A Numerical Implementation of the Finite-Difference Algorithm for solving Conserved Cahn–Hilliard Equation

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Abstract. Phase field modelling technique is critical to contextualizing material microstructures and to represent the composition of microstructural evolution. This work utilizes the periodic boundary condition to numerically solve the Cahn-Hilliard equation. To enhance computation and improve flexibility, Python programming language is introduced to develop and implement the proposed approach. The numerical implementation considered a hypothetical binary system of element A and B using the finite difference method on the conserved order parameter. The work also validates the concentration dependent gradient of the system and the energy coefficient which serves as the first step to show spinodal decomposition in a system. The implementation involves solving the Cahn Hilliard equation in multi-dimensions capturing minimal time steps evolution, thus serving as an esplanade, an approach into crystallization. The system shows that the element A and B can be used to describe evolution phases alpha (α) and beta (β) through a persisting thermodynamic variable to form a single phase. The time-dependent phase morphology of the studied system, and the concentration and mobility effects are discussed in this paper.

1. Introduction
The phase-field modelling technique is critical to contextualizing material microstructures which can be used to represent the microstructural evolution of material composition [1]. The importance of modelling a high-fidelity microstructural investigation motivates several advanced modelling tools and techniques, such as kinetic Monte Carlo modelling, and the cellular automation modelling [2]. However, these conventional approaches do not give the highest level of information about grain structure and segregation patterns, and the phase-field model is limited to a small section of the material [2].

Demonstratively, the Cahn-Hilliard equation has remained one of the underlying equations of the phase-field approach used to describe the established applications of the phase-field model in compositional and structural domains of microstructures. Represented by functions continuous in space and time that are termed as field variables and these sets of field variables are classified into conserved and non-conserved [3]. They are so termed depending on if they satisfy the local conservation law i.e. \( \frac{\partial \varnothing}{\partial t} = -\nabla J \) where \( \varnothing \) is a field variable and \( J \) is the corresponding flux and sustained inside the phase domain away from the interfaces, where different values of the variables determine different phase domain [4]. Typically, the non-conserved variables contain information on the local (crystal) structure and orientation and the conserved variables of its composition are also considered [5].

However, the approach is limited by computational expense in running large simulations because of the need to resolve the diffuse interface and any numerical error therein [6, 7]. Some advanced
methods were proposed to address the size and interface issues with meshing and an adaptative time-step [8], as presented by Zhang et al. [9] and Baňas, L. et al. [10]. An improvement in the large time step method was also proposed [11], to address accuracy loss when the energy of the system does not decay rapidly. This has been successfully applied to detect microstructural defects in materials, but the achieved efficiency can be improved and the method still needs to be optimized.

Consequently, this work presents a novel numerical implementation of the finite difference algorithm for solving the Cahn-Hilliard equation by discretization of the Euler-Lagrange equation without employing strain on the system motivated by the improvements recorded in recent robust literature [12, 13].

2. Cahn Hilliard

For a certain system, the order of the parameters contributes to a total Gibb’s free energy which is defined for the system, and a variational method is applied to find evolution equations that would evolve the system towards the minimum of the energy functional [14]. The Gibb’s free energy functional is expressed as:

\[ G(c, \nabla c) = \int_V \left[ g_{\text{chem}}(c) + g_{\text{grad}}(\nabla c) \right] dV \]

\[ G(c, \nabla c) = \int_V \left[ f(c) + k(\nabla c)^2 \right] dV \]  

Where \( k \) is the gradient constant, \( k(\nabla c)^2 \) is the gradient energy term, and \( f(c) \) is the chemical free energy.

The gradient energy term helps create a region of interface formation, where concentration varies sharply [15]. The free energy density is constructed to promote phase separation, opposing to the gradient energy term for a stable interface to represent a balance between the phase separation and the interface formation [16].

3. Characteristic of a Phase

For the multiphase system, \( \phi_\alpha \) is a spatially varying order parameter that indicates where the \( \alpha \)-phase exists in a microstructure. Regions of \( \phi_\alpha = 0 \) designate areas where no \( \alpha \)-phase is present, and areas of \( \phi_\alpha = 1 \) correspond to single-phase regions of \( \alpha \). For a system with \( N \) phases, the phase fractions obey a phase fraction constraint [17]:

\[ \sum_{\alpha=1}^{N} \phi_\alpha = 1 \]

And the free energy density at the interfaces is a function of the free energy functions, the components, and the multiple phase fractions. In that, the thermodynamic potential of a multiphase system is equal to the summation of potentials in all present phases [18]. Whilst the linear weighting of the free energy densities by phase fractions is used for the homogeneous free energy of a multiphase system:

4. The Multiphase and Multicomponent Model

Multiphase modelling with a phase-field approach begins with the definition of an interface between two phases and usually in the presence of one or more diffusing solutes [19]. With the assumption that in several systems, a phase is seen as s binary variable that differentiates regions by a sharp interface that is generally considered to be a smoothly varying quantity only for liquid-vapor boundaries close to the critical point. In a diffused interface model, however, phase and composition are modelled as smoothly varying quantities at all interfaces [20]. In the modelling of such an interface, a decision has to be made if to treat the interface as an interpolation between two phases with the same composition, or two phases with different compositions [21].

5. The Numerical Methods for Phase-Field Modelling

To numerically model the phase field, the explicit finite difference and spectral methods were found to be several orders of magnitude more stable. The finite-difference algorithm offers a more direct approach to the numerical solution of partial differential equations than any other method [22].
Because the algorithm is based on the substitution of each derivative by a difference quotient making them simple to code, economic to compute, and easy to parallelize for the distributed computing environments [22].

6. Simulation & Result

![Simulation & Result](image)

**Figure 1.** The time-dependent phase morphology of a binary system for mobility as a function of concentration

The resulting image in Fig. 1 shows the direction of evolution from left to right as a barrier-less phase separation process with minimal thermodynamic conditions such that any alterations to its equilibrium would lead to system evolution suggestive of minimal effect on the spinodal decomposition [23-24]. As the concentration content increases, the nanodomains of $\beta$ increase in size, and its growth is promoted by the gradient energy term which explains the deformation mechanism or evolution. Figure 2 shows the phase evolution at constant mobility. The 3D morphology is developed using the Python language and plotting tools. The figure shows the phase evolution and continuous growth over
different time scales. The spikes in the images show the grid boundary of the crystal structure. At constant mobility, there is a clear distinction between the red solvent rich region and the yellow solute rich region which grows with increasing time (t). In each of these schemes, the crystal structure and orientation of the precipitates and parent phase are sufficiently similar but also show sufficient deformation upon continuous thermal quenching, which are sufficient in revealing the microstructural changes and thus spinodal decomposition resting on the concentration of the system as the relevant microstructural descriptor.

7. Conclusion
This work shows the step-wise application of the numerical approach to the implementation of the finite difference method to solving the Cahn-Hilliard equation and its application to spinodal decomposition. To enhance computation efficiency and improve flexibility, the proposed approach is developed and simulated using Python programming language. The proposed method is applied to study a system behaviour that cannot be solely explained by the Gibbs free energy without the influences of elastic strain energy which will also affect the behaviour of evolution of the system. Simulation results show good consistency in the proposed approach and the conventional approaches. Also, the proposed method has better fidelity in the observed pattern migration in the analysed images. Moreover, the temperature dependence of both the Gibbs energy and diffusion coefficient are considered in the simulations and had initial conditions of a homogeneous β phase. The simulated system is also free from errors that would naturally occur from system impurities.

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