For 1-D

Governing Equation

The governing equation (the non-local Cahn-Hilliard equation) is as follows:

$$\frac{\partial \phi(\mathbf{x}, t)}{\partial t} = \Delta \left(f(\phi(\mathbf{x}, t)) - \epsilon^2 \Delta \phi(\mathbf{x}, t) \right) - \alpha \left(\phi(\mathbf{x}, t) - \bar{\phi} \right)$$

for x in Ω , t in (0, T] where $\Omega = \mathbb{R}^d$ (d = 1, 2, 3) is a domain.

• The Helmholtz free energy $F(\phi)=0.25(\phi^2-1)^2$ with f=F' and global minima $\phi=\pm 1$.

Coefficients in Governing equation

• $\bar{\phi}=\int_{\Omega}\phi d\mathbf{x}/|\Omega|$ is the average concentration of the initial condition

- α : inversely proportional to the square of the total chain length of the copolymer
- ε: the gradient energy coefficient.

Numerical Scheme

 We consider a spectral method with the discrete Fourier transform method. The linear and nonlinear terms treated implicitly and explicit, respectively.

 $x_m = (m-1)L/M$ where m=1,...,M where M is even

$$\phi^k = (\phi_1^k, \cdots, \phi_M^k) , \quad \phi_m^k \approx \phi(x_m, k\Delta t)$$

$$\hat{\phi}_p^k = \sum_{m=1}^M \phi_m^k e^{-ix_m \xi_p}, \quad \phi_m^k = \frac{1}{M} \sum_{p=1-M/2}^{M/2} \hat{\phi}_p^k e^{ix_m \xi_p}$$

where
$$\xi_p = 2\pi(p-1)/L$$

Then,
$$\hat{\phi}_p^{k+1} = \frac{\hat{\phi}_p^k - \Delta t \xi_p^2 \hat{g}_p^k + \Delta t \alpha \bar{\phi}}{1 + \alpha \Delta t + 2\Delta t \xi_p^2 + \epsilon^2 \Delta t \xi_p^4}$$

 By the linear stability analysis, the solution of the governing equation is assumed to have the form of

$$\phi(x,t) = \bar{\phi} + \sum_{k=1}^{\infty} \beta_k(t) \cos(k\pi x)$$

where $|\beta_k(t)| \ll 1$.

 Substituting the above equation into the governing equation, we have

$$\frac{d\beta_k}{dt} = -(k\pi)^2 [3\bar{\phi}^2 - 1 + \epsilon^2 (k\pi)^2] \beta_k + \alpha \beta_k$$

The equation as in the last slide

$$\frac{d\beta_k}{dt} = -(k\pi)^2 [3\bar{\phi}^2 - 1 + \epsilon^2 (k\pi)^2] \beta_k + \alpha \beta_k$$

is up to first order.

• The solution of above one is $\beta_k(t) = \beta_k(0)e^{\eta_k t}$ where

$$\eta_k = -(k\pi)^2 [3\bar{\phi}^2 - 1 + \epsilon^2 (k\pi)^2] - \alpha$$

is the growth rate.

Therefore, we have the maximal growth rate

$$k = \sqrt{1 - 3\bar{\phi}^2} / \left(\sqrt{2}\phi\epsilon\right)$$

• Next, the theoretical growth rate η_k is compared to the numerical growth rate by our proposed scheme with different values of k and α .

Numerical Test

The numerical growth rate is defined by

$$\eta_k = \frac{1}{T} \log \left(\frac{\max_i |\phi_i^n|}{\max_i |\phi_i^0|} \right)$$

• For the numerical test, we let $\bar{\phi}=0$ and an initial condition $\phi(x,0)=0.01\cos(k\pi x)$ with $\epsilon=1/\left(10\sqrt{2}\pi\right)$, $\Delta t=10^{-6}$ and h=0.01 until $T=10^{-4}$.

Numerical Results

- Figure in the next slide will suggests that theoretical values from the linear analysis (solid and dashed line) and numerical values (circle and diamond) are in good agreement.
- Moreover, the result shows that k = 10 is the maximal growth rate which is consistent with the result from the theory.

Figure

