Fourier Spectral Method (III)

For a block copolymer

Block Copolymer

- In this slide, we apply the Fourier Spectral Method to the block copolymer model based on the Cahn-Hilliard equation.

- The original Cahn-Hilliard equation are presented in previous lectures. It is a model of phase-field method and has a bi-harmonic term which makes difficult to solve.

- In block copolymer model, one additional term is added.

Block Copolymer

- This is an equation for the block copolymer model :

$$\frac{\partial \phi}{\partial t} = \frac{\partial^2 f(\phi)}{\partial x^2} - \epsilon^2 \frac{\partial^4 \phi}{\partial x^4} - \alpha(\phi - \bar{\phi})$$

- ϕ is an order parameter for a phase-field method.

- $\bar{\phi} = \frac{1}{|\Omega|} \int_{\Omega} \phi dx$ is an average concentration of initial value.

- $f(\phi) = \frac{\partial}{\partial \phi} \frac{1}{4}(1 - \phi^2)^2 = \phi^3 - \phi$

Fourier Spectral Method

- For even integer M, we discretize in the interval [0, L] as given below

$$\phi_m^n \approx \phi(m\Delta x, n\Delta t)$$

$$\phi^n = (\phi_1^n, \cdots, \phi_M^n)$$

- And we consider the discrete Fourier transformation (DFT) and the inverse discrete Fourier transformation (iDFT).

Fourier Spectral Method

- DFT :

$$\hat{\phi}_p^n = \sum_{m=1}^{M} \phi_m^n e^{-ix_m \xi_p}$$

- iDFT :

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

where they are even expansion and $\xi_p = \dfrac{2\pi(p-1)}{L}$

- Next, we apply the transformation to the block copolymer model.

Fourier Spectral Method

- From the Fourier expansion, we can rewrite the order parameter and its derivatives which are continuous version.

$$\phi = \frac{1}{M} \sum_{p=1-M/2}^{M/2} \hat{\phi}_p e^{ix\xi_p}$$

$$\frac{\partial^2}{\partial x^2}\phi = -\frac{1}{M} \sum_{p=1-M/2}^{M/2} \xi_p^2 \hat{\phi}_p e^{ix\xi_p}$$

$$\frac{\partial^4}{\partial x^4}\phi = \frac{1}{M} \sum_{p=1-M/2}^{M/2} \xi^4 \hat{\phi}_p e^{ix\xi_p}$$

- It is an easy calculation by taking the derivatives.

Numerical Scheme

- For the time discretization, we can use the Runge-Kutta method or any other improved method, however, we just use the simple forward difference method in here.

- For the space discretization, we use the non-linearly stabilized splitting scheme which was presented by Eyre. It is proved that the scheme is unconditionally gradient stable and has a unique solution from the convexity of the energy functional.

Numerical Scheme

- So,

$$\frac{\phi_m^{n+1} - \phi_m^n}{\Delta t} = 2\frac{\partial^2}{\partial x^2}\phi_m^{n+1} - \epsilon^2 \frac{\partial^4}{\partial x^4}\phi_m^{n+1} + \frac{\partial^2}{\partial x^2} g_m^n - \alpha\left(\phi_m^{n+1} - \bar{\phi}\right)$$

where

$$g_m^n = f(\phi_m^n) - 2\phi_m^n$$

- Since f has a non-linear term, we use g, instead. If we apply the Fourier transform to f, then we should calculate the cube of summation which is too complicated to calculate.

$$\left(\sum_p \hat{\phi}_p e^{ix\xi_p}\right)^3$$

Fourier Transformation

- Applying the Fourier transformation,

$$\frac{1}{M}\sum_p \frac{\hat{\phi}_p^{n+1}-\hat{\phi}_p^n}{\Delta t}e^{ix_m\xi_p} = -\frac{2}{M}\sum_p \xi_p^2\hat{\phi}_p^{n+1}e^{ix_m\xi_p} - \frac{\epsilon^2}{M}\sum_p \xi_p^4\hat{\phi}_p^{n+1}e^{ix_i\xi_p}$$

$$+\frac{1}{M}\sum_p \xi_p^2\hat{g}_p^n e^{ix_m\xi_p} - \frac{\alpha}{M}\sum_p \hat{\phi}_p^{n+1}e^{ix_m\xi_p}$$

$$+\frac{\alpha}{M}\sum_p \bar{\phi}e^{ix_m\xi_p}$$

We can cancel out M, summation and exponential terms from the orthogonality in the Fourier space.

Fourier Transformation

- The result is

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

- And it can be represented as

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