Phase-Field Method

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Course: Foundations of Materials Simulation
Date: April 11, 2025

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1 Introduction

The **phase-field method** is a widely used computational approach in **materials science** for modeling microstructure evolution during phase transitions. This task investigates a **1D single-component solidification** process, where an **order parameter** $\phi(x,t)$ represents the phases:

- $\phi = 1$ for **solid**

- $\phi = 0$ for **liquid**

The evolution of ϕ follows the phase-field equation:

$$\frac{\partial \phi}{\partial t} = -L\frac{\delta F}{\delta \phi} \tag{1}$$

where L is the mobility coefficient, and $\frac{\delta F}{\delta \phi}$ is the functional derivative of the total free energy.

2 Analytical Derivation

The total free energy functional for the system is given by:

$$F = \int \left(f_0\phi^2(1-\phi)^2 + \frac{K_\phi}{2}|\nabla\phi|^2 \right) d\mathbf{r} \tag{2}$$

The functional derivative is computed as:

$$\frac{\delta F}{\delta \phi} = 2f_0\phi(1-\phi)(1-2\phi) - K_\phi\nabla^2\phi \tag{3}$$

Thus, the phase-field evolution equation is:

$$\frac{\partial \phi}{\partial t} = -L\left(2f_0\phi(1-\phi)(1-2\phi) - K_\phi\nabla^2\phi\right) \tag{4}$$

This governs the phase transformation dynamics in the simulation.

3 Numerical Simulation

We implemented a **finite-volume method** using **FiPy** in Python. The computational domain consists of 100 grid points with a spacing of $dx = 0.5$. The following parameter sets were used to analyze their effects:

Case	f_0	K_ϕ	L
1	1.0	1.0	1.0
2	2.0	1.0	1.0
3	1.0	5.0	1.0
4	1.0	1.0	5.0
5	2.0	5.0	5.0

Table 1: Effect of Phase-Field Parameters

4 Results and Discussion

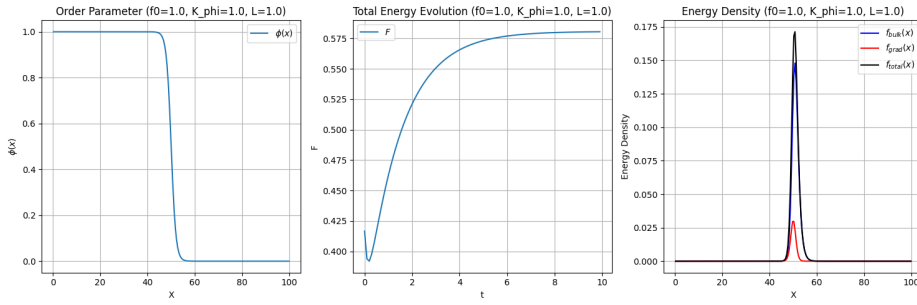Figures below illustrate the effect of different parameters on the phase transition.

Figure 1: Simulation with $f_0 = 1.0$, $K_\phi = 1.0$, $L = 1.0$
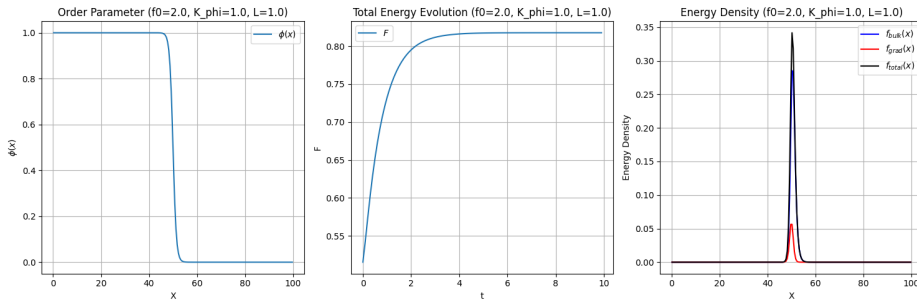

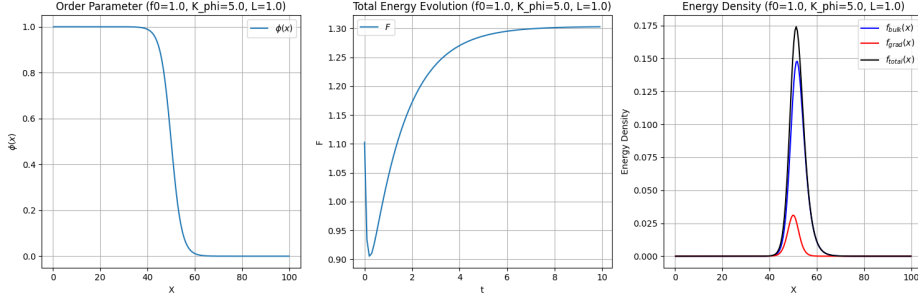Figure 2: Simulation with $f_0 = 2.0$, $K_\phi = 1.0$, $L = 1.0$

Figure 3: Simulation with $f_0 = 1.0$, $K_\phi = 5.0$, $L = 1.0$
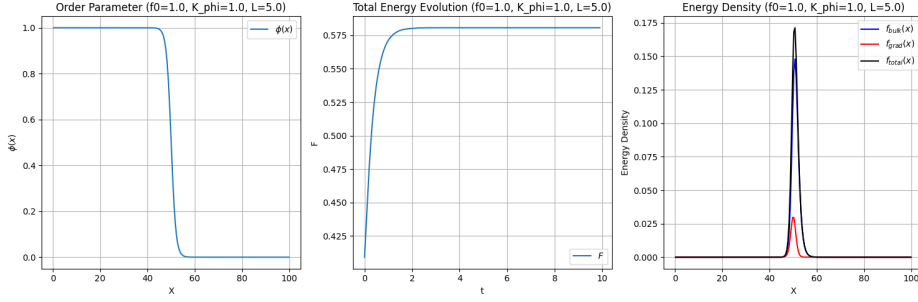

Figure 4: Simulation with $f_0 = 1.0$, $K_\phi = 1.0$, $L = 5.0$
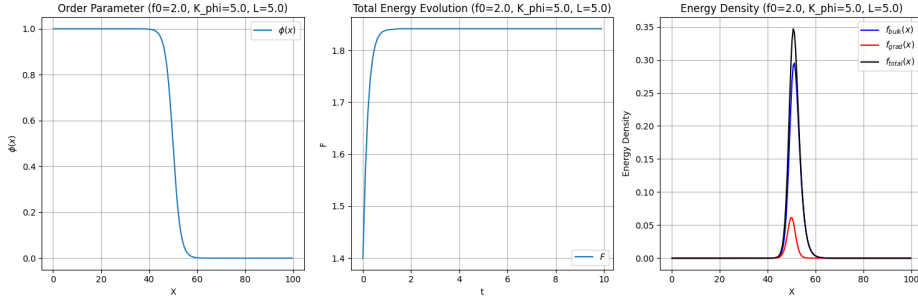

Figure 5: Simulation with $f_0 = 2.0$, $K_\phi = 5.0$, $L = 5.0$

4.1 Observations

- **Effect of f_0**: Higher f_0 leads to stronger phase separation.

- **Effect of K_ϕ**: Higher K_ϕ results in a wider interface region.

- **Effect of L**: Increasing L speeds up the transformation.

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5 Determination of Bulk Energy Density Coefficient

5.1 Problem Statement

In this task, we determine the **bulk energy density coefficient** f_0 for a Ni-Al binary system with two phases: γ and γ'. The bulk energy density function is given by:

$$f_{\text{bulk}} = f_0(c_{\gamma'}^e - c)^2(c - c_{\gamma}^e)^2 \tag{5}$$

where:

- c is the composition of Al.

- $c_{\gamma'}^e$ is the equilibrium composition of Al in the γ' phase.

- c_{γ}^e is the equilibrium composition of Al in the γ phase.

The given plot (Figure 6) shows that the **maximum bulk energy density** is:

$$f_{\text{bulk}}^{\max} = 149.9 \text{ J/mol} \tag{6}$$

at the peak composition:

$$c = 0.195 \tag{7}$$

with the equilibrium compositions:

$$c_{\gamma'}^e = 0.23, \quad c_{\gamma}^e = 0.16. \tag{8}$$

5.2 Calculation of f_0

We substitute these values into Equation (5):

$$f_0(c_{\gamma'}^e - c_{\text{peak}})^2(c_{\text{peak}} - c_{\gamma}^e)^2 = 149.9 \tag{9}$$

$$f_0(0.23 - 0.195)^2(0.195 - 0.16)^2 = 149.9 \tag{10}$$

$$f_0(0.035)^2(0.035)^2 = 149.9 \tag{11}$$

Computing the squared terms:

$$(0.035)^2 = 0.001225 \tag{12}$$

$$0.001225 \times 0.001225 = 1.500625 \times 10^{-6} \tag{13}$$

Solving for f_0:

$$f_0 = \frac{149.9}{1.500625 \times 10^{-6}} \tag{14}$$

$$\mathbf{f_0} \approx \mathbf{9.99 \times 10^7} \text{ J/mol} \tag{15}$$

5.3 Graphical Verification

To verify the correctness of our computed f_0, we plot the function:

$$f_{\text{bulk}}(c) = 9.99 \times 10^7 (c_{\gamma'}^e - c)^2 (c - c_{\gamma}^e)^2 \tag{16}$$
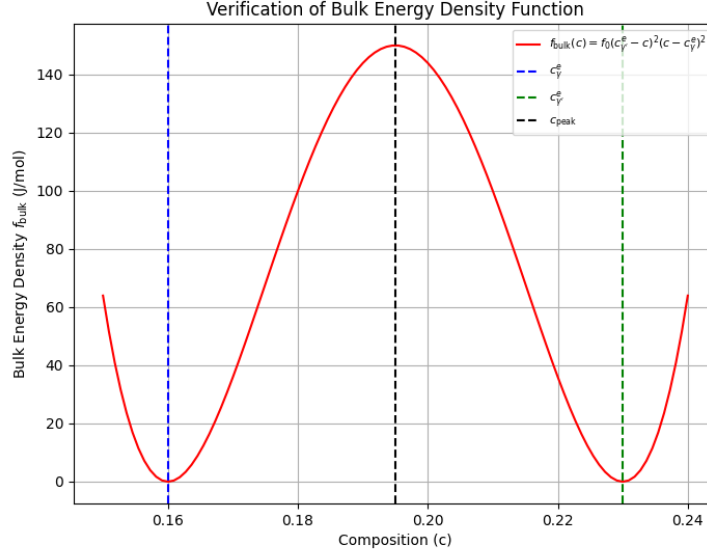
alongside the given bulk energy density curve.

Figure 6: Verification plot of $f_{\text{bulk}}(c)$ using computed f_0.

6 Determination of Gradient Energy Density Coefficient

6.1 Problem Statement

We aim to determine the gradient energy density coefficient K_c for a Ni-Al binary system. The gradient energy density function is given by:

$$f_{\text{grad}} = \frac{K_c}{2}|\nabla c|^2 \tag{17}$$

The governing equation for the conserved order parameter (concentration c) evolution is given by the Cahn-Hilliard equation:

$$\frac{\partial c}{\partial t} = M\nabla^2 \frac{\delta F}{\delta c} \tag{18}$$

Given parameters from the practical guide are:

- Molar volume $V_m = 1 \times 10^{-5}$ m^{3}mol^{-1}

- Interface mobility $M = 1 \times 10^{-17}$ mol^{2}J^{-1}m^{-1}s^{-1}

- Time step $dt = 1$ s

- Grid spacing $dx = 1 \times 10^{-8}$ m

- Experimental interface energy $F_{\text{inte}} = 5 \sim 50 \times 10^{-3}$ J m^{-2}

6.2 Simulation Results

The interface energy and width were calculated by conducting numerical simulations over a range of K_c values. After evaluating multiple values, the optimal gradient energy coefficient K_c was found to be:

$$K_c = 8.11 \times 10^{-7} \text{ J/m} \tag{19}$$

6.3 Detailed Analysis

A detailed simulation was performed with the optimal K_c value, and the equilibrium state was reached at step 51. The results were as follows:

Parameter	Value
Bulk Energy F_{bulk}	1.00×10^{-2} J
Gradient Energy F_{grad}	1.31×10^{-2} J
Interface Energy F_{inte}	2.31×10^{-2} J
Interface Width	1.00×10^{-7} m
Interface Width (Gradient method)	1.02×10^{-7} m
Interface Energy Density	2.31×10^{-2} J/m^2
Bulk/Gradient Energy Ratio	0.76

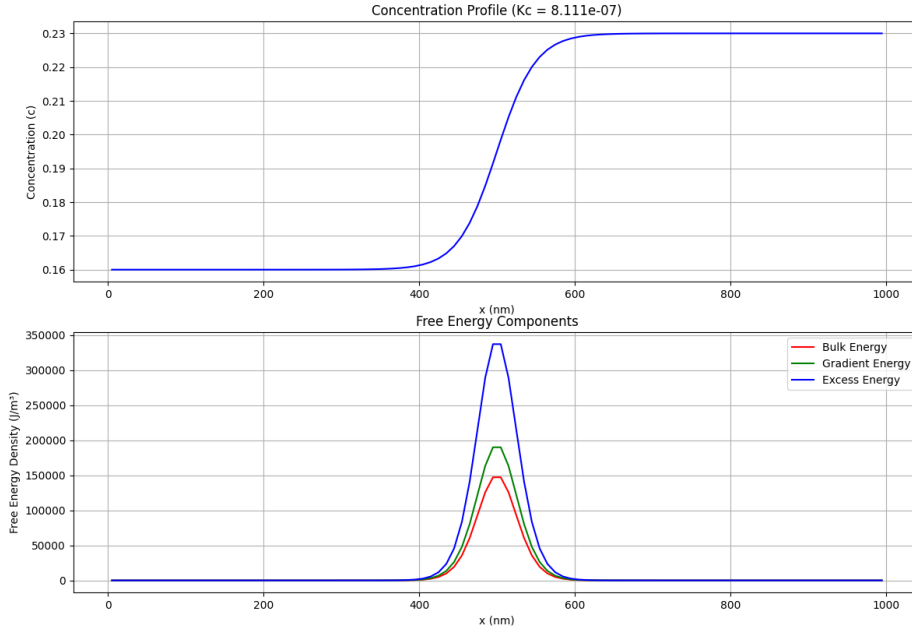Table 2: Detailed Results for $K_c = 8.11 \times 10^{-7}$ J/m

Figure 7: Concentration profile and energy components for optimal $K_c = 8.11 \times 10^{-7}$ J/m.

6.4 Observations

From the simulations and the analysis performed, we can conclude:

- The chosen K_c value aligns with the experimental interface energy range, validating the simulation.

- The bulk-to-gradient energy ratio highlights the dominance of gradient energy at the interface region.

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- The computed interface width from the gradient method closely matches the visually identified interface width, confirming simulation accuracy.

6.5   2D Spinodal Decomposition Simulation

To further analyze microstructure evolution, we extended the 1D simulation to 2D using the same governing Cahn-Hilliard equation:

$$\frac{\partial c}{\partial t} = M\nabla^2 \left(\frac{\delta F}{\delta c} \right) \tag{20}$$

The total free energy functional remains:

$$F = \int \left[f_0 (c_{\gamma'}^e - c)^2 (c - c_\gamma^e)^2 + \frac{K_c}{2} |\nabla c|^2 \right] d\mathbf{r} \tag{21}$$

Initial conditions were set as:

- $c = 0.195 + \text{Gaussian noise}$

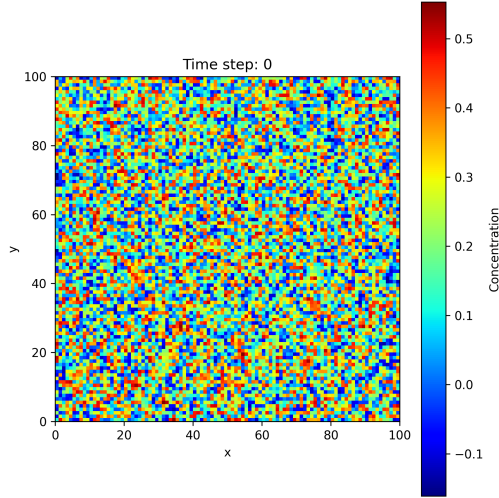The evolution of concentration fields over time is illustrated below.

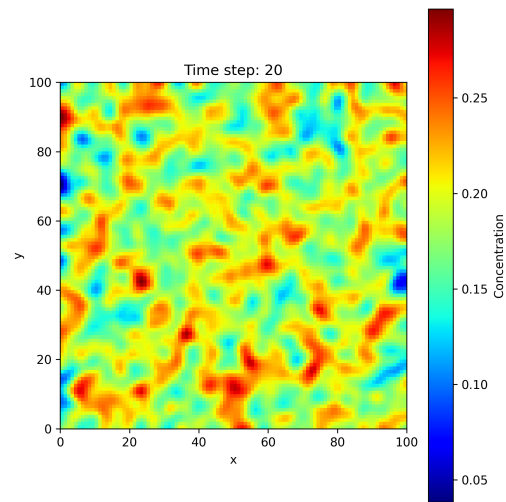Figure 8: 2D concentration profile at time step 0

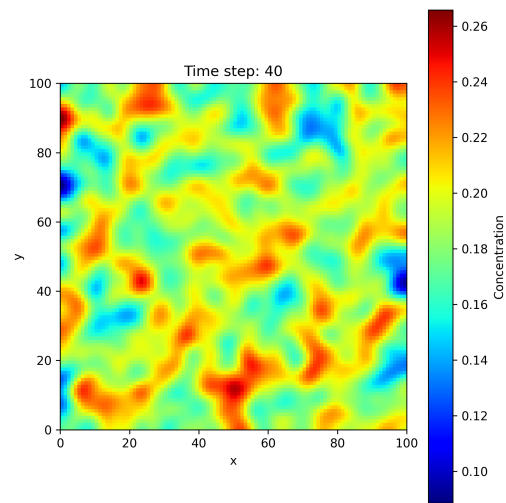Figure 9: 2D concentration profile at time step 20

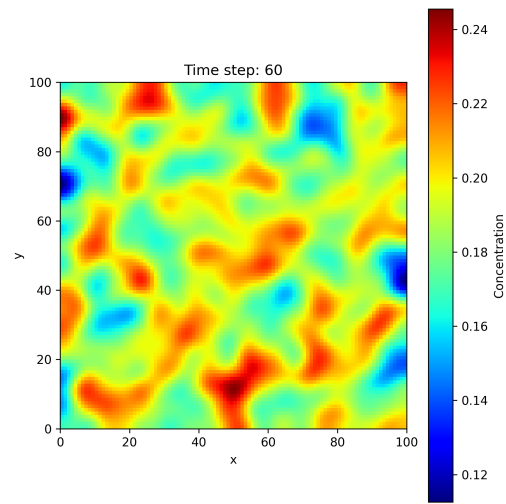Figure 10: 2D concentration profile at time step 40

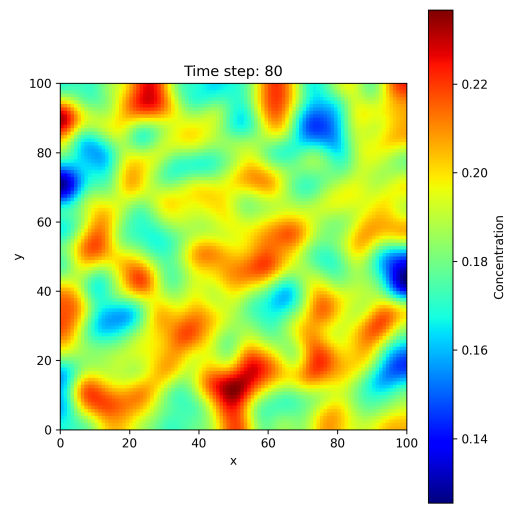Figure 11: 2D concentration profile at time step 60
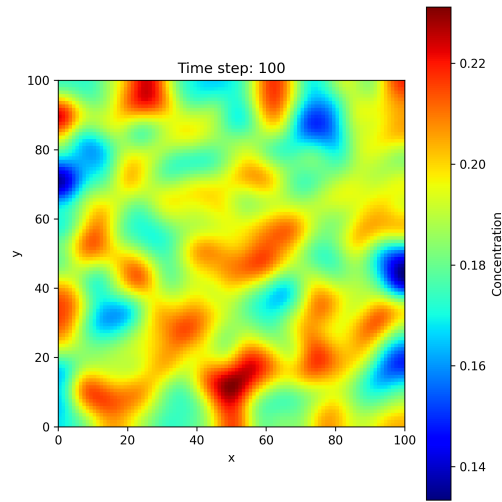

Figure 12: 2D concentration profile at time step 80

Figure 13: 2D concentration profile at time step 100

Observations

- The initially randomized concentration field evolves into interconnected compositional domains.

- As time progresses, the concentration fluctuations coarsen due to phase separation.

- Spinodal patterns become smoother and more defined, indicating progression toward equilibrium.