# Binary Alloy Simulation: A phase-field model study using semi Implicit Fourier spectral Algorithm

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## Abstract

Phase field modelling, a robust computational approach for modelling, predicting microstructure evolution and to speculate mesoscale morphological in various materials. In this study, we have discretized the time variable using semi-implicit instead of explicit scheme, semi-implicit scheme is known to allow a larger time step sizes than explicit schemes. Meanwhile, the discretization of the space variable is carried out using a Fourier spectral method, having a convergence rate that is exponential when compared to the second order Finite-difference method. Meanwhile, a numerical implementation of Cahn-Hilliard equation via semi-implicit Fourier spectral algorithm for conserved quantities was also demonstrated for binary alloy simulation. However, Isothermal conditions are considered and Non-dimmensionalisation is done. Lastly, we implemented a MATLAB code to solve the phase field equation and visualize our model.

## Keywords

Binary alloy, Phase-field, Microstructure Evolution, Fourier spectral method, Cahn-Hilliard equation, semi-implicit

## 1. Introduction

Researchers are increasingly relying on computational technologies to help in simulating and modelling properties of advanced materials, computational modelling has functioned as tools at the disposition of engineers and scientists, aiding them to a have better grasp of different process parameters influence on microstructural evolution, and optimizing the material in the process to obtain very specific material properties. Inexpensive personnel resources, lesser time to get the product to the market and aggressive margin depleting pricing has been the hallmark of computational material science, under which phase field modelling is categorized(Olanipekun et al. 2017).

Phase-field method surfaced as an outstanding and effective predicting computational method for the morphology and mesoscale evolution of the microstructure in a material. However, phase field method has replaces distinctive interface model within nonzero thickness transition regions that has interfacial forces evenly distributed (Badalassi et al. 2003). A phase-field principles and procedures are based on the orchestration of a Cahn–Hilliard and Ginzburg–Landau energy or entropy functional or Cahn Allen. A variational set of partial derivatives suitable thermodynamic quantities namely temperature, concentrations in conjunction and reaction–diffusion equation for the phase-field variable, often derived from the functional (Penrose and Fife 1990).

In the work of Britta Nestler(Janssens et al. 2010), they explained that phase-field model represent a continuous order parameter, describing the state of the system in space and time. Meanwhile, different states show smooth transition, when using diffuse interface to represent two distinct. With the formulation of the diffuse interface, a phase-field model is found to require much less curtailment on the topology of the grain and phase boundaries. L,Q Chen and Jie shen (Chen and Shen 1998), discretized time variable by using semi-implicit schemes, as time step sizes is possible with semi-implicit than explicit schemes. The discretization of the space variable is carried out using a Fourier spectral method, that has a convergence rate that is exponential when compared to the second order finite-difference method.

W.M. Feng (Feng et al. 2006) and his co-workers suggested approach for representation of spectral field variable continuous spatial profile to achieve high accuracy in space e.g. Fourier series for a periodic system, and adaptive mesh approach using dense grid points in the conjunction regions where the field variables have large gradients. They also went further in their work to state that the spectral method and its semi-implicit implementation have proved to be effective for systems in which, the form and microstructures are influenced by long-range elastic interactions.

Hyun Geun and June-Yub (Lee and Lee 2014) explained that researchers have been able to improve Phase field model effectiveness by employing semi-implicit Fourier spectral (SIFS) methods, paving a way for larger time steps than explicit scheme.

Phase-Field Crystal Method has linked the conventional phase-field theory to the atomistic scale, allowing simulations on diffusive time scales which may not be obtainable with atomistic simulations (Biner 2017).

The focus of this paper is to simulate a binary alloy using spinodal decomposition with semi-implicit Fourier spectral algorithm. However, this was demonstrated by implementing numerically a semi-implicit Fourier spectral algorithm for a conserved Cahn–Hilliard equation solution in phase-field modeling.

## 2. Phase-field Model

A phase-field model depicts a microstructure (structural domains and composition) with some field variables (Biner 2017). In agreement to Cahn-Hilliard (Cahn and de Fontaine 1961, Cahn and Hilliard 1958), we have conserved field variable and non-conserved field variable. Non-conserved field variables developed with the time-dependent Ginzburg–Landau equation or Allen–Cahn relaxation equation while conserved field variables temporal evolution is regulated by the Cahn–Hilliard nonlinear diffusion equation and the (Allen and Cahn 1972, Allen and Cahn 1973). Notably, the two kinetic equations have their foundation from physics rudiment of phase-field models.

In the work of Bulent Biner(Biner 2017), he represented Cahn Hilliard equation by equation (1) below.

$$\frac{\partial c_i}{\partial t} = \nabla M_{ij} \nabla \frac{\delta F}{\delta c_j(r,t)} \quad (1)$$

Equation (1) is first Non-dimmensionalised

Where $r$ is the position, $t$ is the time, $M_{ij}$ is the diffusivities of the species or Mobility, and $c_1, c_2 \dots \dots c_n$ are the conserved field variables, $F$ is the system free energy (Biner 2017).

The total free energy is given as,

$$F = \int_v \left[ f(c) + \frac{1}{2} k (\nabla c)^2 \right] dv \quad (2)$$

However, k is the gradient energy coefficient and $f(c)$ is the chemical/bulk energy represented by:

$$f(c) = Ac^2(1-c)^2 \quad (3)$$

Which is the simple phenomenological double-well potential. An energy barrier between two equilibrium phases is controlled by $A$, which is a positive constant, depicted with a concentration values of $c = 0.0$ and $c = 1.0$ (Biner 2017).

### 3. Numerical Analysis of the Governing Equation

From Equation (1) which is the semi-implicit algorithm implementation, we take its functional derivative, which gives evolution equation below(Biner 2017).

$$\frac{\partial c}{\partial t} = \nabla^2 M\left[\frac{\delta f}{\delta c} - k\nabla^2 c\right] \quad (4)$$

The Fourier transform of both side of Equation (4) is taken, the spatial discretization becomes:

$$\frac{\partial\{c\}_k}{\partial t} = -k^2 M\left[\{\frac{\delta f}{\delta c}\}_k + k^2 k\{c\}_k\right] \quad (5)$$

The Fourier transform of the quantity inside the bracket is represented by $\{\cdot\}_k$ and $k$ represent the vector in Fourier space, k= $(k_1, k_2,)$ with a magnitude $\sqrt{k_1^2 + k_2^2}$ . Expanding Equation (5) we have $\frac{\partial\{c\}_k}{\partial t} = -k^2 M\left\{\frac{\delta f}{\delta c}\right\}_k - k^4 M k\{c\}_k$ (6)

Fourth-order and linear operators are treated implicitly while the non-linear terms are treated explicitly, the semi-implicit form for Equation (6) will now be:

$$\frac{\{c\}_k^{n+1} - \{c\}_k^n}{\Delta t} = k^2 M\left\{\frac{\delta f}{\delta c}\right\}_k^n - k^4 M k\{c\}_k^{n+1} \quad (7)$$

Where $\Delta t$ is the time increment between time steps $n\ and\ n+1$. Regrouping the equation, it becomes,

$$\{c\}_k^{n+1} = \frac{\{c\}_k^n - \Delta t k^2 M\left\{\frac{\delta f}{\delta c}\right\}_k^n}{1 + \Delta t k^4 M k} \quad (8)$$

### 4. Simulation steps

A code was developed in MATLAB using the mentioned algorithm steps below. Periodic boundary conditions were used.

**Algorithm for microstructural evolution:**

- Given a composition profile at time t = 0, we evaluate Fourier transform of $\frac{\delta f}{\delta c}$ and as well as the Fourier transform of $c$.
- Using equation (8), we calculate the composition profile or spatial variation of $c$ in Fourier space at some future time t + Δt.
- The inverse Fourier transform of $c$(t+Δt) gives the composition profile at time t + Δt.
- Above steps are repeated to process a given number of steps in time.

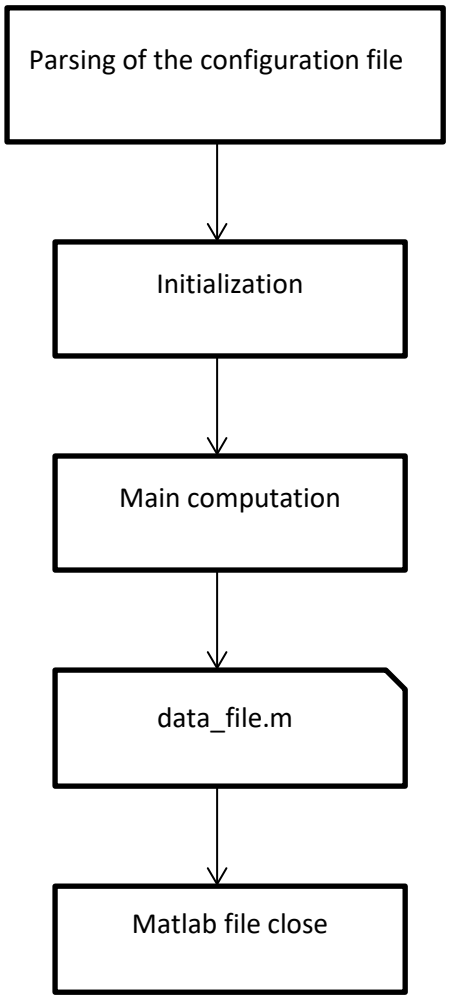


Figure 1. Program structure of the phase-field simulation code

**Inputs needed for the simulation are as follows:**

$N_x, N_y$ size of the mesh
N Noise strength
$dx, dy$ distance between the nodes in x & y direction
$dt$ Length of time step
A free energy barrier
$M$ Mobility
Kappa gradient energy coefficient
$c$ $(N_x, N_y)$ Initial composition field information

**Table 1.** The non-dimensional values of the parameters used in the simulations.

| $A$ | $M$ | Kappa | N | $t$ | $c$ |
|---|---|---|---|---|---|
| 1.0 | 1.0 | 1.0 | $0.5\times 10^{-1}$ , $0.5\times 10^{-2}$ | 63,150 | 0.5 |

## 5. Results and Discussion

Microstructural evolution showing phases was depicted by figure 2. Also, time values are in non-dimensional format. The simulation was carried out using a spatial mesh of $N_x = 250$ by $N_y = 250$ and with dx=dy=1.0, also using all non-dimensional parameter.

From Fig 2(a), we were able to show a homogenous binary mixture at time t=3, that first separate, followed by slow coarsening with relatively fine microstructure that contain many precipitates. Meanwhile, as the time frame increases, as shown by fig 2(b) snapshot at time t=63, there is a noticeable second phase coarsening through the phase boundaries migration, merging and dislocation. Thus, the grain boundary movement and diffusion that leads to grain growth, which can be explained by Oswald ripening process, as explained by Moelans and co-workers (Moelans et al. 2008) explaining how small precipitate dissolve and absolve the lager precipitate through Oswald ripening process. However, at t time t= 123, at the later stage the coarsening tends to be very slow as the interface of the microstructure reduces, noticeable in the total free energy change rate.

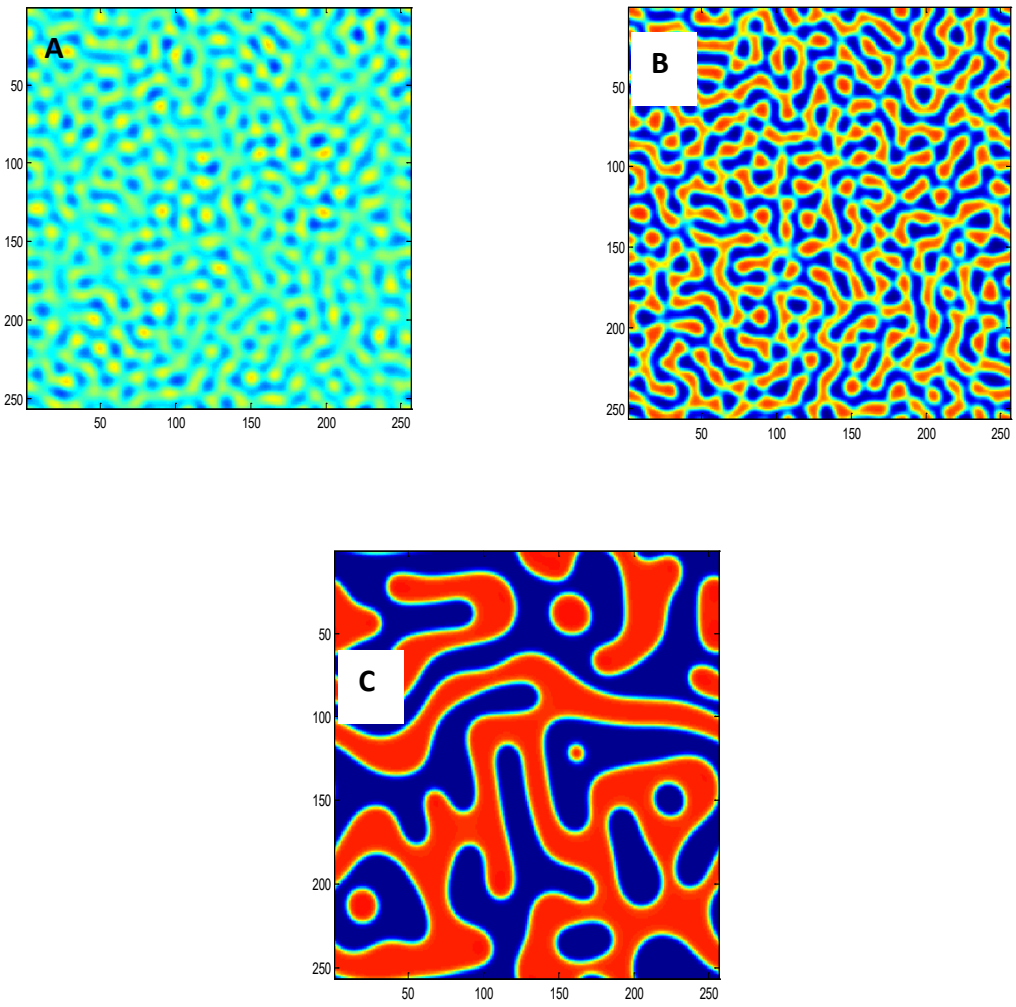


Figure 2: Microstructure showing phase separation in tandem with time evolution, with corresponding non-dimensional times using a noise factor $0.5\times 10^{-1}$ (a) 3, (b) 63, and (c)123.

## Conclusion

In this work we have been able to study microstructural evolution in a binary alloy using semi implicit, Fourier spectral algorithm phase field model developed in MATLAB. A Phase field method was used to present the numerical solution, using fewer equations that are relatively lesser than the number of particles in the system. Therefore, themo-physical parameters like Mobility that explains or control the composition field ($N_x, N_y$) of the system, anisotropy, time, internal energy coefficient, gradient energy co-efficient, has played larger part to control microstructural evolution, in terms of grain coarsening, morphology changes.
The parameters used is not specific to any material. Lastly, the present studies vividly show microstructure evolution of binary alloy due to complex interactions of thermophysical properties and parameter. Meanwhile, we were able to validate the contribution of Oswald ripening process explaining the microstructural evolution.

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## Biographies

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