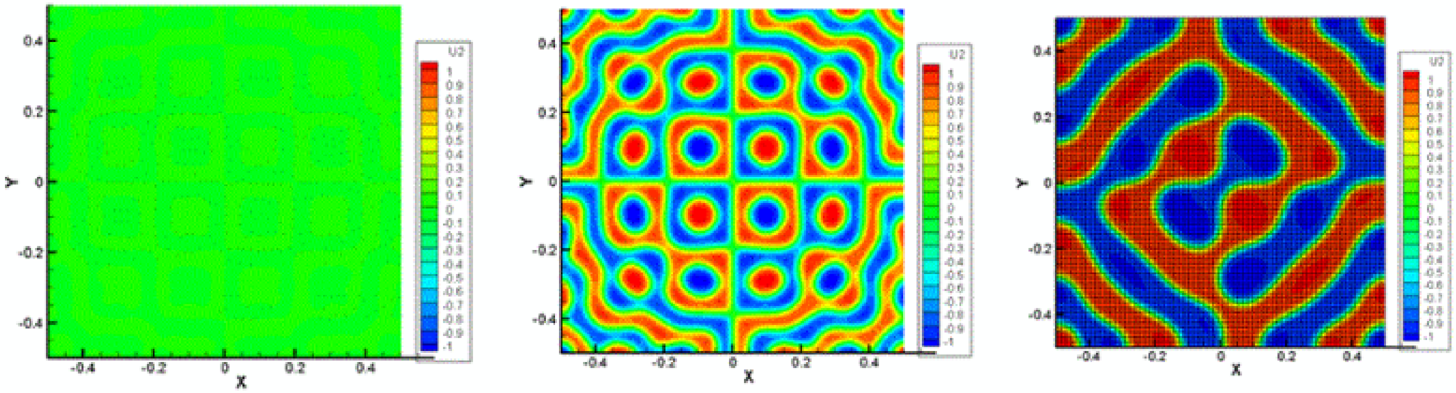


$\theta = 0 \quad \Delta t = 10^{-3} \quad D = 1, \quad \kappa = 0.0001$

(unstable even for very small timesteps)

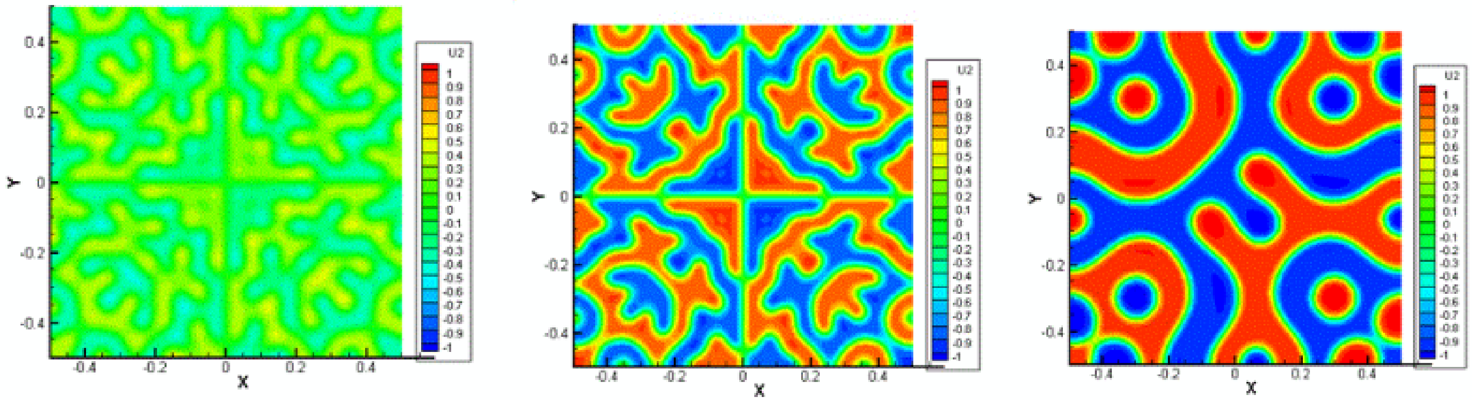
$\theta > 0.5$ is stable

$\theta = 0.5$ gives best accuracy



$\theta = 0.5 \quad \Delta t = 10^{-3} \quad D = 1, \quad \kappa = 0.0001$

$\theta = 1$ gives best stability

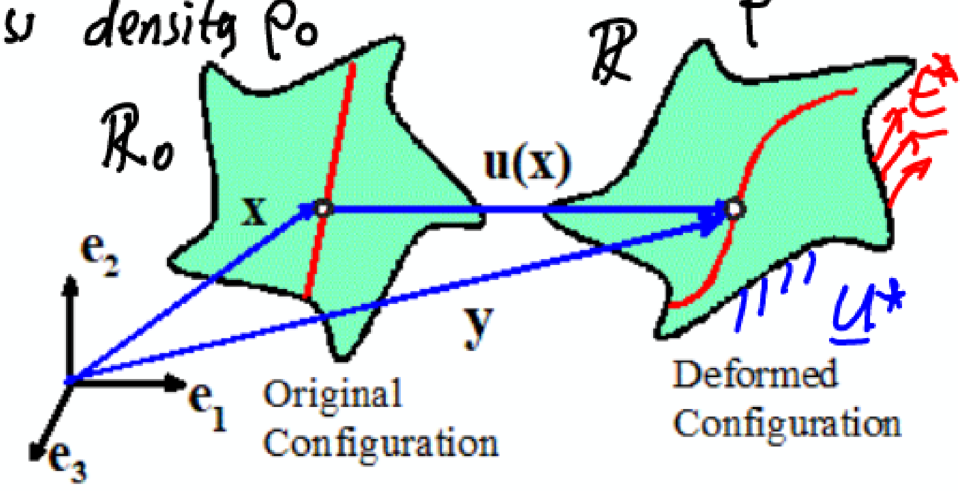


$\theta = 1 \quad \Delta t = 10^{-3} \quad D = 1, \quad \kappa = 0.0001$

$\Rightarrow$ Instability problems sensitive to choice

8.2 Solving Dynamic problems in solids

mass density ρ_0



Governing Equations

BLM: $$\frac{\partial \sigma_{ij}}{\partial y_j} = \rho \left.\frac{\partial^2 u_i}{\partial t^2}\right|_{\underline{x}=\text{const}}$$

Initial conditions

$$u_i = \mathring{u}_i \qquad \frac{\partial u_i}{\partial t} = \mathring{v}_i \qquad t=0$$

$$\rho_0 = J\rho \qquad J = \det(F)$$

Boundary conditions $\sigma_{ij} n_j = t_i^*$ on S_2 $\qquad u_i = u_i^*$ S_1

Constitutive equation (eg linear elasticity)

$$\sigma_{ij} = C_{ijkl} \frac{\partial u_k}{\partial x_l}$$ (other models ok too)

Weak form of BLM is

$$\int_{R_0} J\sigma_{ij}\frac{\partial \eta_i}{\partial y_j}\,dV_0 + \int_{R_0}\rho_0\frac{\partial^2 u_i}{\partial t^2}\eta_i\,dV_0 = \int_{S_{20}} t_i^*\eta_i\,dA_0 \quad \forall \eta_i$$

Discretize : Use usual interpolations $u_i = N^a u_i^a \quad \eta_i = N^a\eta_i^a$

Subst into weak form

$$M_{ab}\ddot{u}_i^b + R_i^a[u_k^b] = F_i^a(t) \qquad *$$

$$M_{ab} = \int_{R_0}\rho_0 N^a N^b\,dV_0 \quad - \text{ mass matrix}$$

$$R_i^a = \int_{R_0} J\sigma_{ij}\frac{\partial N^a}{\partial y_j}\,dV_0 \qquad F_i^a = \int_{S_2} t_i^* N^a\,dA$$

This is all just like statics, except that we need to integrate BLM (*) wrt t

FEA usually uses "Newmark" time-stepping

Two versions : (1) "Implicit" dynamics

(2) "Explicit" dynamics

Also for linear elasticity – "Modal dynamics"

Newmark Time Integration

Given $\underline{u}^n$ $\underline{v}^n$ $\underline{a}^n$. at time t_n $\{\underline{u}, \underline{v}, \underline{a}\}$ are FEA vectors

Goal: get $\underline{u}^{n+1}$, $\underline{v}^{n+1}$ $\underline{a}^{n+1}$ at $t_{n+1} = t_n + \Delta t$

Simple time-stepping

$$\underline{v}^{n+1} = \underline{v}^n + \Delta t \{(1-\beta_1)\underline{a}^n + \beta_1 \underline{a}^{n+1}\}$$

$$\underline{u}^{n+1} = \underline{u}^n + \Delta t \underline{v}^n + \frac{\Delta t^2}{2}\left((1-\beta_2)\underline{a}^n + \beta_2 \underline{a}^{n+1}\right)$$

$0 < \beta_1 < 1$ $\qquad$ $0 < \beta_2 < 1$

$\boxed{\beta_2 = 0 \text{ — Explicit Dynamics}}$

We find $\underset{\sim}{a}^{n+1}$ from momentum balance

$$[M]\underset{\sim}{a}^{n+1} + \underset{\sim}{R}\left[\underset{\sim}{u}^{n} + \Delta t \underset{\sim}{v}^{n} + \frac{\Delta t^2}{2}(1-\beta_2)\underset{\sim}{a}^{n} + \frac{\Delta t^2}{2}\beta_2 \underset{\sim}{a}^{n+1}\right] = \underset{\sim}{F}(t+\Delta t)$$

For $\beta_2 \neq 0$ this is a nonlinear system for $\underset{\sim}{a}^{n+1}$

Solve with Newton-Raphson

(1) Guess $\underset{\sim}{a}^{n+1} = \underset{\sim}{w}$; Correct

(2) $\left\{[M] + \frac{\Delta t^2}{2}\beta_2 [K]\right\} d\underset{\sim}{w} = -[M]\underset{\sim}{w} - \underset{\sim}{R}(\underset{\sim}{a}^{n+1} = \underset{\sim}{w}) + \underset{\sim}{F}(t+\Delta t)$ **

(3) $\underset{\sim}{w} \rightarrow \underset{\sim}{w} + d\underset{\sim}{w}$; check convergence ; repeat

$[K] = \dfrac{\partial \underset{\sim}{R}}{\partial \Delta \underset{\sim}{u}}$ (same as static stiffness matrix)

(Small change to statics equation system

Newmark algorithm:

Initialize: $\underset{\sim}{u}^0$, $\underset{\sim}{v}^0$ - given $\qquad \underset{\sim}{a}^0 = [M]^{-1}\left(\underset{\sim}{F} - R(\underset{\sim}{u}^0)\right)$

Time step: (general)

(1) Solve ** for $\underset{\sim}{a}^{n+1}$ (Newton - Raphson)

(2) $\underset{\sim}{v}^{n+1} = \underset{\sim}{v}^n + \Delta t\left((1-\beta_1)\underset{\sim}{a}^n + \beta_1 \underset{\sim}{a}^{n+1}\right)$

(3) $\underset{\sim}{u}^{n+1} = \underset{\sim}{u}^n + \Delta t \underset{\sim}{v}^n + \frac{\Delta t^2}{2}\left((1-\beta_2)\underset{\sim}{a}^n + \beta_2 \underset{\sim}{a}^{n+1}\right)$

For $\beta_2 = 0$ $\qquad \underset{\sim}{a}^{n+1} = [M]^{-1}\left(\underset{\sim}{F} - R(\underset{\sim}{u}^{n+1})\right)$

("Explicit" update) $\qquad$ only depends on $\underset{\sim}{a}^n$

Mass Matrices

$$m_{ab} = \int_{\mathcal{R}_0} \rho_0 N^a N^b \, dV_0$$

- Compute using usual quadrature ~ 1 order higher integration

"Consistent" mass matrix

"Lumped" mass matrix – for explicit dynamics we replace m_{ab} with a diagonal approximation so $[M]^{-1}$ is easy

Lumping schemes:

(1) "Row Sum" $\quad \tilde{m}_{aa} = \sum_b m_{ab} \qquad m_{ab} = 0 \quad a \neq b$

(2) "Diagonal Scaling $\quad \tilde{m}_{aa} = c\, m_{aa} \qquad c = \dfrac{\sum_a \tilde{m}_{aa}}{\sum_a \sum_b m_{ab}}$

(3) Compute m_{ab} with int pts @ nodes

Lumped mass matrices for 2D elements

eg for linear quad

$$[M]^{el} = \text{mass of el} \begin{bmatrix} 1/4 & 1/4 \\ 1/4 & 1/4 \end{bmatrix}$$

Different methods give different answers

- Choose the most sensible one!

- Linear elements generally preferable in explicit.