



Phase Separation Dynamics of Metallic Glass Using Cahn-Hilliard Equation: A Computational Study

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Introduction

The study of alloys and their properties has generated significant interest in recent times. When these alloys are mixed at a high temperature and quenched, the metal does not get enough time to form an ordered structure. Thus an amorphous metal is created. In the last few decades there has been development of various alloys which allow for low critical cooling rates and result in an amorphous structure which can be up to several millimetres thick. These alloys are known as bulk metallic glasses. They possess electrical and physical properties that are of great interest.

Phase field modelling is the method used to study the phase transformations in these alloy systems. When the alloy is cooled at a very slow rate the system spontaneously phase separates without a nucleation barrier forming a microstructure which gives the metallic glass certain interesting properties. Evidence of this was first discovered in 1940s by Bradley[1] as sidebands in the Bragg peaks of Cu-Ni-Fe alloy. The phase separation was initially thought of as an uphill diffusion or negative diffusion coefficient but when used with the Fick's law for diffusion, negative diffusion produces incorrect results. What Fick's law and the classical diffusion equation fails to account for is the interfacial energy term which was presented by Cahn [2] along with a term for the effect of coherency strains which dictates why spinodal decomposition happens in some alloys and not in others. [3]

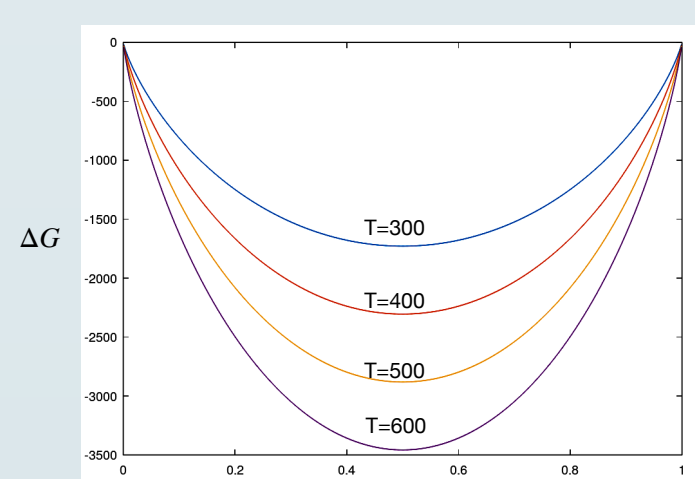
- We start by considering a binary alloy with atom types A and B.
- Basis for our model is the minimisation of Gibbs Free Energy. $G = H - TS$. Considering $H \approx U$, we get $\Delta G^{mix} = \Delta U^{mix} - T\Delta S^{mix}$ where temperature and pressure are kept constant.
- $\Delta G^{mix} = \Omega(1 - \chi_B)\chi_B + RT[(1 - \chi_B)\ln(1 - \chi_B) + \chi_B\ln\chi_B]$

Theory

Ordered Solution $\Omega < 0$
 $\Rightarrow E_{AB} < \frac{1}{2}(E_{AA} + E_{BB})$

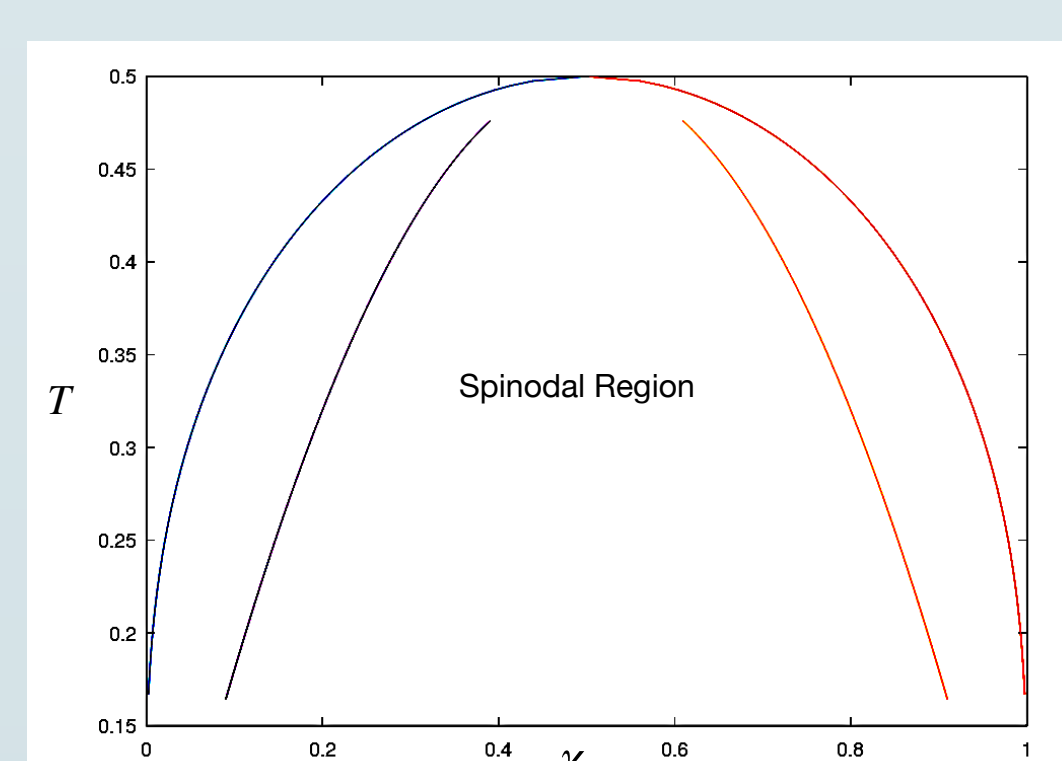
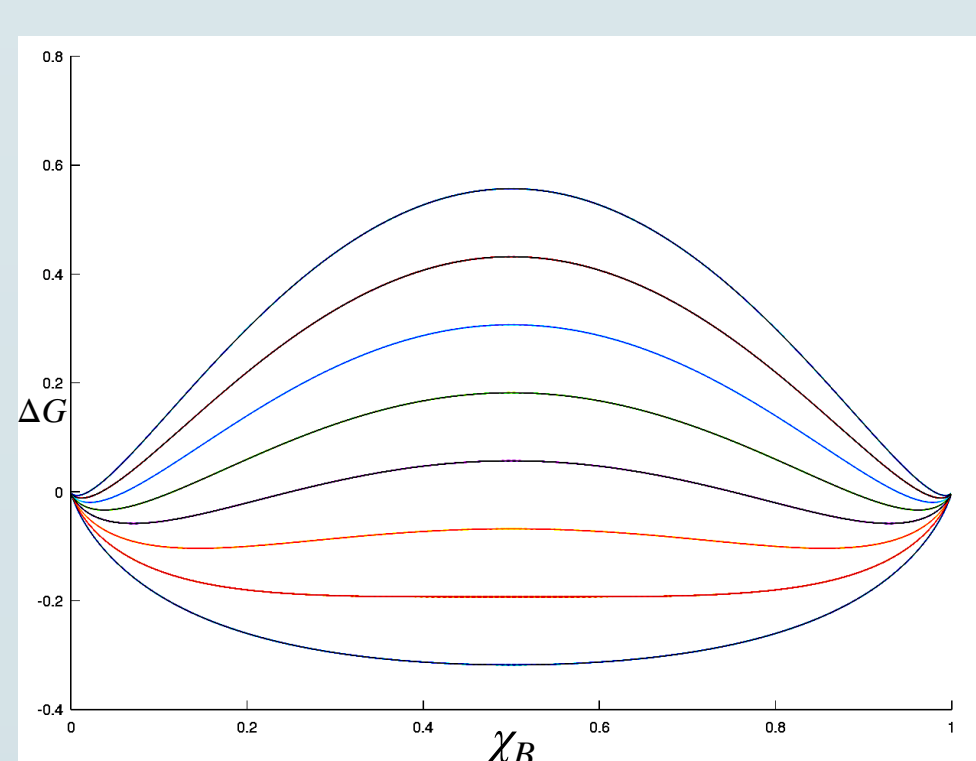
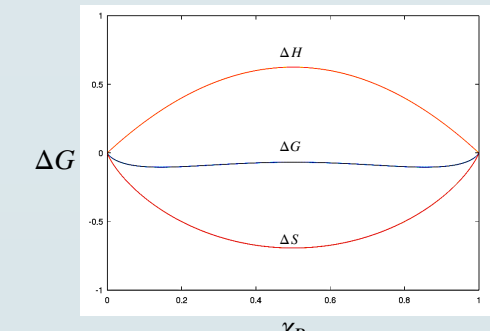
If we have AA or BB bonds, the system will break them and form AB bonds. At lower temperatures the system might become ordered or phase separated

Ideal solution $\Omega = 0$
This model does not differentiate between AA or BB or AB bonds as the enthalpy of mixing is 0.



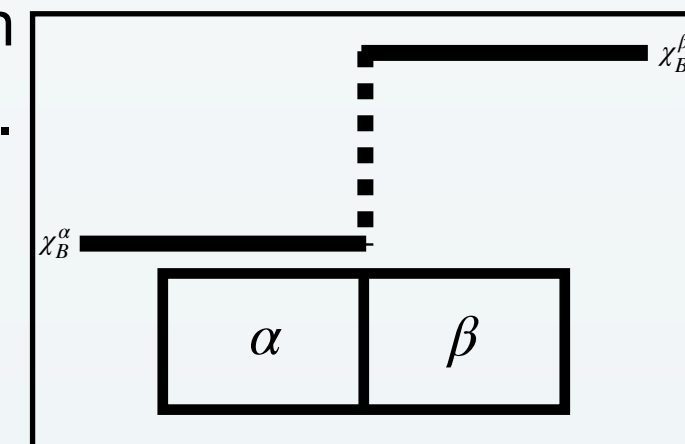
Spinodal decomposition $\Omega > 0$
 $\Rightarrow E_{AB} > \frac{1}{2}(E_{AA} + E_{BB})$

System Phase separates
AB bonds require more energy to form/break than AA or BB bonds
Thus it is more favourable for the system to form AA and BB bonds than AB bonds

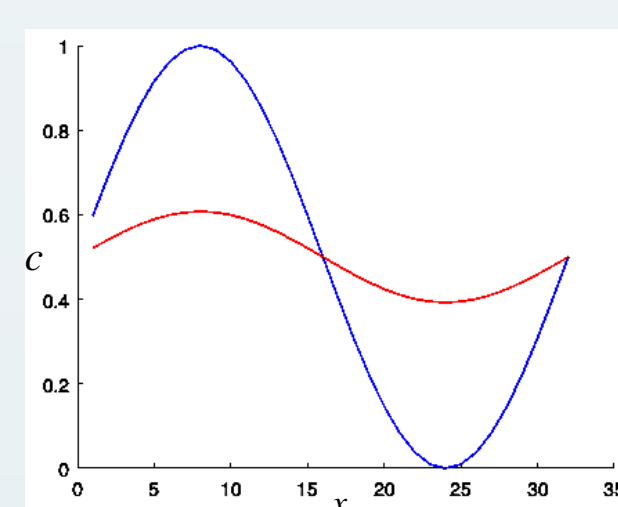


Cahn-Hilliard Equation

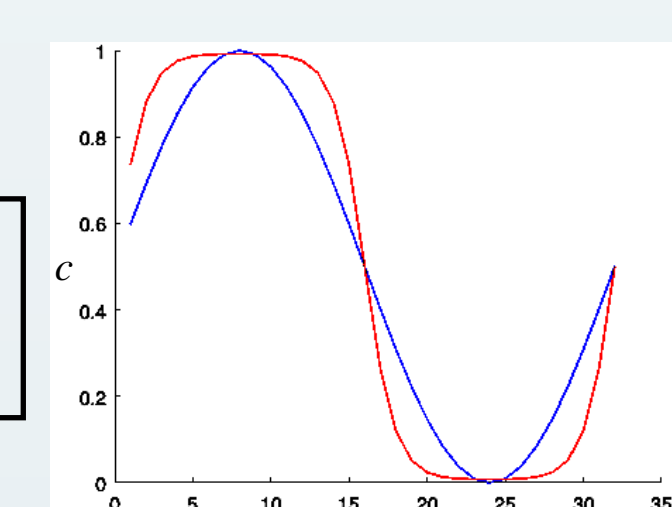
- The interface is the plane of discontinuity between the two phases α and β .
- This sudden change in composition can contribute some energy.
- There is a cost associated with making the interface more diffused as compared to keeping it sharp.
- What the classical free energy function misses is the contribution from the interface of the discontinuity. Even if we have a continuous curve the gradient will start contributing to the free energy. This gradient needs to be accounted for.



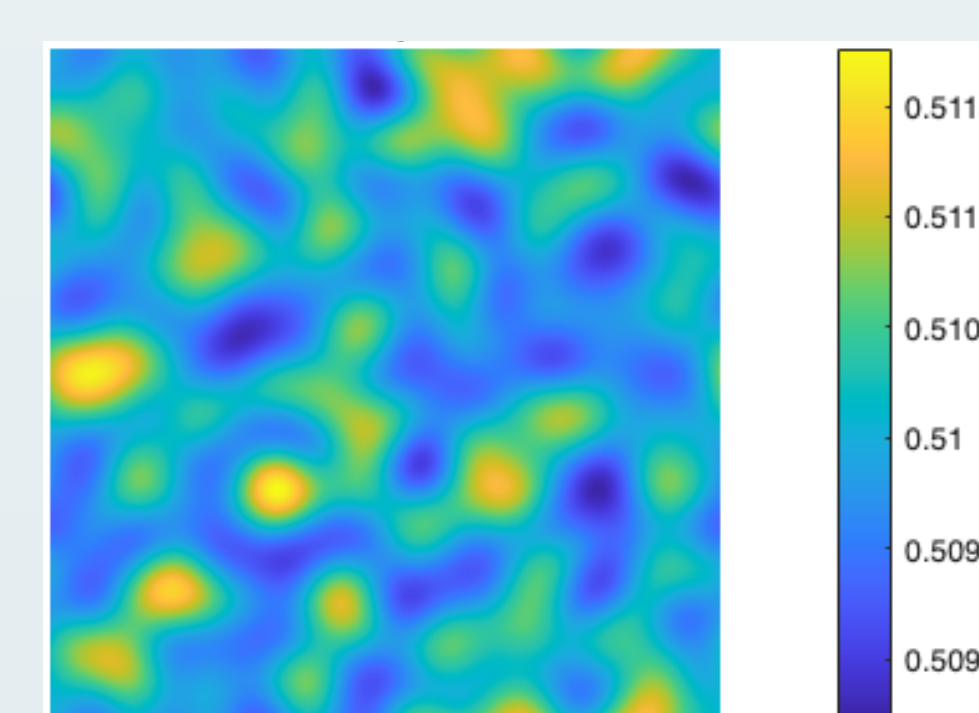
Instead of considering Gibbs Free Energy as a function of concentration, we consider it to be a functional of concentration and its derivatives [3]



$$F = \int [f(c) + k \nabla^2 c] dV$$
$$\frac{\partial c}{\partial t} = D \nabla^2 \left[\frac{\partial f}{\partial c} - 2k \nabla^2 c \right]$$



Fickian Diffusion



Cahn Hilliard Diffusion

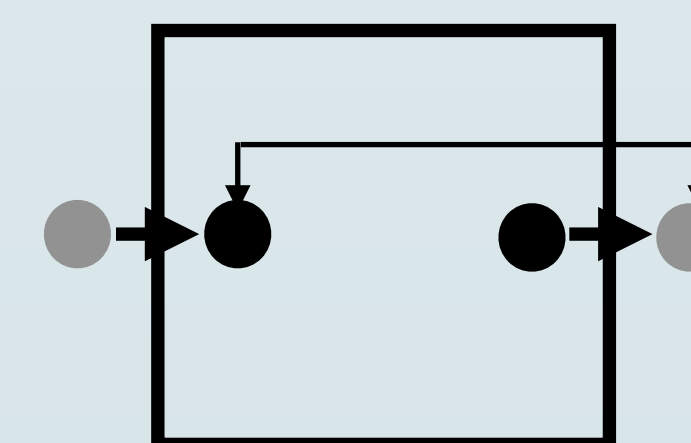


Computational Methods

- The Gibbs free energy is a function of temperature and concentration. The derived equation for free energy includes logarithmic terms which are computationally expensive.
- To reduce the computational cost we assume free energy term $f(c)$ as $f(c) = Ac^2(1 - c)^2$.

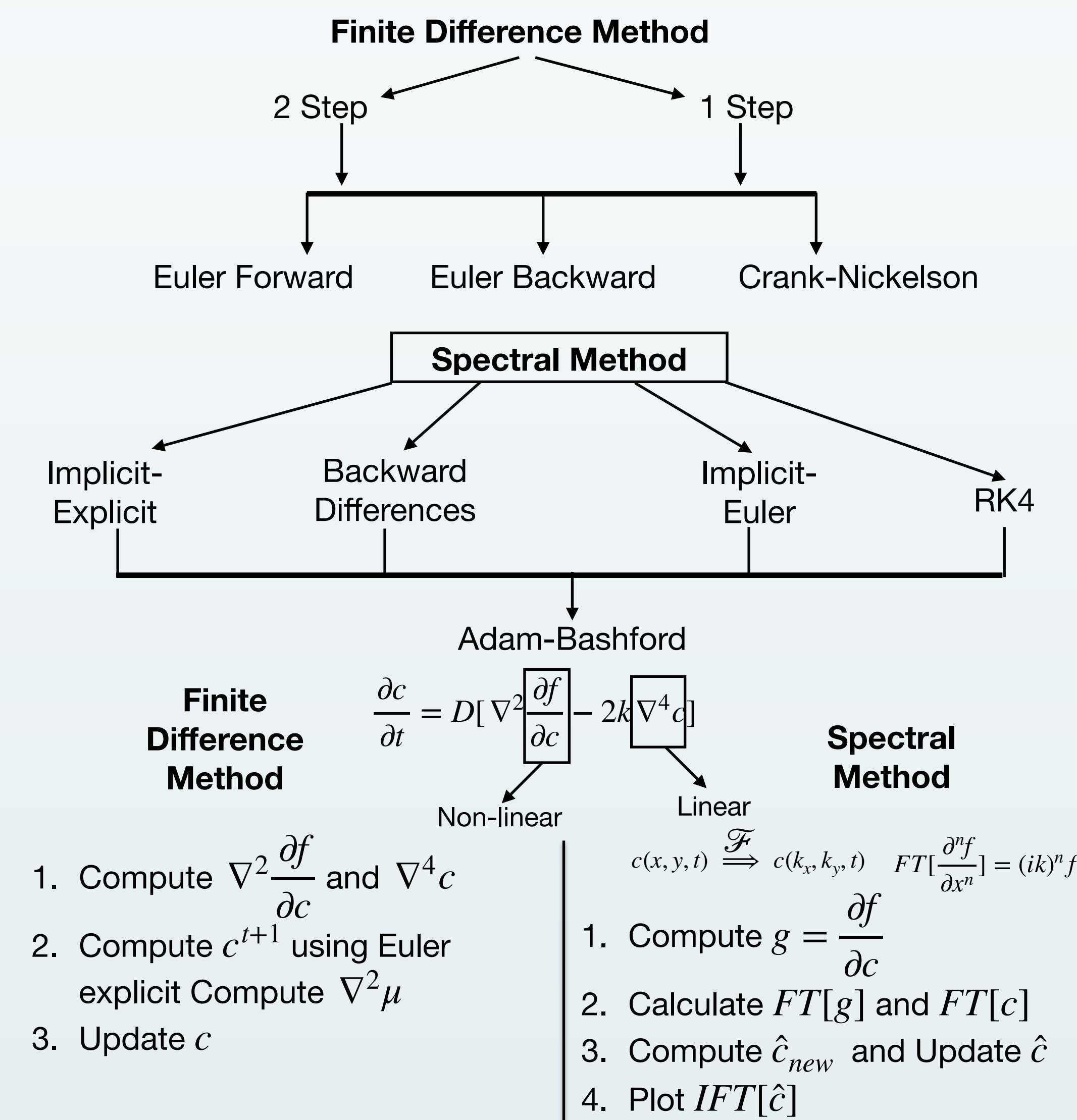
Boundary Conditions

- We can use a number of boundary conditions like Dirichlet, Neumann or Periodic Boundary Conditions.
- We are assuming a system with periodic boundary conditions.



- Various numerical methods can be used to computationally solve the Cahn-Hilliard equation.
- The Spectral method uses the Fast Fourier Transform (FFT) to calculate the derivatives while the finite difference method uses the finite difference approximation to calculate the derivatives.
- Spectral Method takes the composition to Fourier space where derivatives can easily be calculated, thus it is a more stable and computationally less expensive technique.

Numerical Methods



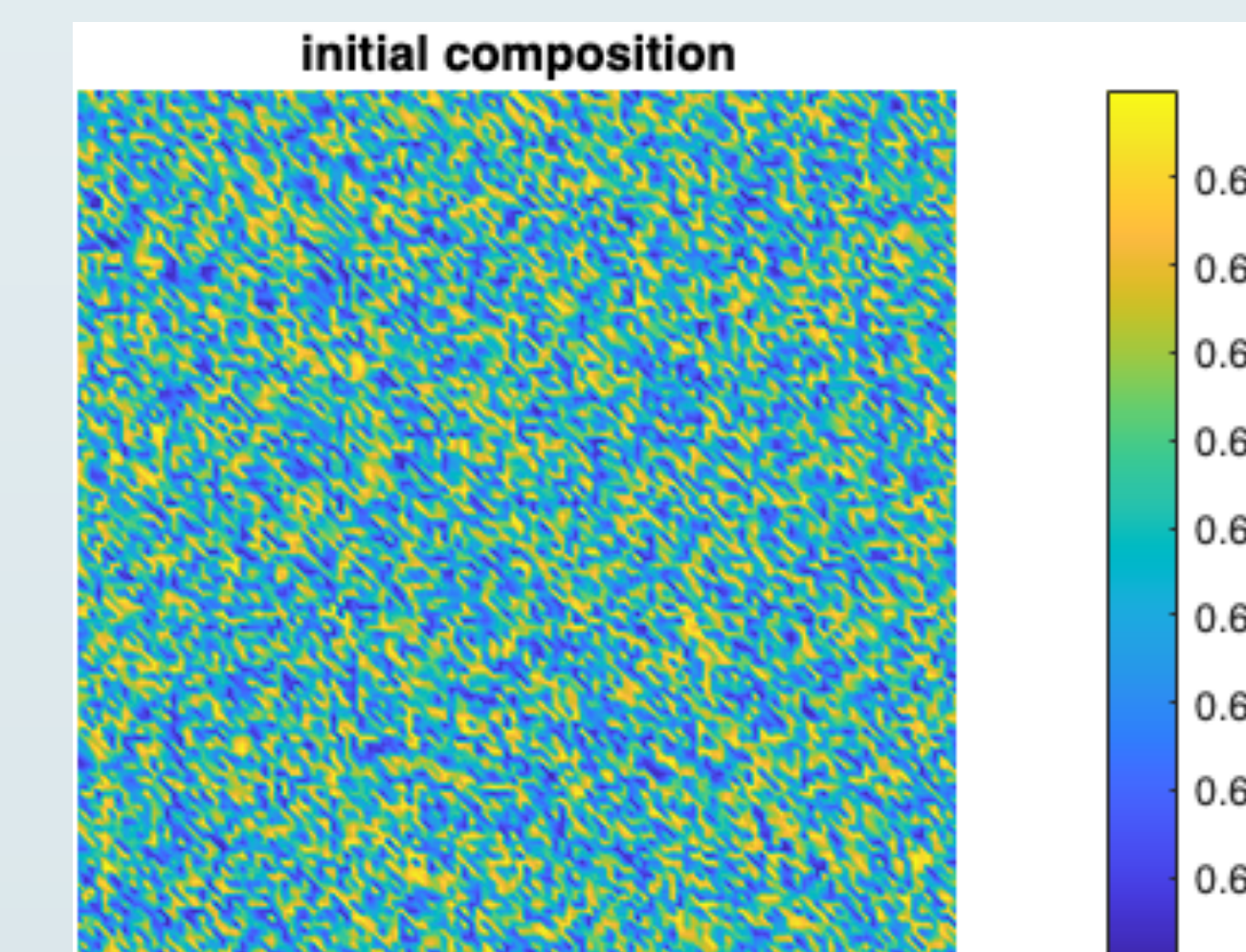
1. Compute $\nabla^2 \frac{\partial f}{\partial c}$ and $\nabla^4 c$
2. Compute c^{t+1} using Euler explicit Compute $\nabla^2 \mu$
3. Update c

1. Compute $g = \frac{\partial f}{\partial c}$
2. Calculate $FT[g]$ and $FT[c]$
3. Compute \hat{c}_{new} and Update \hat{c}
4. Plot $IFT[\hat{c}]$

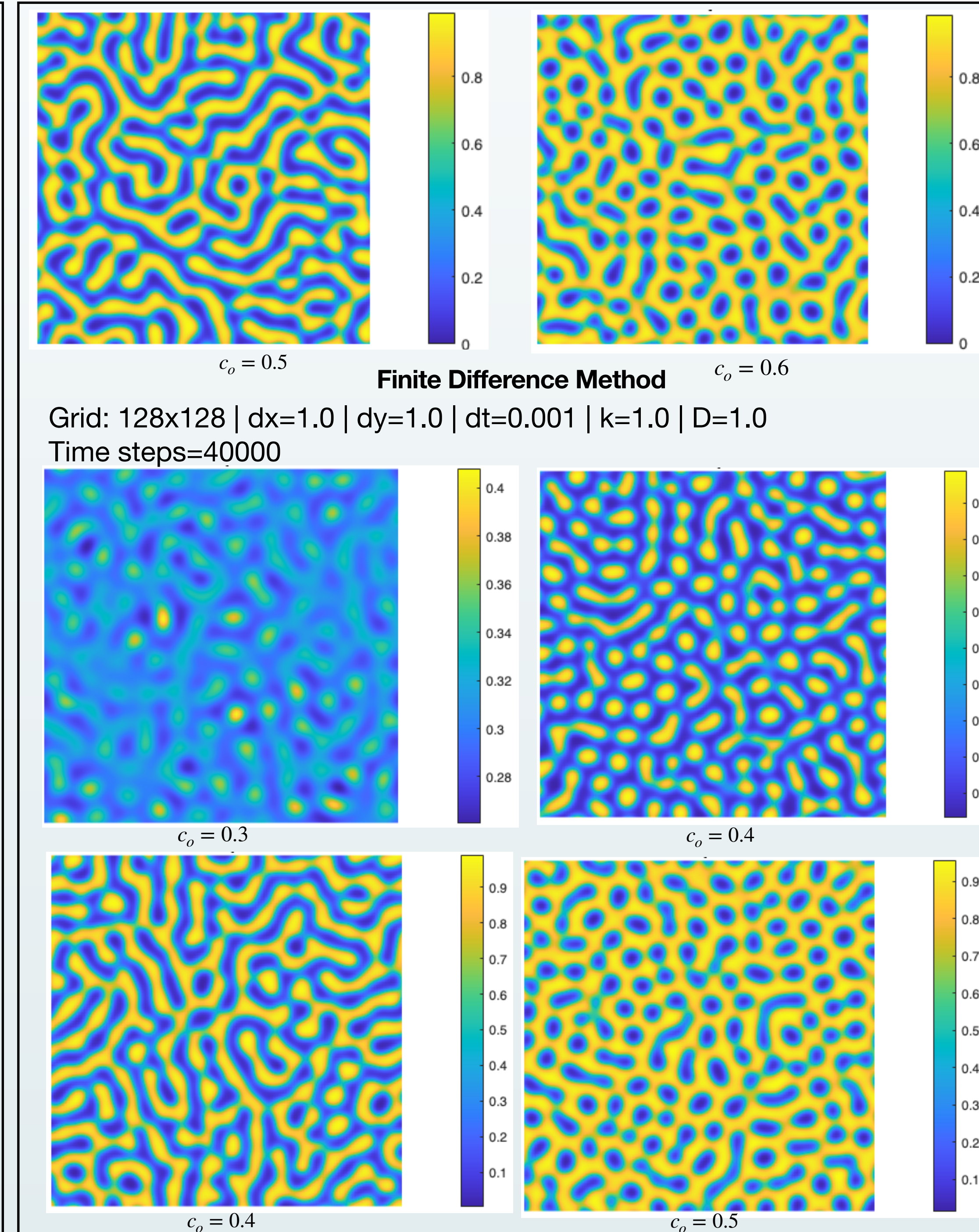
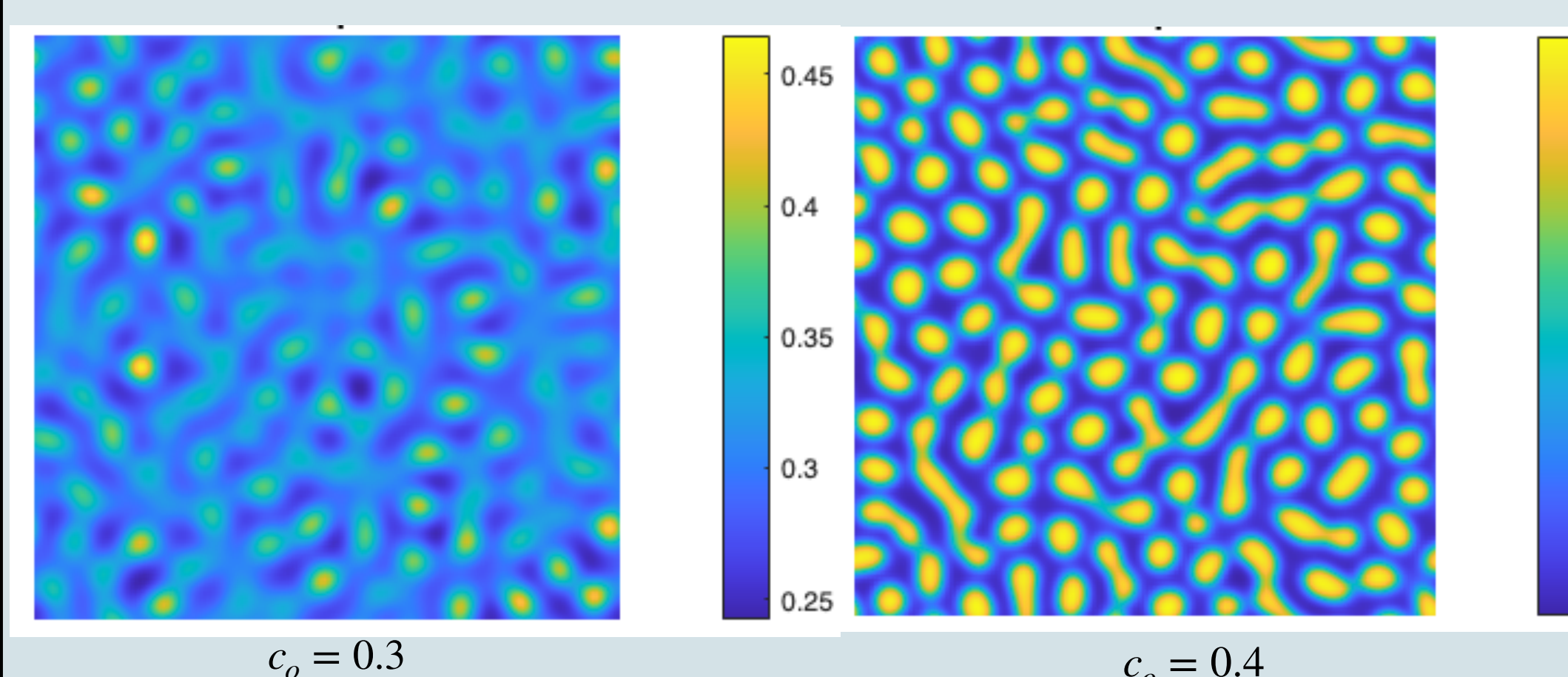
Results

Spectral Method - IMEX

Grid : 128x128
dx=1.0
D=1.0
k=1.0
dt=0.5
Time steps =80



Final compositions after starting from various initial composition values



Conclusion and Future Scope of Work

1. Spectral method yields results much faster and is much more stable than finite difference methods. Finite difference method is highly sensitive to large time steps. Time steps need to be extremely small for the simulation to converge.
 2. We can see that spinodal decomposition takes place for an initial concentration of ~0.4.
- Further work can be carried out by replacing the actual Gibbs free energy function with the assumption taken in this project. Other thermodynamical models like Flory-Huggins models can also be used.

Acknowledgement

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References

- [1] Daniel et. al. *Series A, Mathematical and Physical Sciences*, vol. 181, no. 987, pp. 368-78 (1943)
- [2] J. W. Cahn, *Acta Materialia*, 9, 795 (1961)
- [3] Phase Transformations: Papers Presented at a Seminar of the American Society for Metals, (1968)