Lec. 59,60,61,62,63,64
Prof. Gururajan Date: 24/2/2016

$$\frac{\partial c}{\partial t} = \frac{M}{N_v} f'' \frac{\partial^2 c}{\partial x^2}$$ 1D diffusion equation

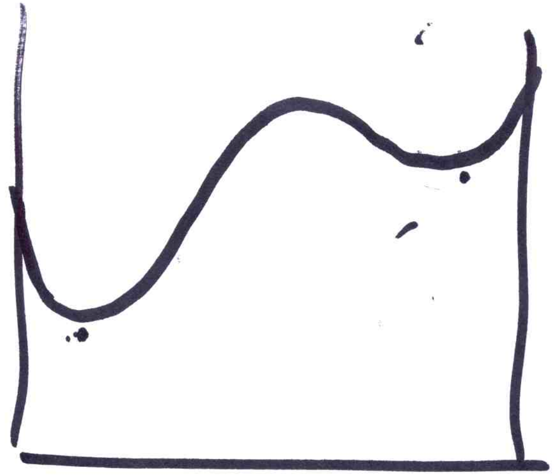
$$\frac{\partial c}{\partial t} = \frac{M}{N_v} \left[f'' \frac{\partial^2 c}{\partial x^2} - 2K \frac{\partial^4 c}{\partial x^4} \right]$$ 1D Cahn Hilliard equation

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2}$$

$$\Delta f = \Omega x(1-x) + RT \left(x \ln x + (1-x) \ln(1-x) \right)$$

$$F = \int \left\{ \underline{\underline{f_0}} + K |\nabla c|^2 \right\} dV$$

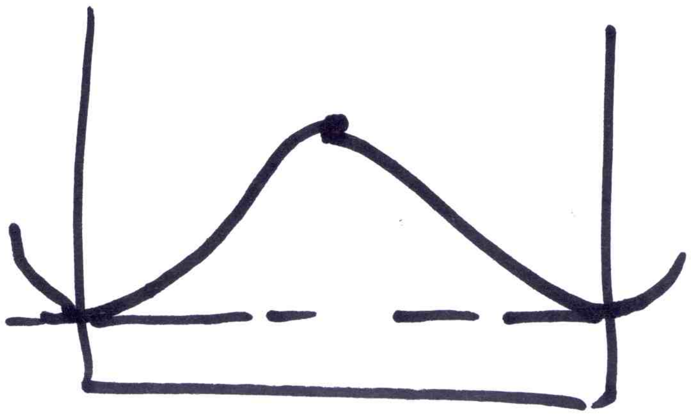
$$f_0 = A c^2 (1-c)^2$$



$c = 0$

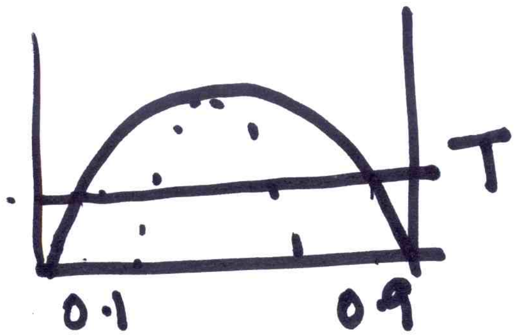
$c = 0.5$

$c = 1.0$



$$f = AC^2(1-C)^2 \quad \text{Isothermal}$$

$$G(x, T)$$



$$f' = 2AC(1-C)^2$$
$$- 2AC^2(1-C)$$
$$= 2AC(1-C)\left[1-C-C\right]$$
$$= 2AC(1-C)(1-2C)$$
$$2AC(1-C)(1-2C) = 0 \quad \begin{array}{l} C=0 \\ C=1 \\ C=1/2 \end{array}$$

$$
\begin{aligned}
f'' = {} & 2A(1-c)(1-2c) \\
& - 2Ac(1-2c) \\
& - 4Ac(1-c)
\end{aligned}
$$

$$
\left.
\begin{array}{l}
f''\Big]_{c=0} = 2A. \quad > 0 \\[2ex]
f''\Big]_{c=1} = +2A \quad > 0
\end{array}
\right\} \text{Minima}
$$

$$
f''\Big]_{c=0.5} = -4A\,\frac{1}{2}\,\frac{1}{2} = -A < 0 \;\Big\}\; \text{Maxima.}
$$

$$\frac{\partial c}{\partial t} = \frac{M}{N_V} f'' \frac{\partial^2 c}{\partial x^2}$$

$$c - c_0 = A(\beta, t) \exp(i\beta x)$$

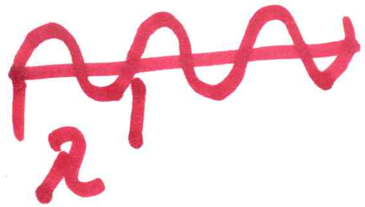
$$\frac{dA}{dt} . \exp i\beta x = -A \frac{M}{N_V} f'' \beta^2 \exp(i\beta x)$$

$$\frac{dA}{dt} = -\underbrace{\frac{M}{N_V} f'' \beta^2}_{R(\beta)} . A$$

$$A(\beta,t) = A(\beta,0) \exp(R(\beta) t)$$

$$\frac{\partial c}{\partial t} = \frac{M}{N_V}\left[f'' \frac{\partial^2 c}{\partial x^2} - 2\kappa \frac{\partial^4 c}{\partial x^4}\right]$$

$$\beta = \frac{2\pi}{\lambda}$$



$$\frac{dA}{dt} = -\underbrace{\frac{M}{N_V}\left[f'' \beta^2 - 2\kappa \beta^4\right]}_{R(\beta)} A$$

$$A(\beta,t) = A(\beta,0) \exp(R(\beta)\, t)$$

$$A(\beta,t) = A(\beta,0)\exp(R(\beta)\,t)$$

$$R(\beta) = -\frac{M}{N_V} f''\beta^2$$

If $f'' < 0$,

$$R(\beta) > 0$$

$$R(\beta) = \frac{-M}{N_V}\left[f''\beta^2 - 2k\beta^4\right]$$

If $f'' < 0$,

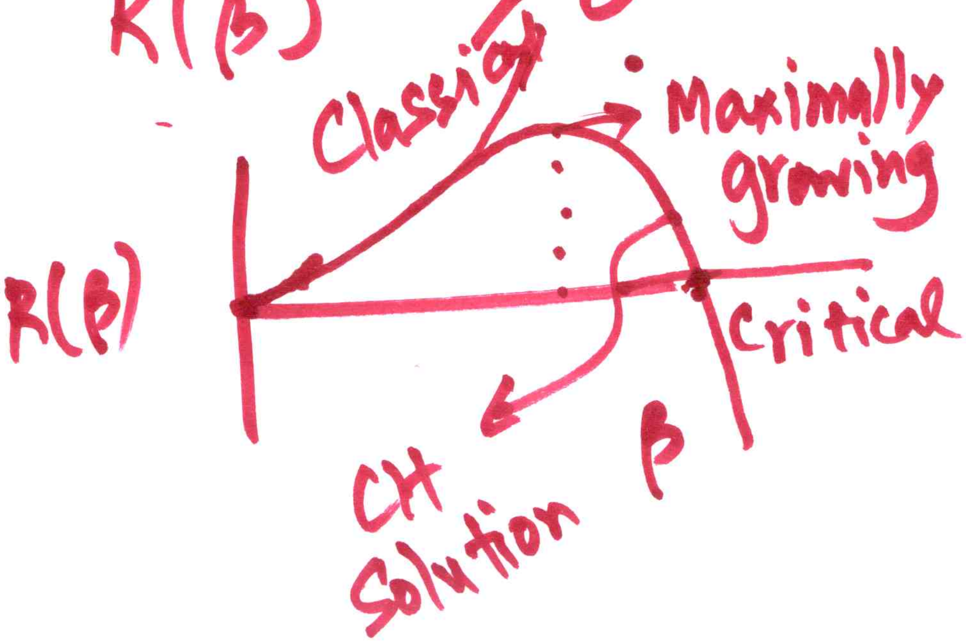
$$\frac{M}{N_V}|f''|\beta^2 + \frac{2kM}{N_V}\beta^4$$

$$A(\beta,t) = A(\beta,0)\exp(R(\beta)\,t)$$

$$R(\beta) = -\frac{M}{N_V} f'' \beta^2 \qquad R(\beta) = -\frac{M}{N_V}\left[f''\beta^2 + 2k\beta^4\right]$$

$\underline{\underline{f'' < 0}}$

$R(\beta) > 0$



$f'' < 0$

$$R(\beta) = -\frac{M}{N_V}\left[2k\beta^4 - |f''|\beta^2\right]$$

$\beta = \dfrac{2\pi}{\lambda}$ Small β, $R(\beta) > 0$

Large β, Small λ

$R(\beta) < 0$

$$\frac{\partial C}{\partial t} = \underset{\underset{1}{\downarrow}}{\tilde{D}} \, \frac{\partial^2 C}{\partial x^2}$$

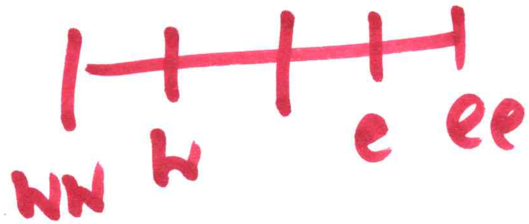
Finite difference

$$\frac{C_i^{t+\Delta t} - C_i^{t}}{\Delta t} = \tilde{D} \, \frac{C_{i-1}^{t} - 2C_i^{t} + C_{i+1}^{t}}{(\Delta x)^2}$$

$$C_i^{t+\Delta t} = C_i^{t} + \frac{D \Delta t}{(\Delta x)^2} \cdot \left[C_{i-1}^{t} - 2C_i^{t} + C_{i+1}^{t} \right]$$

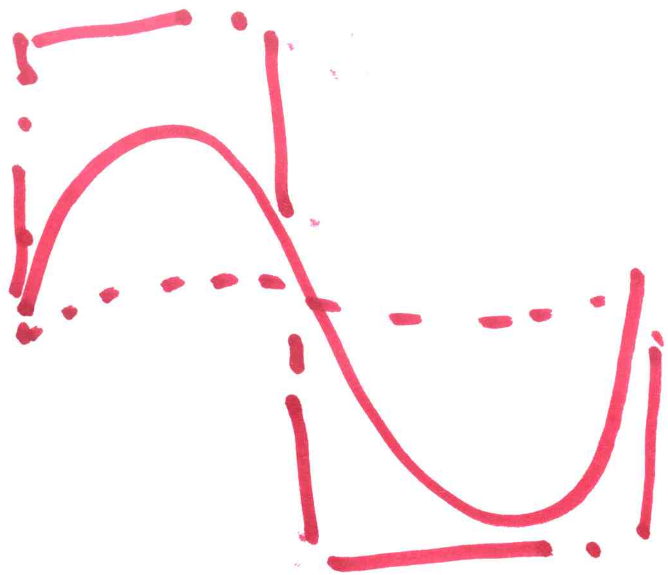
$$\frac{\partial c}{\partial t} = \underbrace{\frac{M}{N_v}}_{\tilde{D}}\left[\frac{\partial^2}{\partial x^2}\frac{\partial f_0}{\partial c} - 2K\frac{\partial^4 c}{\partial x^4}\right] \qquad f''\frac{\partial^2 c}{\partial x^2}$$

$$\frac{\partial^2}{\partial x^2}g(c) \qquad g(c) = 2Ac(1-c)(1-2c)$$



$$\frac{C_i^{t+\Delta t} - C_i^{t}}{\Delta t} = \cancel{g(c)^t_i - 2K}\ \frac{g_{i+1}^t - 2g_i^t + g_{i-1}^t}{(\Delta x)^2} - 2K\frac{\left[C_{ww} - 4C_w + 6C_i - 4C_e + C_{ee}\right]}{(\Delta x)^4}$$

$$C_i^{t+\Delta t} = C_i^t + \underbrace{\frac{\tilde{D}\Delta t}{(\Delta x)^2}}_{B_1}\cdot\left(g_{i-1}^t + g_{i+1}^t - 2g_i^t\right) - \overbrace{\frac{2K\Delta t}{(\Delta x)^4}}^{B_2}\left[C_{ww} - 4C_w + 6C_i - 4C_e + C_{ee}\right]$$



$$\frac{\partial c}{\partial t} = \tilde{D}\,\frac{\partial^2 c}{\partial x^2}$$

$$\frac{\tilde{c}^{\,t+\Delta t} - \tilde{c}^{\,t}}{\Delta t} = -\tilde{D}\,k^2\,\tilde{c}^{\,t+\Delta t}$$

$$\tilde{c}^{\,t+\Delta t} = \frac{\tilde{c}^{\,t}}{1+\tilde{D}k^2\Delta t}$$

$$\frac{\partial c}{\partial t} = \tilde{D}\left[\nabla^2 g - 2\kappa\nabla^4 c\right]$$

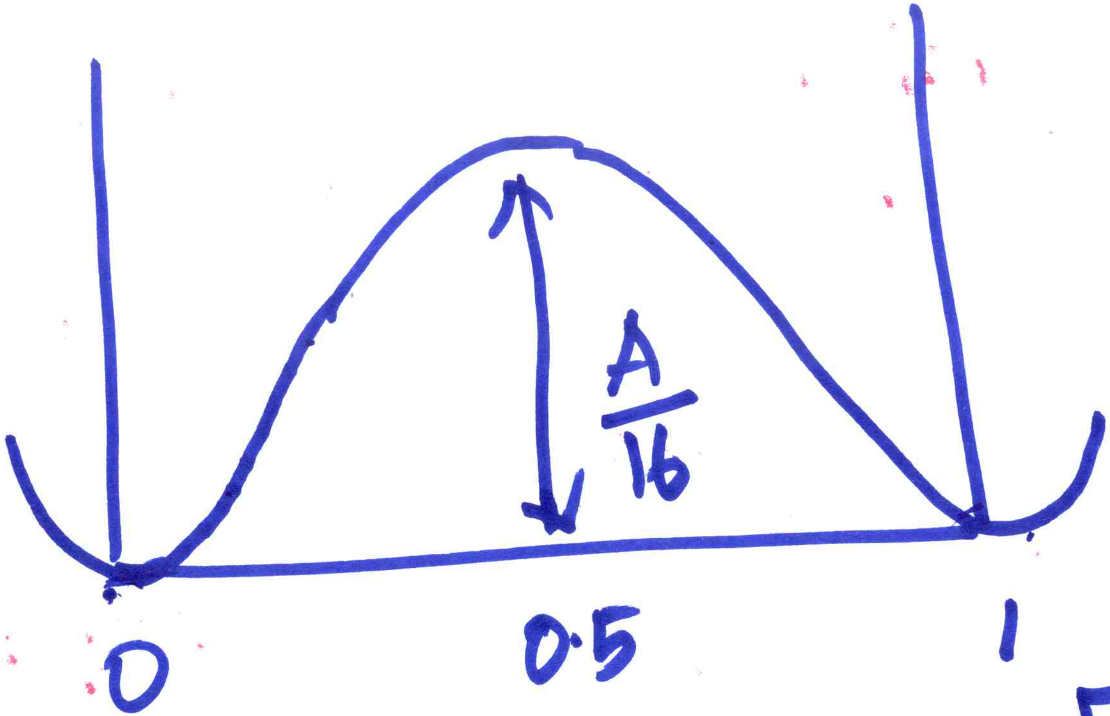
$$\frac{\partial f_0}{\partial c}$$

$$g = 2Ac(1-c)(1-2c)$$

$$\frac{\tilde{c}^{\,t+\Delta t} - \tilde{c}^{\,t}}{\Delta t} = \tilde{D}\left(-k^2\tilde{g}^{\,t}\right) - 2\kappa k^4\,\tilde{c}^{\,t+\Delta t}.$$

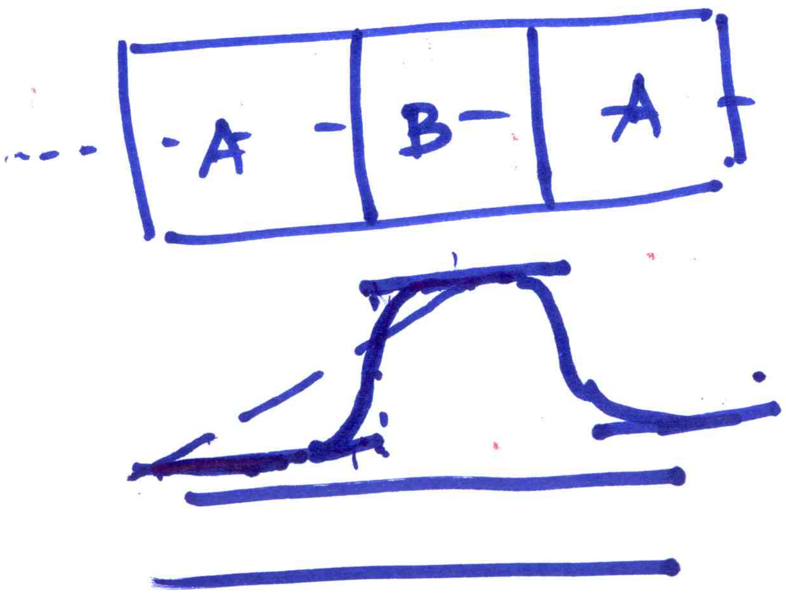
$$\tilde{c}^{\,t+\Delta t} = \frac{\tilde{c}^{\,t} - \tilde{D}k^2\Delta t\,\tilde{g}^{\,t}}{1+2\kappa k^4\Delta t}$$

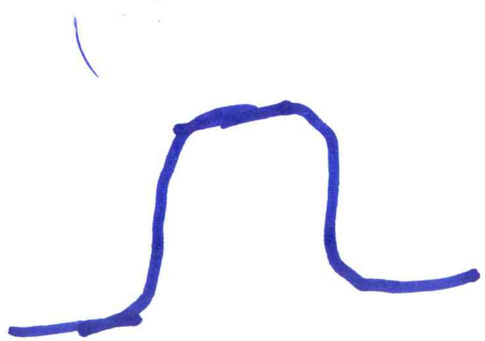
Semi-implicit



$$F = \iiint f_0 + \kappa |\nabla c|^2 \, dV$$

$$Ac^2(1-c)^2$$





$\tilde{c}$

$$\frac{d\tilde{c}}{dx} = ik\tilde{c}$$

$$c \rightarrow \tilde{c}$$