MSE 203
Introduction to Computational Materials
Assignment 4

Dreamy Jain (23110106)
Course Instructor: Prof. Raghavan Ranganathan

Department of Material Science and Engineering
IIT Gandhinagar

PROBLEM 1: DOUBLE WELL POTENTIAL

(a) The free energy density for a binary system is modelled using a double-well potential of the form:

$$f(\phi) = a\,\phi^2(1-\phi)^2$$

where ϕ is the composition (phase field variable), and a is a parameter controlling the depth of the wells. For this problem, we set $a = 2$.
The plot of the double-well potential over the range $\phi \in [-0.2, 1.2]$ is shown in **Figure 1**. It can be observed that the energy has two minima at $\phi = 0$ and $\phi = 1$, corresponding to the two stable phases.
The energy barrier occurs at $\phi = 0.5$, where the energy reaches a maximum:

$$f(0.5) = 2 \cdot (0.25)^2 = 0.5$$

Hence, the energy barrier between the two phases is 0.5.

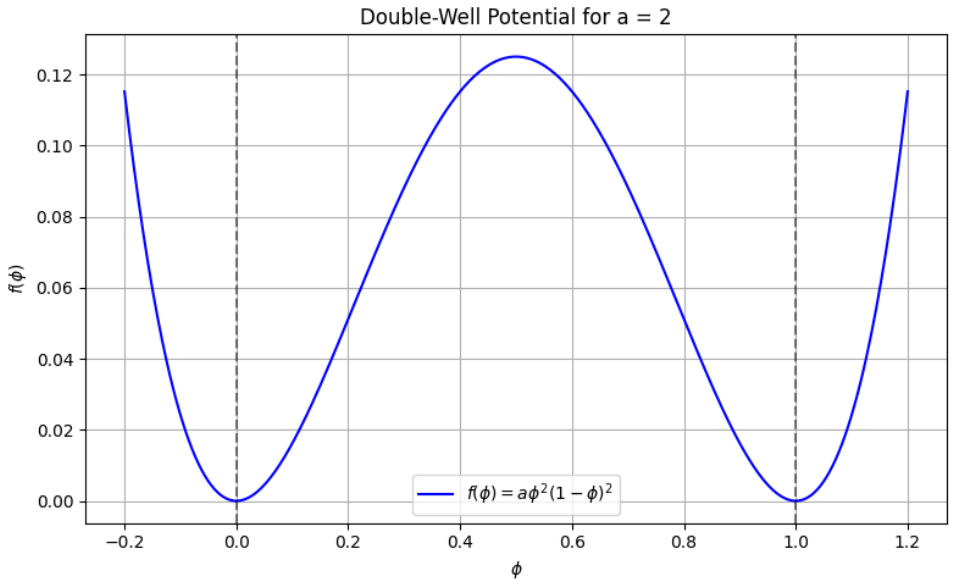

Figure 1: Double Well Potential $f(\phi)$ for $a = 2$

(b) To determine the spinodal region, we solve for the points where the second derivative of the free energy becomes zero:

$$\frac{d^2 f}{d\phi^2} = a(2 - 12\phi + 12\phi^2)$$

Setting this to zero and solving the quadratic:

$$\phi^2 - \phi + \frac{1}{6} = 0 \Rightarrow \phi = \frac{1 \pm \sqrt{1 - \frac{2}{3}}}{2} \approx 0.21 \text{ and } 0.79$$

Thus, the spinodal region is defined as:

$$0.21 < \phi < 0.79$$

In this region, the system is thermodynamically unstable, and spontaneous phase separation occurs without nucleation.

PROBLEM 2: MICROSTRUCTURE EVOLUTION OVER TIME

In this simulation, the spinodal decomposition of a binary system is modelled using the Cahn–Hilliard equation, implemented via the `FiPy` finite volume solver. The phase field variable ϕ, representing the local composition, evolves in time, starting from an initially random distribution.

- $a = D = \epsilon = 1$
- *Grid:* 50×50
- *Initial* $\phi \approx 0.5$, *random noise*
- *Total simulation time* $= 400$
- *Intermediate time* $= 50, 100, 200, 300$

The snapshots for different time:

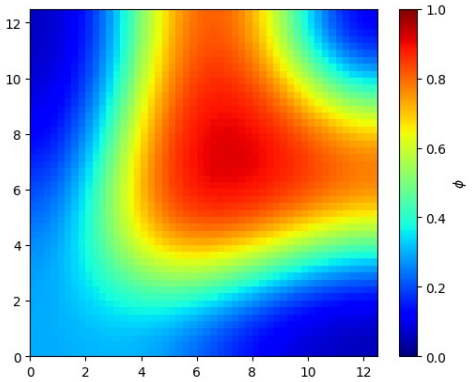

Figure 2: For t = 50

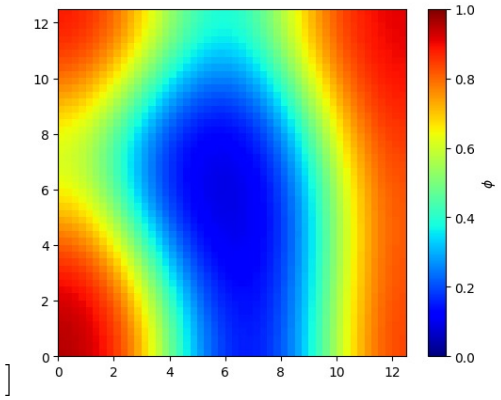

Figure 3: For t = 100

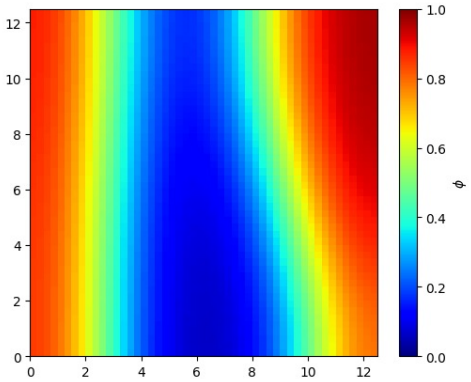

Figure 4: For t = 200

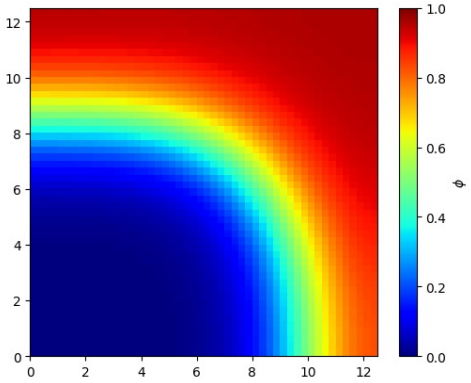

Figure 5: For t = 300

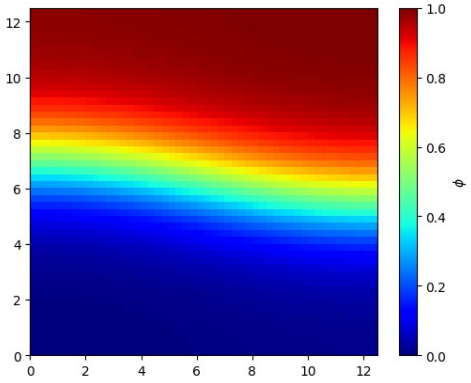

Figure 6: For t = 400

PROBLEM 3: EFFECT OF SYSTEM SIZE

In this problem we varied the grid sizes in both x and y for varying the system size.

- $a = 1$
- $D = \epsilon = 1$
- *Initial* $\phi \approx 0.5$, *random noise*
- *Total simulation time* $= 400$
- *Grid sizes* $= nx = ny = 30, 60, 100, 500$

The snapshots for different system sizes:

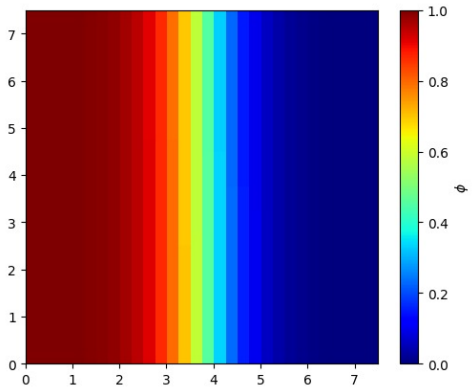

Figure 7: $nx = ny = 30$

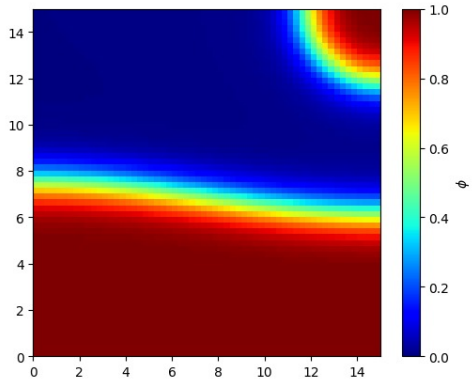

Figure 8: $nx = ny = 60$

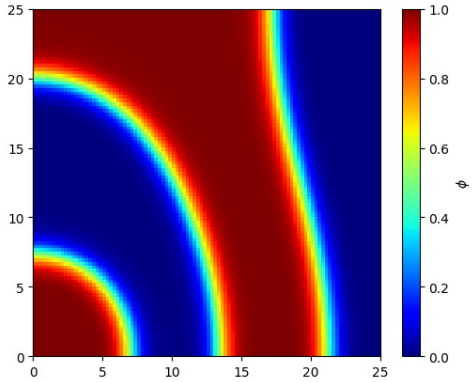

Figure 9: $nx = ny = 100$

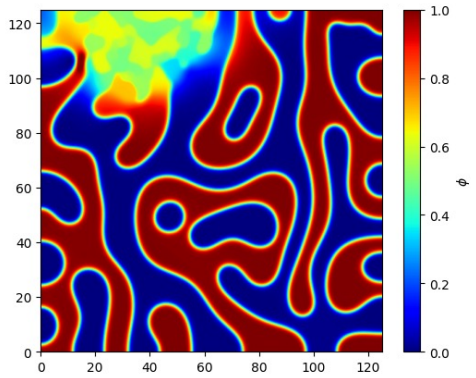

Figure 10: $nx = ny = 500$

Does the microstructure change as a function of system size?
Yes, the microstructure does change as a function of system size.
As the system size increases (from 30×30 to 500×500), the simulation allows for more fluctuation modes and spatial freedom. In smaller systems (e.g., 30×30), fewer domains form, and their growth is limited due to the confined space. The resulting microstructure appears simpler and more uniform.
In contrast, larger systems (e.g., 100×100 and 500×500) show:

- More intricate domain patterns
- Increased number of nucleated regions
- A more realistic representation of spinodal decomposition

Thus, the morphology and number of domains are significantly affected by the system size.

What is the width of the interface? Does it depend on the system size?
The width of the interface is determined by the gradient energy coefficient ϵ, and does not depend on the system size.
In the Cahn–Hilliard model, the interface thickness is related to ϵ approximately by:

$$\text{Interface width} \propto \epsilon$$

Since ϵ is kept constant in all simulations, the observed interface width remains the same across all grid sizes. Although the number and layout of domains change, the sharpness of the phase boundaries is constant, confirming that interface width is independent of the overall system size.

PROBLEM 4: EFFECT OF 'a' PARAMETER

In this problem we varied the parameter a, keeping the other parameters as following:

- $D = \epsilon = 1$
- *Initial* $\phi \approx 0.5$, *random noise*
- *Total simulation time* $= 400$
- *Grid sizes* $= nx = ny = 60$
- $a = 0.5, 1.0, 1.5$

The snapshots for different $'a'$

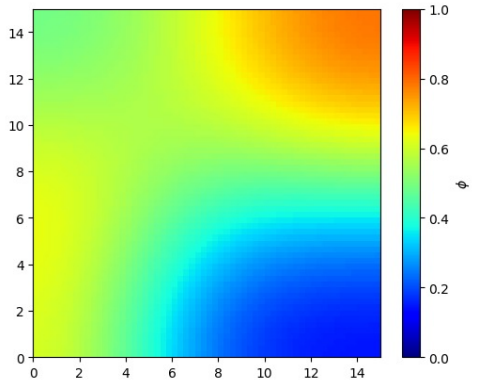

Figure 11: a=0.5

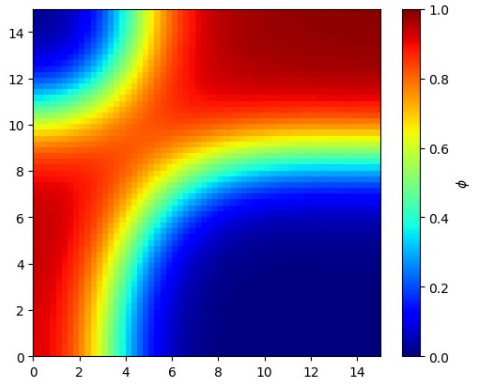

Figure 12: a=1

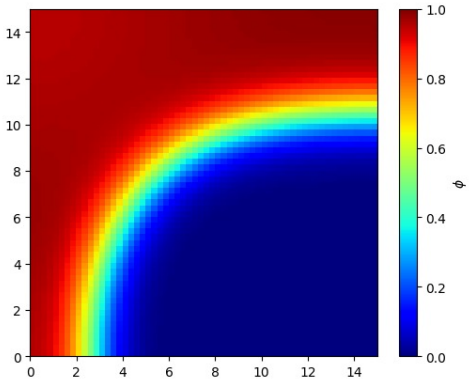

Figure 13: a=1.5

Question: *How does the microstructure change and why?*
Answer: The parameter a in the double-well potential

$$f(\phi) = a\phi^2(1-\phi)^2$$

controls the **depth of the energy wells**, and therefore the thermodynamic driving force for phase separation.
As a increases from $0.5 \rightarrow 1.0 \rightarrow 1.5$, the microstructure changes as follows:

- **Domain contrast increases:**
  Higher a leads to **sharper phase separation**, as the free energy penalty for intermediate ϕ values becomes steeper. This causes the system to drive more strongly toward pure phases ($\phi \approx 0$ and $\phi \approx 1$).
- **Interface thickness decreases:**
  The transitions between domains become **narrower and more defined**, as the system penalizes intermediate states more heavily.
- **Domain shapes become more regular:**
  With larger a, the system more quickly eliminates curved or diffused interfaces, resulting in smoother, sharper domain boundaries.

In summary, **as a increases**, the system shows **stronger segregation**, **sharper interfaces**, and **higher thermodynamic contrast** between phases — leading to more distinct and well-separated microstructures.

PROBLEM 5: VERIFYING PHASE BOUNDARIES

To verify that the simulation correctly captures the phase boundaries, we initialized the system with five different average compositions:

$$\phi_0 = 0.1, \quad 0.25, \quad 0.5, \quad 0.75, \quad 0.9$$

All simulations were performed with:

- Grid size: 100×100
- Parameters: $a = D = \epsilon = 1$

- Initial condition: random noise centered around each composition
- Simulation time: 400 units

According to **Problem 1(b)**, the spinodal region lies between:

$$\phi \in (0.21,\ 0.79)$$

This means that only compositions **inside** this range are thermodynamically unstable and will undergo **spontaneous spinodal decomposition**, whereas compositions **outside** will remain mostly homogeneous (or evolve minimally).
Final Microstructres:

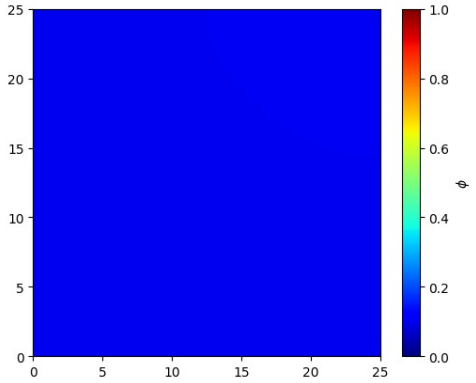

Figure 14: $\phi = 0.1$

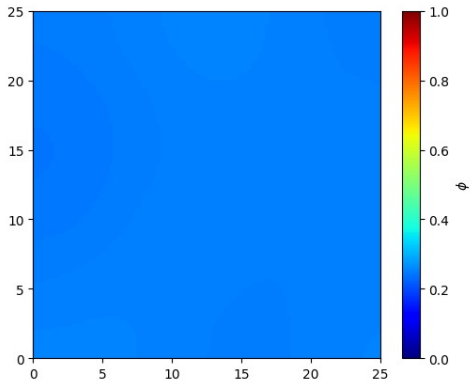

Figure 15: $\phi = 0.25$

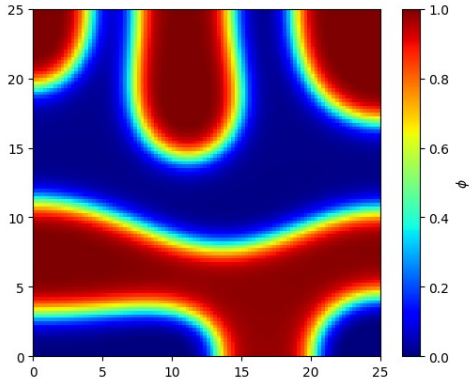

Figure 16: $\phi = 0.5$

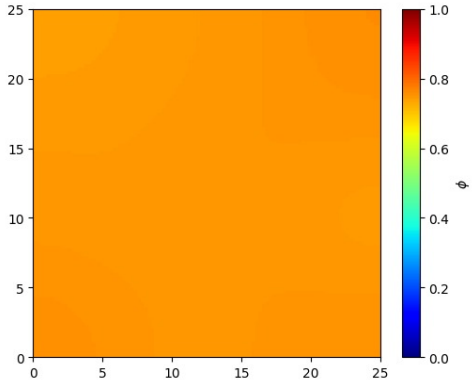

Figure 17: $\phi = 0.75$

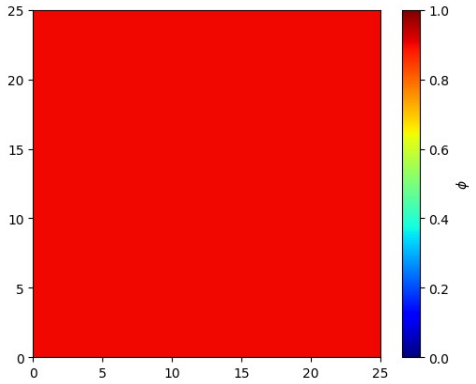

Figure 18: $\phi = 0.9$

Phase separation was observed clearly at $\phi = 0.5$.
For $\phi = 0.25$ and $\phi = 0.75$, phase separation was present but hard to distinguish.
No visible phase separation was observed at $\phi = 0.1$ and $\phi = 0.9$.

PROBLEM 6: MASS CONSERVATION

To verify mass conservation, we computed the spatial average of the phase field variable ϕ at each time step during the simulation. In the Cahn-Hilliard model, mass conservation is expected because the evolution equation is written in a conservative form.

We tracked the total average ϕ using:

$$\bar{\phi}(t) = \frac{1}{N} \sum_{i=1}^{N} \phi_i(t)$$

where N is the total number of grid points.
The plot of $\bar{\phi}$ versus time is shown in Figure 19. The average value remains nearly constant throughout the simulation, with only negligible numerical fluctuations. This confirms that the simulation respects the conservation of total concentration.

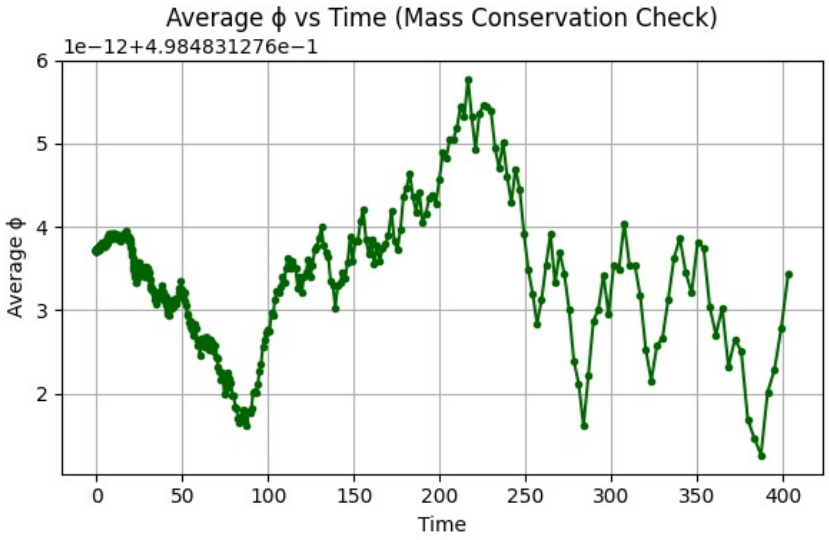

Figure 19: Plot of average ϕ as a function of time. The curve remains flat, confirming that the simulation conserves the total composition, as expected from the Cahn-Hilliard model.