

**EFFICIENT NUMERICAL STRATEGIES
FOR SOLVING PHASE-FIELD
DENDRITIC CRYSTAL GROWTH MODEL**

BY

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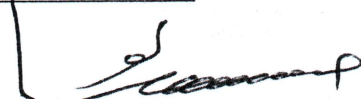
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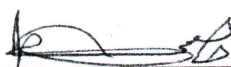
DEANSHIP OF GRADUATE STUDIES

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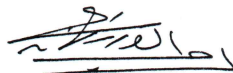
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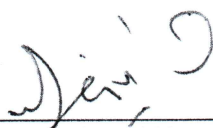
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To my beloved mother, father, and sister

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THESIS ABSTRACT

NAME: Muhammad Habibur Rahman

TITLE OF STUDY: EFFICIENT NUMERICAL STRATEGIES FOR SOLVING PHASE-FIELD DENDRITIC CRYSTAL GROWTH MODEL

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This study develops a phase-field model for simulating dendritic crystal growth, utilizing a non-uniform grid to improve both accuracy and computational efficiency. The model is based on the Allen-Cahn equation, with a curvilinear transformation applied to map the physical domain, where grid points are locally concentrated near high-growth regions into a uniformly spaced computational domain. This transformation facilitates localized refinement, enabling higher resolution in critical areas of crystal growth while maintaining a consistent numerical framework. By addressing the limitations of uniform grids, which require significant computational resources to resolve fine morphological details across the entire domain, the proposed approach achieves a balance between precision and efficiency.

Simulations conducted with the non-uniform grid demonstrate its ability to effectively capture fine morphological details, particularly in regions of rapid growth, and match the results obtained on a uniform grid. The non-uniform grids provides flexibility by allowing the resolution to be focused on areas of high-growth area, enabling the model to resolve complex growth patterns without unnecessary computational expense. Key observations from the simulations include the influence of latent heat, relaxation time, and interface width on dendritic morphology and growth rates. These results showcase the effectiveness of non-uniform grids in precisely modeling dendritic solidification, emphasizing their value in enhancing the understanding of crystal growth behavior within phase-field simulations.

ملخص الرسالة

الاسم: محمد حبيب الرحمن

عنوان الدراسة: استراتيجيات عددية فعالة لحل نموذج نمو البلورات الشجرية في مجال الطور

التخصص: الرياضيات

تاريخ الدرجة العلمية: ديسمبر 2024

تتناول هذه الدراسة تطوير نموذج مجال الطور لمحاكاة نمو البلورات الشجرية، (Dendritic) مع الاستفادة من شبكة غير منتظمة لتحسين كل من الدقة والكفاءة الحسابية. يستند النموذج إلى معادلة "ألين-كان" (Allen-Cahn) حيث يتم تطبيق تحويل منحني لرسم خريطة المجال الفيزيائي، يتم فيه تركيز نقاط الشبكة محلياً بالقرب من المناطق ذات النمو السريع إلى مجال حسابي ذي توزيع متساوٍ. يسهل هذا التحويل تحسين التوضيح الموضوعي، مما يتيح تحقيق دقة أعلى في المناطق الحرجة لنمو البلورات مع الحفاظ على إطار عددي متماسك. ومن خلال معالجة القيود المرتبطة بالشبكات المنتظمة، التي تتطلب موارد حسابية كبيرة لحل التفاصيل الشكلية الدقيقة عبر المجال بأكمله، يحقق النهج المقترح توازناً بين الدقة والكفاءة.

أظهرت المحاكاة التي أُجريت باستخدام الشبكة غير المنتظمة قدرتها على النقاط التفاصيل الشكلية الدقيقة بشكل فعال، خصوصاً في المناطق ذات النمو السريع، ومطابقة النتائج التي تم الحصول عليها باستخدام الشبكات المنتظمة. توفر الشبكات غير المنتظمة مرونة بتمكين التركيز على المناطق ذات النمو السريع، مما يسمح للنموذج بحل الأنماط النمو المعقدة دون نفقات حسابية غير ضرورية. من بين الملاحظات الرئيسية التي تم استخلاصها من المحاكاة تأثير الحرارة الكامنة، وزمن الاسترخاء، وعرض الواجهة على مورفولوجيا البلورات ومعدلات النمو. تظهر هذه النتائج مزايا الشبكات غير المنتظمة في محاكاة عمليات التصلب البلوري بدقة، مما يبرز إمكانياتها في تحسين فهم ديناميكيات نمو البلورات في محاكاة مجال الطور.

CHAPTER 1

INTRODUCTION

1.1 Dendritic Crystal Growth

Crystal growth is a fundamental physical phenomenon that produces complex, spontaneous patterns found in a wide range of natural and industrial processes. Among the various form of crystal structures, dendritic growth—a branch-like pattern—emerges prominently when a supercooled liquid undergoes solidification. This growth pattern results from molecular attachment to the interface between solid and liquid phases. Dendritic crystals are commonly observed in the solidification processes of metals and alloys, where their growth is affected by temperature gradients and material properties [2], [3]. The growth direction and rate significantly affect the morphology of crystal. Notably, this morphology play a critical role in determining the material's final properties and applications.

In fluid dynamics, the dendritic growth rate and branching behavior are governed by local fluid flow, as well as concentration and temperature distributions within the material. A clear understanding of these factors influencing dendritic growth is essen-

tial for controlling the microstructure of solidified crystal, especially in industrial processes [4]. For instance, by understanding and manipulating these variables, engineers and scientists can tailor specific properties in metal and alloys, such as microstructural stability, uniformity, resilience, and strength. The microscopic features of dendritic crystals, including their morphology and distribution, directly influence macroscopic characteristics like durability, toughness, and yield strength, making them crucial for optimizing the performance of metals and alloys.

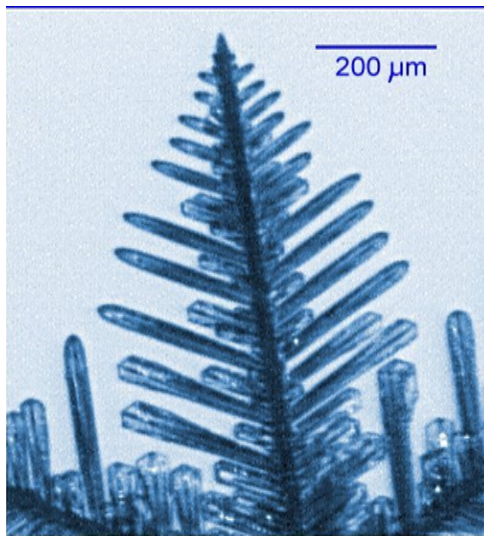


Figure 1.1: Dendritic structures on crystal solidification [1].

Crystal structures formed during solidification processes can be categorized into two types: equilibrium forms and growth forms. Equilibrium crystal forms arise when free surface energy is minimized, resulting spherical shapes under isotropic conditions, where the properties are uniform in all directions, and polyhedral shapes under anisotropic conditions, where the properties vary with directions [5]. In contrast, dendritic crystals represent growth forms, developing when the surface tension and thermodynamic driving forces reach a balance during the solidification process [6].

This type of growth is noticeable under anisotropic conditions, where directional variations in crystal properties affect the overall shape and complexity of the structure [7]. Anisotropy plays a substantial role in the final form of the crystal, leading to highly ordered, branched patterns that contribute to a material's mechanical and thermal properties [8]. By studying these variations, researchers can gain insights into optimizing material properties through controlled crystal growth and solidification processes.

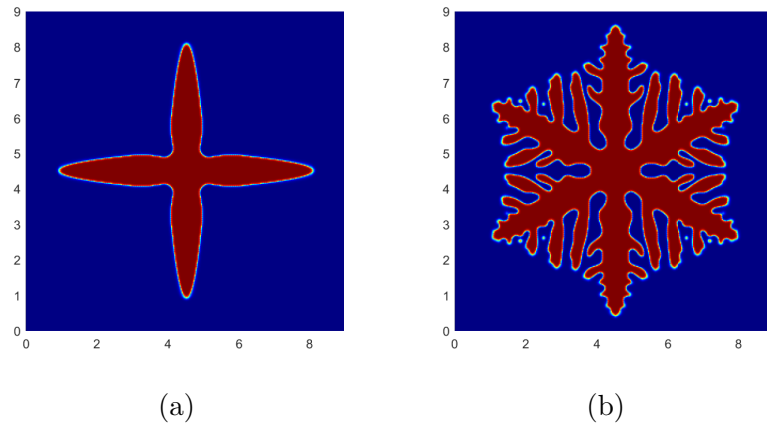


Figure 1.2: Snapshots of dendritic crystal with (a) 4-mode, and (b) 6-mode anisotropy.

1.2 Thesis Structure

This thesis is organized into five chapters, each addressing a key aspect of the research on the phase-field model for dendritic crystal growth, specifically incorporating a non-uniform grid into its numerical computations to enhance accuracy and efficiency.

- **Chapter 1** introduces the thesis topic, providing a broad background on dendritic crystal growth. This chapter establishes the importance of understanding and modeling dendritic patterns in crystal solidification, discusses the motivation for this research, and offers a structural overview of the thesis.

- **Chapter 2** covers the foundational concepts and key literature related to models of dendritic crystal growth. Special attention is given to the Kobayashi model [9], a widely recognized phase-field model that describes dendritic crystal growth phenomena. This chapter contextualizes the Kobayashi model within broader dendritic growth research and highlights its limitations and areas for potential adaptation.
- **Chapter 3** details the transformation of the phase-field model for dendritic crystal growth into a curvilinear framework. This chapter explains how a non-uniform grid is integrated to improved resolution in regions of interest within the model. This transformation allows for better computational efficiency and accuracy within simulating complex, branching structure typical of dendritic growth.
- **Chapter 4** presents the numerical discretization techniques employed in the simulations, describing in detail the specific methods used for the phase-field model on a non-uniform grid. This chapter also provides the computational results, including graphical illustration and analyses of dendritic crystal growth patterns. Additionally, a qualitative study observes the behavior of dendritic structures within the curvilinear coordinates.
- **Chapter 5** concludes the thesis by summarizing the primary findings and contributions of the research. This chapter also proposes directions for future work, emphasizing areas where the model could be further refined or adapted to study other crystal growth scenarios.

CHAPTER 2

PHASE-FIELD MODEL OF DENDRITIC CRYSTAL GROWTH

2.1 Overview

The phase-field modeling is a powerful technique widely used for simulating microstructure evolution processes, including solidification and dendritic growth [10]. By employing a diffuse-interface approach, phase-field models capture the morphological evolution of dendritic crystal at the solid-liquid interface, where the dynamics are governed by the release of latent heat during solidification, as represented in the thermal conductivity equation [11]. Pioneering work by Collins, et.al., [12] and Kobayashi [9] introduced a coupled system of parabolic partial differential equations that describe the interactions between the phase-field and temperature-field, forming the founda-

tion for modern phase-field modeling of dendritic growth. Ongoing research seeks to refine phase-field methods to achieve greater accuracy and computational efficiency for solving this model.

Shah, et.al., [13] introduced an adaptive time-stepping technique combined with an implicit scheme for spatial discretization, which enhanced computational stability and efficiency. Jeong and Kim [14] proposed a fast and accurate adaptive time-stepping method through a hybrid explicit approach, while Li, et.al., [15] developed a high-order stable scheme applicable to a variety of gradient flows. Wang, et.al., [16] contributed an energy-stable algorithm that ensures computational speed while preserving energy consistency. Zhang, et.al., [17] combined stabilized energy minimization with a novel decoupling technique to efficiently solve the nonlinear equations in dendritic crystal growth model. Furthermore, Guo, et.al., [18] utilized a Fourier spectral method for spatial discretization, effectively stabilizing the scheme across a range of applications. In order to achieve high resolution in regions of steep gradient, we will apply algebraic stretching functions that optimize grid density in areas requiring finer detail [19].

2.2 Dendritic Crystal Growth Model

The mathematical model for dendritic crystal growth, as proposed by Ryo Kobayashi [9], involves two variables: a phase field $p(\mathbf{x}, t)$ which represents an ordering parameter at position $\mathbf{x}$ and time t , and a temperature field $T(\mathbf{x}, t)$. In this model, when $p = 0$, the phase is liquid, and when $p = 1$, it is solid. The solid-liquid interface, characterized by a thickness ε , is represented as a steep layer of p that transitions between the values

0 and 1. The model explains the formation of dendritic patterns by considering only the diffusion field resulting from the temperature gradient and the concentration of the pure material undergoing growth.

Figure 2.1 illustrates the difference between a sharp interface and a diffusive interface. In (a), the sharp interface model represents an abrupt transition between two phases, where the order parameter p changes discontinuously at the interface (denoted by the dashed line). In contrast, (b) shows a diffusive interface model, where the order parameter p varies smoothly across the interface. This diffuse transition is characteristic of the phase-field method, which eliminates the need to explicitly track the interface location. Instead, the interface is naturally defined by the region where p transitions between its two bulk values (e.g., 0 and 1).

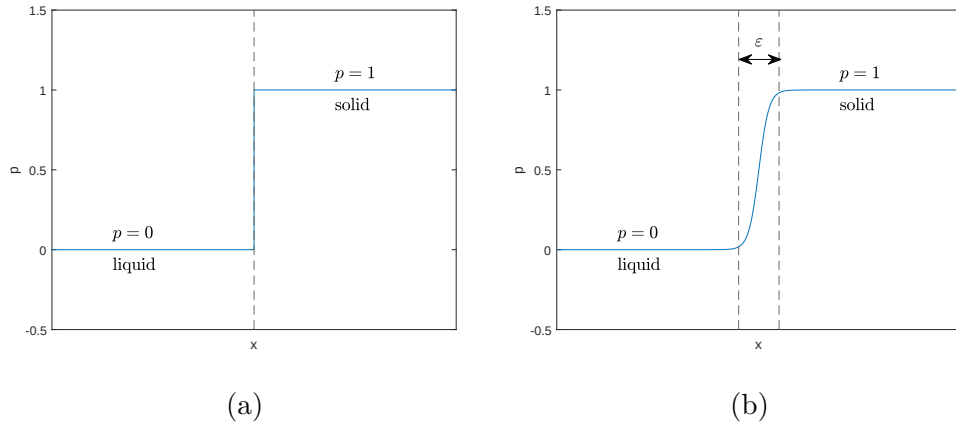


Figure 2.1: Phase-field profile with (a) sharp-interface, and (b) diffuse-interface.

The diffusive interface approach provides several advantages, including numerical stability and the ability to handle complex interface morphologies, such as branching. This smooth variation also incorporates the effects of interface thickness into the model, making it ideal for simulations of dendritic crystal growth.

The following Ginzburg-Landau [9] form of free energy is utilized to maintain the profile of p :

$$\Phi [p; m] = \int_{\Omega} \frac{1}{2} \varepsilon^2 |\nabla p|^2 + F(p; m) d\mathbf{x}, \quad (2.1)$$

where ε is a small parameter that determines the interface thickness and m provides a thermodynamic driving force. The term F represents a double-well potential with two local minima at $p = 0$ and $p = 1$, defined by [9]:

$$F(p; m) = \frac{1}{4} p^4 - \left(\frac{1}{2} - \frac{1}{3} m \right) p^3 + \left(\frac{1}{4} - \frac{1}{2} m \right) p^2. \quad (2.2)$$

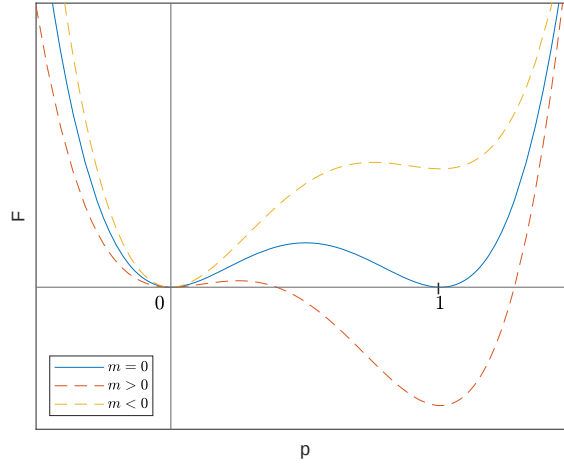


Figure 2.2: Generalized sketch of the double-well potential F .

Figure 2.2 illustrates the double-well potential, a key component in the phase-field model, as a function of the order parameter p . The double-well potential is used to define the free energy density of the system, encouraging the phase-field variable p to take on stable values corresponding to the minima of the potential. These minima represent the two stable phases of the system, typically at $p = 0$ for liquid-phase and $p = 1$ for solid-phase. The parameter m influences the two minima values, which

arises from the phenomena of chemical potentials given by

$$m(T) = \frac{\alpha}{\pi} \tan^{-1} [\gamma (T_e - T)], \quad (2.3)$$

where α and γ are some material parameters to ensure that $|m| < \frac{1}{2}$ and T_e is an equilibrium temperature, which means that the driving force of interfacial motion is proportional to the supercooling.

Anisotropy occurs when ε is dependent on the direction of the interface's outer normal vector. According to Allen-Cahn formula, the interface evolution equation is given by [11], [9]:

$$\tau \frac{\partial p}{\partial t} = - \frac{\delta \Phi}{\delta p}, \quad (2.4)$$

where τ is a positive constant and $\delta/\delta p$ denotes the variational derivative. In isotropic case, the interface width is not varying, $\varepsilon = C$. Thus, Eq. (2.4) becomes

$$\tau \frac{\partial p}{\partial t} = \varepsilon^2 \Delta p + p(1-p) \left(p - \frac{1}{2} + m \right). \quad (2.5)$$

In anisotropic case, we consider $\varepsilon = \varepsilon(\theta)$ defined as [9]

$$\varepsilon(\theta) = \bar{\varepsilon} (1 + \delta \cos(\beta(\theta - \theta_0))), \quad (2.6)$$

where $\bar{\varepsilon}$ is a computational parameter corresponding to the layer of the solid-liquid interface. The parameter δ denotes the strength of anisotropy, while β indicates the mode number of the anisotropy, θ represents the the direction of the outer normal vector at the interface given by

$$\theta = \tan^{-1} \left(\frac{p_y}{p_x} \right). \quad (2.7)$$

Incorporating all these parameters, we derive the following phase-field equation in two dimensional case [9]:

$$\begin{aligned} \tau \frac{\partial p}{\partial t} = & -\frac{\partial}{\partial x} \left(\varepsilon \varepsilon' \frac{\partial p}{\partial y} \right) + \frac{\partial}{\partial y} \left(\varepsilon \varepsilon' \frac{\partial p}{\partial x} \right) + \frac{\partial \varepsilon^2}{\partial x} \frac{\partial p}{\partial x} + \frac{\partial \varepsilon^2}{\partial y} \frac{\partial p}{\partial y} \\ & + \varepsilon^2 \left(\frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial y^2} \right) + p(1-p) \left(p - \frac{1}{2} + m \right). \end{aligned} \quad (2.8)$$

The diffusion equation for the temperature T is expressed as follows:

$$\frac{\partial T}{\partial t} = \Delta T + K \frac{\partial p}{\partial t}. \quad (2.9)$$

where $T = 0$ corresponds to a fully cooled state. The parameter K represents the latent heat, which is inversely proportional to the cooling strength. A heat source is present along the moving interface, influencing the dynamics of the temperature-field during the phase transition.

We consider that the equations (2.8) and (2.9) are subject to the Neumann boundary conditions

$$\frac{\partial p}{\partial \mathbf{n}}|_{\partial \Omega} = 0, \quad \frac{\partial T}{\partial \mathbf{n}}|_{\partial \Omega} = 0, \quad (2.10)$$

and three different initial conditions:

Case I

$$\begin{cases} p(x, y, 0) &= \frac{1}{2} \left(\tanh \left(\frac{r_0 - ((x-x_0)^2 + (y-y_0)^2)}{\varepsilon_0} \right) + 1 \right), \\ T(x, y, 0) &= 0, \end{cases} \quad (2.11)$$

where $r_0 = 0.005$, $x_0 = y_0 = 4.5$, and $\varepsilon_0 = 0.0005$. This initial condition forms a circular nuclei with radius r_0 , centering at (x_0, y_0) , and the interface thickness is ε_0 .

Case II

$$\begin{cases} p(x, y, 0) = \frac{1}{2} \left(\tanh \left(\frac{r_0 - y}{\varepsilon_0} \right) + 1 \right), \\ T(x, y, 0) = 0, \end{cases} \quad (2.12)$$

with $r_0 = 0.1$, and $\varepsilon_0 = 0.0005$. This initial condition forms a thin layer of solid phase near the boundary $y = 0$.

Case III

$$\begin{cases} p(x, y, 0) = \frac{1}{2} \left(\tanh \left(\frac{r_0 - (y - y_0)^2}{\varepsilon_0} \right) + 1 \right), \\ T(x, y, 0) = 0, \end{cases} \quad (2.13)$$

with $r_0 = 0.005$, $y_0 = 4.5$, and $\varepsilon_0 = 0.0005$. This initial condition forms a thin layer of solid phase near the middle of y -axis at $y = 4.5$.

CHAPTER 3

TRANSFORMATION TO CURVILINEAR COORDINATES

3.1 Motivation

The crystal growth primarily occurs near the center along both axes of the domain, influenced significantly by the fourfold anisotropy of the system. To capture this concentrated growth accurately, we employ a non-uniform grid that clusters grid points more densely in the direction of crystal growth, providing enhanced resolution in regions with higher growth activity. This grid arrangement is achieved through an algebraic transformation that maps the physical domain, (x, y) , where the grid points concentrate at the center, to a computational domain, (ξ, η) . In this transformed domain, we reformulate the governing model equations to facilitate computation on the non-uniform grid. The transformation is given by

$$\begin{aligned}
x &= x(\xi, \eta), \\
y &= y(\xi, \eta).
\end{aligned}
\tag{3.1}$$

In our study, we employ the following algebraic transformation that clusters the grid points towards the direction of the crystal growth.

$$\begin{aligned}
x(\xi) &= \xi + \frac{\mu L}{\pi} \sin\left(\frac{2\pi\xi}{L}\right), \\
y(\eta) &= \eta + \frac{\mu L}{\pi} \sin\left(\frac{2\pi\eta}{L}\right).
\end{aligned}
\tag{3.2}$$

The degree of clustering in the grid is controlled by the parameter μ on the square domain $[0, L] \times [0, L]$. When $\mu = 0$, the grid points are uniformly distributed across the entire domain. As μ increases, the grid points become progressively clustered towards specific regions of interest. This transformation is applied to Case I, where a small nuclei is expected to form at the center and grow in four directions.

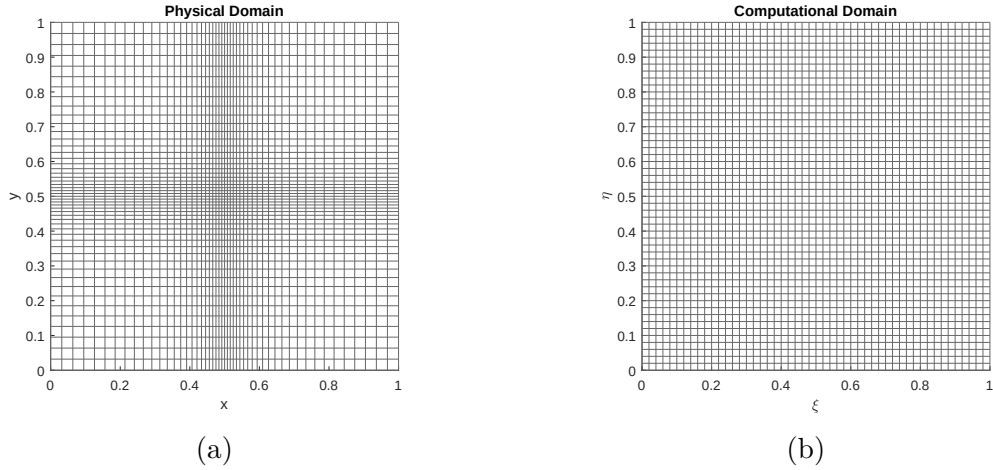


Figure 3.1: (a) Non-uniform grid spacing on physical domain generated by equation (3.2) and (b) its computational domain with uniform grid.

Figure 3.1 illustrates both the physical domain and the corresponding computational domain generated using equations (3.2). As shown, the grid points in the physical domain are more densely distributed near the center along both axes. This non-uniform grid provides increased resolution where crystal growth is most significant, enhancing the accuracy of numerical results in these critical regions.

Another transformation is applied to Case II, where the initial conditions generate a thin layer of solid-phase near $y = 0$, which begins growing upwards. The transformation is as follows.

$$\begin{aligned} x(\xi) &= \xi, \\ y(\eta) &= \eta + \frac{\mu L}{\pi} \sin\left(\frac{\pi \eta}{L}\right). \end{aligned} \tag{3.3}$$

This transformation clusters grid points along the y direction towards $y = 0$, while

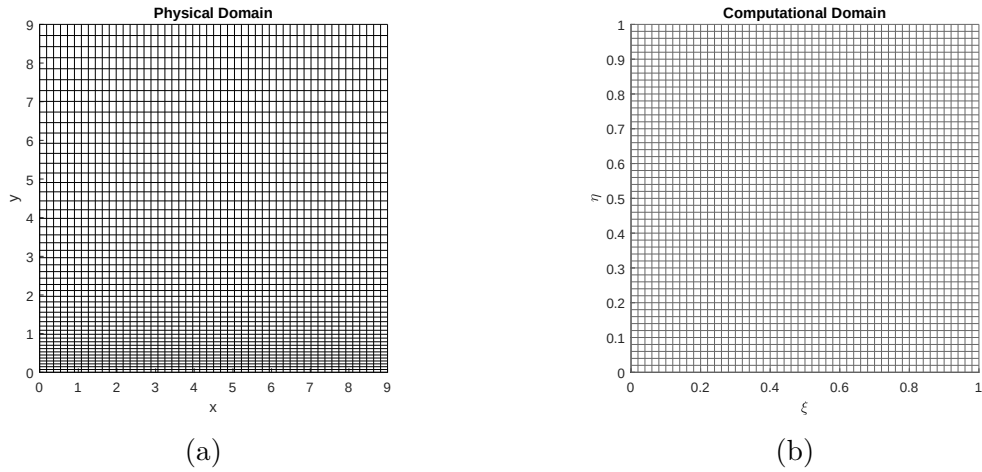


Figure 3.2: (a) Non-uniform grid spacing on physical domain generated by equation (3.3) and (b) its computational domain with uniform grid.

maintaining uniform spacing in the x direction. The resulting grid structures, as shown in Figure 3.2, demonstrates how the transformation concentrates resolution

near $y = 0$, while uniform grid spacing along x .

The last transformation is applied to Case III, where the initial conditions form a thin layer of solid-phase near $y = 4.5$, which grows upwards and downwards. The transformation is as follows.

$$\begin{aligned} x(\xi) &= \xi, \\ y(\eta) &= \eta + \frac{\mu L}{\pi} \sin\left(\frac{2\pi\eta}{L}\right). \end{aligned} \tag{3.4}$$

This transformation clusters grid points along the y direction towards $y = 4.5$, while maintaining uniform grid spacing along x . The resulting grid structures, shown in Figure 3.3, demonstrates the clustered grid near $y = 4.5$.

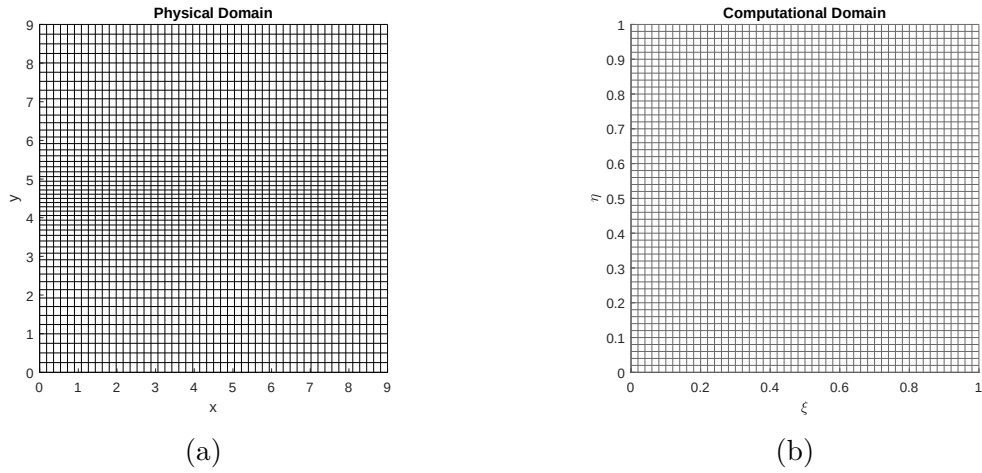


Figure 3.3: (a) Non-uniform grid spacing on physical domain generated by equation (3.4) and (b) its computational domain with uniform grid.

3.2 Curvilinear Coordinates

Reformulating the governing equations to a transformed grid is essential for achieving accurate numerical solutions. Using the transformation described in Eq. (3.2), we map the physical domain to computational coordinates ξ, η , allowing us to rewrite

the governing phase-field model equation (2.8) in terms of these coordinates. This reformulation enables the application of the finite difference method (FDM) directly on the transformed uniform grid, ensuring the accuracy of numerical results while preserving the advantages of the non-uniform grid in the physical domain.

The next step involves deriving the first and second derivatives of p and T . These derivatives will be incorporated into the governing equations, allowing us to integrate the effects of the non-uniform grid into the analysis.

Let u be a function of x and y , $u(x, y)$. We transform the function u in terms of ξ and η by the algebraic transformation (3.1), so that $u(x, y) = u(x(\xi, \eta), y(\xi, \eta)) = u(\xi, \eta)$.

The derivatives of u with respect to ξ and η are derived by chain rule

$$\begin{aligned}\frac{\partial u}{\partial \xi} &= \frac{\partial u}{\partial x} \frac{\partial x}{\partial \xi} + \frac{\partial u}{\partial y} \frac{\partial y}{\partial \xi}, \\ \frac{\partial u}{\partial \eta} &= \frac{\partial u}{\partial x} \frac{\partial x}{\partial \eta} + \frac{\partial u}{\partial y} \frac{\partial y}{\partial \eta}.\end{aligned}\tag{3.5}$$

Solving the system of equation (3.5) gives us

$$\begin{aligned}\frac{\partial u}{\partial x} &= \frac{1}{J} \left(\frac{\partial u}{\partial \xi} \frac{\partial y}{\partial \eta} - \frac{\partial u}{\partial \eta} \frac{\partial y}{\partial \xi} \right), \\ \frac{\partial u}{\partial y} &= \frac{1}{J} \left(\frac{\partial u}{\partial \eta} \frac{\partial x}{\partial \xi} - \frac{\partial u}{\partial \xi} \frac{\partial x}{\partial \eta} \right),\end{aligned}\tag{3.6}$$

where

$$J = \frac{\partial x}{\partial \xi} \frac{\partial y}{\partial \eta} - \frac{\partial x}{\partial \eta} \frac{\partial y}{\partial \xi}.$$

For simplicity, we denote

$$\begin{aligned} u_x &= \frac{\partial u}{\partial x}; u_y = \frac{\partial u}{\partial y}; u_\xi = \frac{\partial u}{\partial \xi}; u_\eta = \frac{\partial u}{\partial \eta}; \\ x_\xi &= \frac{\partial x}{\partial \xi}; x_\eta = \frac{\partial x}{\partial \eta}; y_\xi = \frac{\partial y}{\partial \xi}; y_\eta = \frac{\partial y}{\partial \eta}; \end{aligned} \quad (3.7)$$

Rewriting (3.6), we have

$$\begin{aligned} u_x &= \frac{1}{J} (u_\xi y_\eta - u_\eta y_\xi), \\ u_y &= \frac{1}{J} (u_\eta x_\xi - u_\xi x_\eta), \end{aligned} \quad (3.8)$$

where

$$J = x_\xi y_\eta - x_\eta y_\xi.$$

The transformation of its second derivatives is given by

$$\begin{aligned} u_{xx} &= (u_x)_x = \frac{1}{J} \left((u_x)_\xi y_\eta - (u_x)_\eta y_\xi \right) \\ &= \frac{1}{J} \left[\left(\frac{1}{J} (u_\xi y_\eta - u_\eta y_\xi) \right)_\xi y_\eta - \left(\frac{1}{J} (u_\xi y_\eta - u_\eta y_\xi) \right)_\eta y_\xi \right] \\ &= \frac{1}{J} \left[-\frac{1}{J^2} J_\xi (u_\xi y_\eta - u_\eta y_\xi) y_\eta + \frac{1}{J} (u_\xi y_\eta - u_\eta y_\xi)_\xi y_\eta \right. \\ &\quad \left. + \frac{1}{J^2} J_\eta (u_\xi y_\eta - u_\eta y_\xi) y_\xi - \frac{1}{J} (u_\xi y_\eta - u_\eta y_\xi)_\eta y_\xi \right] \\ &= \frac{1}{J^2} \left[(u_\xi y_\eta - u_\eta y_\xi)_\xi y_\eta - (u_\xi y_\eta - u_\eta y_\xi)_\eta y_\xi \right] \\ &\quad + \frac{1}{J^3} [J_\eta (u_\xi y_\eta - u_\eta y_\xi) y_\xi - J_\xi (u_\xi y_\eta - u_\eta y_\xi) y_\eta] \\ &= \frac{1}{J^2} [u_{\xi\xi} y_\eta^2 - 2u_{\xi\eta} y_\xi y_\eta + u_{\eta\eta} y_\xi^2 + u_\xi (y_{\xi\eta} y_\eta - y_{\eta\eta} y_\xi) + u_\eta (y_{\xi\eta} y_\xi - y_{\xi\xi} y_\eta)] \\ &\quad + \frac{1}{J^3} [J_\eta (u_\xi y_\xi y_\eta - u_\eta y_\xi^2) - J_\xi (u_\xi y_\eta^2 - u_\eta y_\xi y_\eta)], \end{aligned}$$

and

$$\begin{aligned}
u_{yy} &= (u_y)_y = \frac{1}{J} \left((u_y)_\eta x_\xi - (u_y)_\xi x_\eta \right) \\
&= \frac{1}{J} \left[\left(\frac{1}{J} (u_\eta x_\xi - u_\xi x_\eta) \right)_\eta x_\xi - \left(\frac{1}{J} (u_\eta x_\xi - u_\xi x_\eta) \right)_\xi x_\eta \right] \\
&= \frac{1}{J} \left[-\frac{1}{J^2} J_\eta (u_\eta x_\xi - u_\xi x_\eta) x_\xi + \frac{1}{J} (u_\eta x_\xi - u_\xi x_\eta)_\eta x_\xi \right. \\
&\quad \left. + \frac{1}{J^2} J_\xi (u_\eta x_\xi - u_\xi x_\eta) x_\eta - \frac{1}{J} (u_\eta x_\xi - u_\xi x_\eta)_\xi x_\eta \right] \\
&= \frac{1}{J^2} \left[(u_\eta x_\xi - u_\xi x_\eta)_\eta x_\xi - (u_\eta x_\xi - u_\xi x_\eta)_\xi x_\eta \right] \\
&\quad + \frac{1}{J^3} [J_\xi (u_\eta x_\xi - u_\xi x_\eta) x_\eta - J_\eta (u_\eta x_\xi - u_\xi x_\eta) x_\xi] \\
&= \frac{1}{J^2} [u_{\xi\xi} x_\eta^2 - 2u_{\xi\eta} x_\xi x_\eta + u_{\eta\eta} x_\xi^2 + u_\xi (x_{\xi\eta} x_\eta - x_{\eta\eta} x_\xi) + u_\eta (x_{\xi\eta} x_\xi - x_{\xi\xi} x_\eta)] \\
&\quad + \frac{1}{J^3} [J_\xi (u_\eta x_\xi x_\eta - u_\xi x_\eta^2) - J_\eta (u_\eta x_\xi^2 - u_\xi x_\xi x_\eta)].
\end{aligned}$$

Thus we have

$$\Delta u = u_{xx} + u_{yy} = \frac{1}{J^2} [q_1 u_{\xi\xi} - 2q_2 u_{\xi\eta} + q_3 u_{\eta\eta}] + \Delta\xi u_\xi + \Delta\eta u_\eta, \quad (3.9)$$

where

$$q_1 = x_\eta^2 + y_\eta^2,$$

$$q_2 = x_\xi x_\eta + y_\xi y_\eta,$$

$$q_3 = x_\xi^2 + y_\xi^2,$$

$$\Delta\xi = \xi_{xx} + \xi_{yy} = \frac{1}{J^2} [x_{\xi\eta} x_\eta - x_{\eta\eta} x_\xi + y_{\xi\eta} y_\eta - y_{\eta\eta} y_\xi] + \frac{1}{J^3} [-q_1 J_\xi + q_2 J_\eta], \quad (3.10)$$

$$\Delta\eta = \eta_{xx} + \eta_{yy} = \frac{1}{J^2} [x_{\xi\eta} x_\xi - x_{\xi\xi} x_\eta + y_{\xi\eta} y_\xi - y_{\xi\xi} y_\eta] + \frac{1}{J^3} [q_2 J_\xi - q_3 J_\eta], \quad (3.11)$$

$$J_\xi = x_{\xi\xi} y_\eta + x_\xi y_{\xi\eta} - x_{\xi\eta} y_\xi - x_\eta y_{\xi\xi},$$

$$J_\eta = x_{\xi\eta} y_\eta + x_\xi y_{\eta\eta} - x_{\eta\eta} y_\xi - x_\eta y_{\eta\xi}.$$

Equation (3.10) and (3.11) are derived by letting $u = \xi$ and $u = \eta$, so that we have its first and second derivatives as follows.

$$\begin{aligned}
\xi_x &= \frac{1}{J} (\xi_\xi y_\eta - \xi_\eta y_\xi) = \frac{y_\eta}{J}, \\
\xi_y &= \frac{1}{J} (\xi_\eta x_\xi - \xi_\xi x_\eta) = -\frac{x_\eta}{J}, \\
\xi_{xx} &= \frac{1}{J} \left[\left(\frac{y_\eta}{J} \right)_\xi y_\eta - \left(\frac{y_\eta}{J} \right)_\eta y_\xi \right] \\
&= \frac{1}{J} \left[-\frac{1}{J^2} J_\xi y_\eta^2 + \frac{1}{J} y_{\xi\eta} y_\eta + \frac{1}{J^2} J_\eta y_\xi y_\eta - \frac{1}{J} y_{\eta\eta} y_\xi \right] \\
&= \frac{1}{J^2} [y_{\xi\eta} y_\eta - y_{\eta\eta} y_\xi] + \frac{1}{J^3} [J_\eta y_\xi y_\eta - J_\xi y_\eta^2], \\
\xi_{yy} &= \frac{1}{J} \left[\left(-\frac{x_\eta}{J} \right)_\eta x_\xi - \left(-\frac{x_\eta}{J} \right)_\xi x_\eta \right] \\
&= \frac{1}{J} \left[\frac{1}{J^2} J_\eta x_\xi x_\eta - \frac{1}{J} x_{\eta\eta} x_\xi - \frac{1}{J^2} J_\xi x_\eta^2 + \frac{1}{J} x_{\xi\eta} x_\eta \right] \\
&= \frac{1}{J^2} [x_{\xi\eta} x_\eta - x_{\eta\eta} x_\xi] + \frac{1}{J^3} [J_\eta x_\xi x_\eta - J_\xi x_\eta^2], \\
\eta_x &= \frac{1}{J} (\eta_\xi y_\eta - \eta_\eta y_\xi) = -\frac{y_\xi}{J}, \\
\eta_y &= \frac{1}{J} (\eta_\eta x_\xi - \eta_\xi x_\eta) = \frac{x_\xi}{J}, \\
\eta_{xx} &= \frac{1}{J} \left[\left(-\frac{y_\xi}{J} \right)_\xi y_\eta - \left(-\frac{y_\xi}{J} \right)_\eta y_\xi \right] \\
&= \frac{1}{J} \left[\frac{1}{J^2} J_\xi y_\xi y_\eta - \frac{1}{J} y_{\xi\xi} y_\eta - \frac{1}{J^2} J_\eta y_\xi^2 + \frac{1}{J} y_{\xi\eta} y_\xi \right] \\
&= \frac{1}{J^2} [y_{\xi\eta} y_\xi - y_{\xi\xi} y_\eta] + \frac{1}{J^3} [J_\xi y_\xi y_\eta - J_\eta y_\xi^2], \\
\eta_{yy} &= \frac{1}{J} \left[\left(\frac{x_\xi}{J} \right)_\eta x_\xi - \left(\frac{x_\xi}{J} \right)_\xi x_\eta \right] \\
&= \frac{1}{J} \left[-\frac{1}{J^2} J_\eta x_\xi^2 + \frac{1}{J} x_{\xi\eta} x_\xi + \frac{1}{J^2} J_\xi x_\xi x_\eta - \frac{1}{J} x_{\xi\xi} x_\eta \right] \\
&= \frac{1}{J^2} [x_{\xi\eta} x_\xi - x_{\xi\xi} x_\eta] + \frac{1}{J^3} [J_\xi x_\xi x_\eta - J_\eta x_\xi^2].
\end{aligned}$$

Applying this transformation to the coupled equation (2.8) and (2.9) gives us

$$\begin{aligned}
\tau \frac{\partial p}{\partial t} &= -\frac{1}{J} \left[\left(a \left[\frac{1}{J} (p_\eta x_\xi - p_\xi x_\eta) \right] \right)_\xi y_\eta - \left(a \left[\frac{1}{J} (p_\eta x_\xi - p_\xi x_\eta) \right] \right)_\eta y_\xi \right] \\
&\quad + \frac{1}{J} \left[\left(a \left[\frac{1}{J} (p_\xi y_\eta - p_\eta y_\xi) \right] \right)_\eta x_\xi - \left(a \left[\frac{1}{J} (p_\xi y_\eta - p_\eta y_\xi) \right] \right)_\xi x_\eta \right] \\
&\quad + \left[\frac{1}{J} (b_\xi y_\eta - b_\eta y_\xi) \right] \left[\frac{1}{J} (p_\xi y_\eta - p_\eta y_\xi) \right] + \left[\frac{1}{J} (b_\eta x_\xi - b_\xi x_\eta) \right] \left[\frac{1}{J} (p_\eta x_\xi - p_\xi x_\eta) \right] \\
&\quad + \frac{b}{J^2} [q_1 u_{\xi\xi} - 2q_2 u_{\xi\eta} + q_3 u_{\eta\eta}] + b\Delta\xi u_\xi + b\Delta\eta u_\eta + p(1-p) \left(p - \frac{1}{2} + m \right) \\
&= \frac{b}{J^2} [q_1 p_{\xi\xi} - 2q_2 p_{\xi\eta} + q_3 p_{\eta\eta}] + \left[b\Delta\xi + \frac{a_\eta}{J} + \frac{1}{J^2} b_\xi q_1 - \frac{1}{J^2} b_\eta q_2 \right] p_\xi \\
&\quad + \left[b\Delta\eta - \frac{a_\xi}{J} - \frac{1}{J^2} b_\xi q_2 + \frac{1}{J^2} b_\eta q_3 \right] p_\eta + p(1-p) \left(p - \frac{1}{2} + m \right), \tag{3.12}
\end{aligned}$$

$$\frac{\partial T}{\partial t} = \frac{1}{J^2} [q_1 T_{\xi\xi} - 2q_2 T_{\xi\eta} + q_3 T_{\eta\eta}] + \Delta\xi T_\xi + \Delta\eta T_\eta + K \frac{\partial p}{\partial t}, \tag{3.13}$$

where

$$a = \varepsilon\varepsilon', \quad \text{and} \quad b = \varepsilon^2.$$

Equations (3.12) and (3.13) are the general phase-field model for dendritic crystal growth in curvilinear coordinates.

Employing the algebraic transformation (3.2) to the model gives us

$$\begin{aligned}
\tau \frac{\partial p}{\partial t} &= \frac{b}{J^2} [y_\eta^2 p_{\xi\xi} + x_\xi^2 p_{\eta\eta}] + \left[\frac{a_\eta}{J} + \frac{1}{J^2} b_\xi y_\eta^2 - \frac{1}{J^3} b x_\xi y_\eta^3 \right] p_\xi \\
&\quad + \left[-\frac{a_\xi}{J} + \frac{1}{J^2} b_\xi x_\xi^2 - \frac{1}{J^3} b x_\xi^3 y_{\eta\eta} \right] p_\eta + p(1-p) \left(p - \frac{1}{2} + m \right), \tag{3.14}
\end{aligned}$$

$$\frac{\partial T}{\partial t} = \frac{1}{J^2} [y_\eta^2 T_{\xi\xi} + x_\xi^2 T_{\eta\eta}] - \frac{1}{J^3} x_\xi y_\eta^3 T_\xi - \frac{1}{J^3} x_\xi^3 y_{\eta\eta} T_\eta + K \frac{\partial p}{\partial t}. \tag{3.15}$$

Our aim is to solve equations (3.14) and (3.15) numerically. For this purpose, a numerical scheme is developed in the next chapter and implemented in MATLAB.

CHAPTER 4

NUMERICAL DISCRETIZATION AND COMPUTED RESULTS

In this chapter, we establish a numerical scheme to discretize the phase-field model for dendritic crystal growth, equations (3.14) and (3.15), employing a second-order central difference scheme for spatial discretization and a forward Euler method for time evolution.

4.1 Central Difference for Spatial Discretization

For spatial discretization, we employ a second order central difference scheme, which can be derived from the Taylor series expansion. To begin, we discretize the domain of the problem. Let $[a, b] \subset \mathbb{R}$ be the domain and let N be a positive integer. We divide the interval $[a, b]$ into N equal parts,

$$[a, b] = [x_0, x_1] \cup [x_1, x_2] \cup \dots \cup [x_{N-1}, x_N],$$

where $a = x_0 < x_1 < \cdots < x_{N-1} < x_N = b$ are the grid points. We denote the step size as $h = (b - a) / N$, so that the node points are given by

$$x_i = a + ih, \quad 0 \leq i \leq N.$$

Let u is a function of x and denote $u_i = u(x_i)$, for $0 \leq i \leq N$. Let U_i be the numerical approximation of the exact (true) solution of $u(x_i)$. The Taylor expansion of u around x_i is given by

$$u_{i+1} = u_i + hu'_i + \frac{h^2}{2}u''_i + \frac{h^3}{6}u'''_i + \frac{h^4}{24}u^{(4)}_i + O(h^5), \quad (4.1)$$

$$u_{i-1} = u_i - hu'_i + \frac{h^2}{2}u''_i - \frac{h^3}{6}u'''_i + \frac{h^4}{24}u^{(4)}_i + O(h^5). \quad (4.2)$$

Subtracting Eq. (4.2) from Eq. (4.1) yields

$$u_{i+1} - u_{i-1} = 2hu'_i + \frac{h^3}{3}u'''_i + O(h^4),$$

which can be rearranged as

$$u'_i = \frac{u_{i+1} - u_{i-1}}{2h} + O(h^2).$$

This equation leads to an approximation:

$$U'_i \approx \frac{u_{i+1} - u_{i-1}}{2h}. \quad (4.3)$$

Eq. (4.3) is known as the central difference approximation for the first derivative with second-order convergence.

Now, adding Eq. (4.1) to Eq. (4.2) gives us

$$u_{i+1} + u_{i-1} = 2u_i + h^2u''_i + \frac{h^4}{12}u^{(4)}_i + O(h^5).$$

This can be rearranged as

$$u_i'' = \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + O(h^2).$$

This equation yields an approximation:

$$U_i'' \approx \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2}. \quad (4.4)$$

Eq. (4.4) is referred to as the central difference approximation for the second derivative with second-order convergence.

Let us denote the central difference operators as follows:

$$\begin{aligned} \delta_\xi p_{ij} &= \frac{p_{i+1,j} - p_{i-1,j}}{2h}, \\ \delta_\eta p_{ij} &= \frac{p_{i,j+1} - p_{i,j-1}}{2h}, \\ \delta_\xi^2 p_{ij} &= \frac{p_{i+1,j} - 2p_{ij} + p_{i-1,j}}{h^2}, \\ \delta_\eta^2 p_{ij} &= \frac{p_{i,j+1} - 2p_{ij} + p_{i,j-1}}{h^2}. \end{aligned}$$

The semidiscrete scheme for phase-field equation (3.14) is expressed as

$$\tau \left(\frac{\partial p}{\partial t} \right)_{ij} + [R_{ij} \delta_\xi^2 + S_{ij} \delta_\eta^2 + T_{ij} \delta_\xi + U_{ij} \delta_\eta] p_{ij} = F_{ij}, \quad (4.5)$$

where the coefficients $R_{ij}, S_{ij}, T_{ij}, U_{ij}$, and F_{ij} are defined by

$$\begin{aligned} R_{ij} &= -\frac{b_{ij}}{J_{ij}^2} y_{\eta ij}^2, \\ S_{ij} &= -\frac{b_{ij}}{J_{ij}^2} x_{\xi ij}^2, \\ T_{ij} &= -\frac{\delta_\eta a_{ij}}{J_{ij}} - \frac{1}{J_{ij}^2} \delta_\xi b_{ij} y_{\eta ij}^2 + \frac{1}{J_{ij}^3} b_{ij} x_{\xi ij} y_{\eta ij}^3, \\ U_{ij} &= \frac{\delta_\xi a_{ij}}{J_{ij}} - \frac{1}{J_{ij}^2} \delta_\eta b_{ij} x_{\xi ij}^2 + \frac{1}{J_{ij}^3} b_{ij} x_{\xi ij}^3 y_{\eta ij}, \\ F_{ij} &= p_{ij} (1 - p_{ij}) \left(p_{ij} - \frac{1}{2} + m_{ij} \right), \end{aligned}$$

and the semidiscrete scheme for temperature equation (3.15) is given by

$$\left(\frac{\partial T}{\partial t}\right)_{ij} + [V_{ij}\delta_\xi^2 + W_{ij}\delta_\eta^2 + X_{ij}\delta_\xi + Y_{ij}\delta_\eta] T_{ij} = K \left(\frac{\partial p}{\partial t}\right)_{ij}, \quad (4.6)$$

where the coefficients V_{ij} , W_{ij} , X_{ij} , and Y_{ij} are defined by

$$\begin{aligned} V_{ij} &= -\frac{1}{J_{ij}^2} y_{\eta ij}^2, \\ W_{ij} &= -\frac{1}{J_{ij}^2} x_{\xi ij}^2, \\ X_{ij} &= \frac{1}{J_{ij}^3} x_{\xi ij} y_{\eta ij}^3, \\ Y_{ij} &= \frac{1}{J_{ij}^3} x_{\xi ij}^3 y_{\eta ij}. \end{aligned}$$

4.2 Time-Stepping Scheme

In this section, we consider the forward Euler method for discretization in terms of time variable. Consider the semidiscrete schemes (4.5) and (4.6) with the initial condition $p(x, y, 0) = p_0$ and $T(x, y, 0) = T_0$ as in Eq. (2.11) on $t \in [0, T]$. Let us divide the interval $[0, T]$ into N_t equal parts,

$$[0, T] = [t_0, t_1] \cup [t_1, t_2] \cup \dots [t_{N_t-1}, t_{N_t}],$$

where $0 = t_0 < t_1 < \dots < t_{N_t-1} < t_{N_t} = T$ are the grid points in time. We denote the step size as $\Delta t = T/N_t$, so that the node points are given by

$$t_n = n\Delta t, \quad 0 \leq n \leq N_t.$$

Let U_{ij}^n be the approximation of $u(x_i, y_j, t_n)$. The forward Euler scheme for time

derivative of u is given as

$$\left(\frac{\partial u}{\partial t}\right)_{ij}^n \approx \frac{U_{ij}^{n+1} - U_{ij}^n}{\Delta t}. \quad (4.7)$$

This yields to the fully discrete problem

$$\begin{cases} \tau \left(\frac{p_{ij}^{n+1} - p_{ij}^n}{\Delta t} \right) + [R_{ij}^n \delta_\xi^2 + S_{ij}^n \delta_\eta^2 + T_{ij}^n \delta_\xi + U_{ij}^n \delta_\eta] p_{ij}^n &= F_{ij}^n, \\ \frac{T_{ij}^{n+1} - T_{ij}^n}{\Delta t} + [V_{ij}^n \delta_\xi^2 + W_{ij}^n \delta_\eta^2 + X_{ij}^n \delta_\xi + Y_{ij}^n \delta_\eta] T_{ij}^n &= K \left(\frac{p_{ij}^{n+1} - p_{ij}^n}{\Delta t} \right). \end{cases} \quad (4.8)$$

4.3 Results and Discussion

In this section, we present two-dimensional simulations to investigate the influence of the parameter μ on the formation of a fourfold anisotropic dendritic pattern. Specifically, we examine how varying μ impacts the crystal growth dynamics and morphology. The simulations are conducted on a domain $[0, 9] \times [0, 9]$ with a grid resolution of $N = 300$. The parameter values for the simulations are set as follows: $\tau = 0.0003$, $\alpha = 0.9$, $\gamma = 10$, $\bar{\varepsilon} = 0.01$, $\delta = 0.02$, $\beta = 4$, $T_e = 1$, and $K = 1.8$.

Figure 4.1 shows snapshots of the phase variable p at various time levels in Case I, illustrating the progression of crystal growth from an initial nucleus. The initial profile of p begins as a small circular region, representing the crystal nucleus, which subsequently develops into a dendritic structure. The characteristic fourfold anisotropy emerges as the crystal grows, consistent with results from uniform grid simulations. Here, we set a value of $\mu = 0.01$ for the non-uniform grid, allowing for higher resolution around the center of the domain.

We also examine the temperature-field T at selected time points $t = 0$, $t = 0.2$, and $t = 0.4$, as shown in Figure 4.2. The temperature distribution around the growing

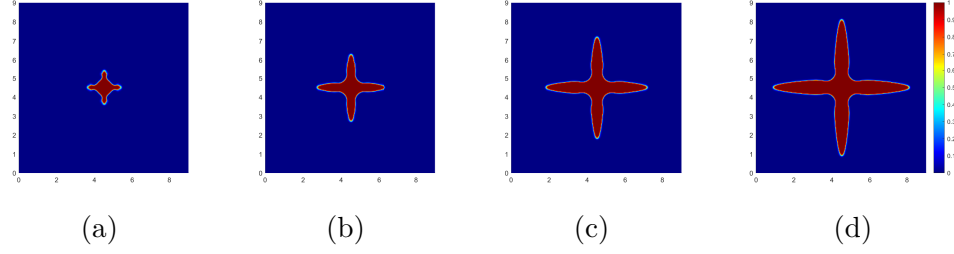


Figure 4.1: The snapshots of phase-field at (a) $t = 0.1$, (b) $t = 0.2$, (c) $t = 0.3$, and (d) $t = 0.4$.

dendrite reveals thermal gradients that drive the anisotropic growth, with the highest temperature near the solid-liquid interface due to the latent heat release during solidification. These thermal gradients play a critical role in defining the dendritic growth morphology and maintaining the fourfold symmetry.

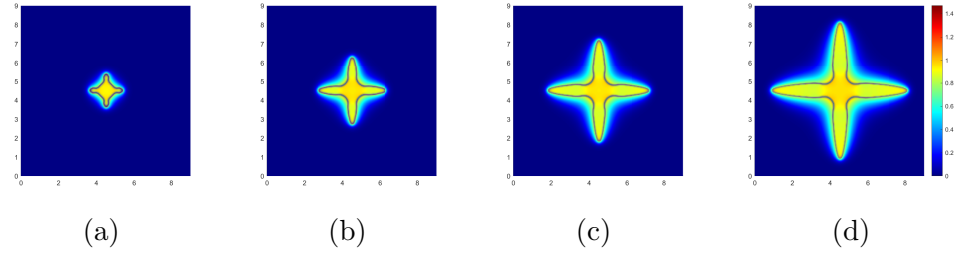


Figure 4.2: The snapshots of temperature-field at (a) $t = 0.1$, (b) $t = 0.2$, (c) $t = 0.3$, and (d) $t = 0.4$.

The comparison of initial profiles highlights the advantages of using clustered grids over uniform grids in accurately resolving the crystal geometry at the beginning of the simulation. As shown in Figure 4.3, the initial crystal profile on a clustered grid represented by blue line is visibly smoother and more accurately defined compared to that on a uniform grid represented by red line. Clustered grids provide enhanced resolution in critical regions, such as near the solid-liquid interface, by clustering grid points where rapid changes in morphology are expected. This leads to a more precise representation of the initial crystal geometry, which is essential for capturing fine

morphological details during the subsequent growth process.

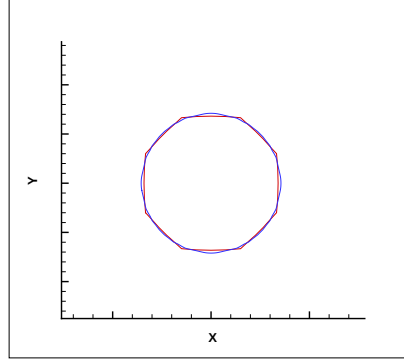


Figure 4.3: Comparison on initial profile of phase-field

The use of clustered grids enables accurate results even with a reduced number of grid points, significantly lowering computational costs. By concentrating resolution where it is most needed, the clustered grid approach strikes a balance between accuracy and efficiency, making it a valuable tool for simulations of dendritic growth processes.

The results for Case II, obtained by implementing the algebraic transformation (3.3) into the model, are presented in Figures 4.4 and 4.5, showing snapshots of the evolution of the phase-field and temperature-field respectively. In this case, the solidification process begins with an initial condition where the solid-phase is initialized along one boundary of the domain, near $y = 0$. The solid-phase grows upwards, driven by the solid-liquid interface dynamics, leading to the formation of dendritic patterns.

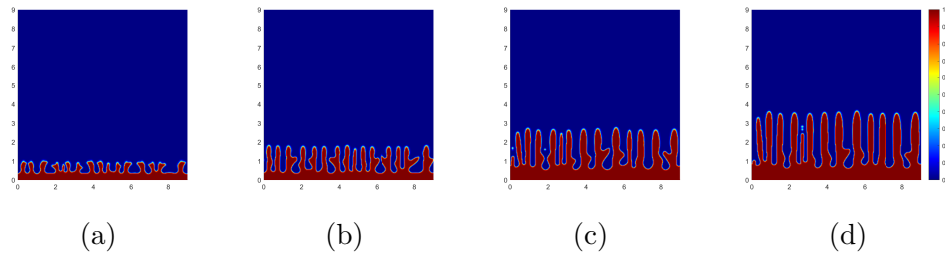


Figure 4.4: The snapshots of phase-field at (a) $t = 0.1$, (b) $t = 0.2$, (c) $t = 0.3$, and (d) $t = 0.4$.

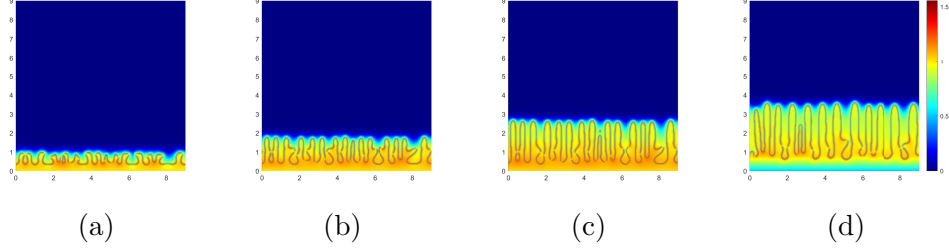


Figure 4.5: The snapshots of temperature-field at (a) $t = 0.1$, (b) $t = 0.2$, (c) $t = 0.3$, and (d) $t = 0.4$.

The results for Case III, obtained by implementing the algebraic transformation (3.4) into the model, are shown in Figures 4.6 and 4.7, presenting snapshots of the evolution of the phase-field and temperature-field, respectively. In this case, the solidification process begins with an initial condition where the solid-phase is initialized as a thin layer near $y = 4.5$. The solid-phase grows both upwards and downwards, forming branching dendritic patterns over time. Together with Case II, these results demonstrate the consistency of the curvilinear framework when applied to varying initial conditions and algebraic transformations.

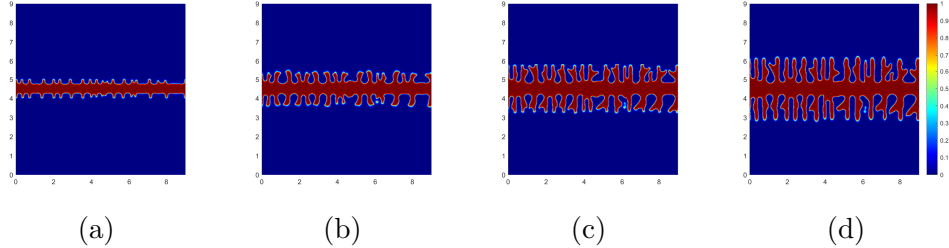


Figure 4.6: The snapshots of phase-field at (a) $t = 0.05$, (b) $t = 0.1$, (c) $t = 0.15$, and (d) $t = 0.2$.

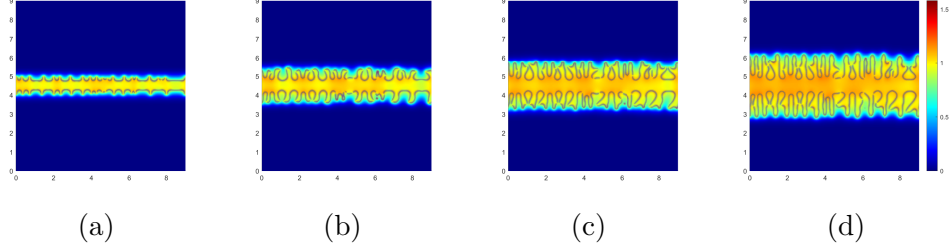


Figure 4.7: The snapshots of temperature-field at (a) $t = 0.05$, (b) $t = 0.1$, (c) $t = 0.15$, and (d) $t = 0.2$.

4.4 Parametric Study

In this section, we explore and analyze the influence of various physical and numerical parameters to validate the performance of the proposed numerical method. Dendritic solidification, a key phenomenon in crystal growth studies, is used as a benchmark to assess the method's accuracy and sensitivity to different parameters. By comparing the simulated results with the expected physical behaviors observed in dendritic solidification, we can evaluate the effectiveness and stability of the method.

The parameters under study include latent heat, relaxation time, and interface width. Each of these parameters plays a critical role in determining the morphology and dynamics of crystal growth.

4.4.1 Effect of Latent Heat

Latent heat is the energy released during the phase transition from liquid to solid. In the context of dendritic growth, it affects the thermal field around the growing crystal, influencing the growth rate and the stability of the dendrite arms. We examine how varying latent heat impacts the crystal growth velocity and the overall shape of the dendrite.

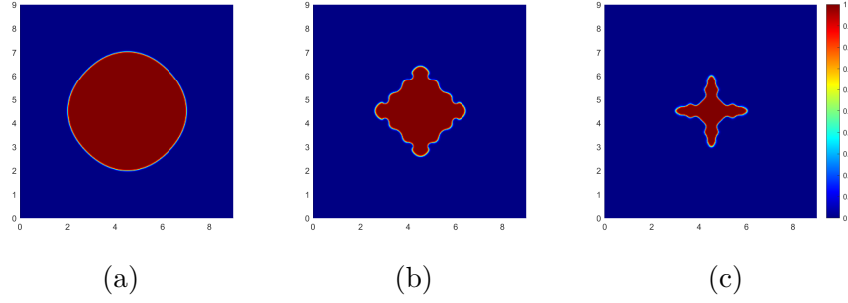


Figure 4.8: Crystal growth with (a) $K = 0.8$, (b) $K = 1.2$, and (c) $K = 1.6$.

Figure 4.8 illustrates how the crystal shape changes as the latent heat parameter K increases, under 4-mode anisotropy. For $K = 0.8$ (a), the crystal grows in a nearly circular shape, as the growth is mostly the same in all directions. When K increases to 1.2 (b), the crystal starts showing fourfold symmetry, forming a diamond-like shape. At this stage, small dents appear at the edges of the crystal, showing the effect of anisotropy. For $K = 1.6$ (c), the crystal develops a branching structure, with the arms extending along specific directions. The branches become thinner and more defined as K increases. This progression shows how the crystal transitions from a circular shape to a more structured and complex dendritic pattern as the value of K increases, driven by the increasing influence of anisotropy.

4.4.2 Effect of Relaxation Time

Relaxation time is a parameter related to the phase-field model, affecting how quickly the interface adapts to changes in the fields. Shorter relaxation times lead to faster interface responses, potentially altering the shape and stability of dendrite tips and branches. We discuss the implications of relaxation time adjustments on the morphological accuracy of the dendritic structures.

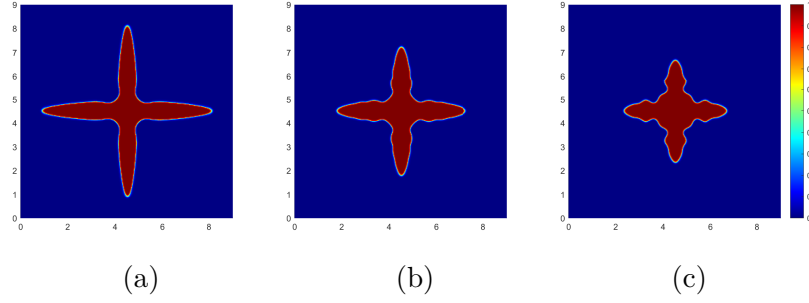


Figure 4.9: Crystal growth with (a) $\tau = 0.0003$, (b) $\tau = 0.0004$, and (c) $\tau = 0.0005$.

Figure 4.9 illustrates the effect of the relaxation time parameter τ on dendritic crystal growth morphology under 4-mode anisotropy. The parameter τ is observed for three values: $\tau = 0.0003$, $\tau = 0.0004$, and $\tau = 0.0005$. As τ increases, the size of the crystal arms decreases, transitioning from elongated and well-defined branches for $\tau = 0.0003$ (a) to shorter, thicker branches for $\tau = 0.0004$ (b), and finally to compact, broader structures for $\tau = 0.0005$ (c). Lower values of τ allow the interface to respond more quickly to gradients, resulting in faster growth and sharper, more directional patterns along the primary axes. Conversely, higher values of τ slow down the interface response, leading to less pronounced dendritic structures and more rounded growth. This progression demonstrates the significant role of relaxation time in controlling the speed and morphology of dendritic crystal growth.

4.4.3 Effect of Interface Width

Interface width defines the spatial extent of the phase-field interface between the solid and liquid-phase. A narrow interface width generally provides a sharper, more detailed depiction of the dendrite shape, while a wider interface can smooth out small features. The sensitivity of the crystal morphology to interface width adjustments is examined.

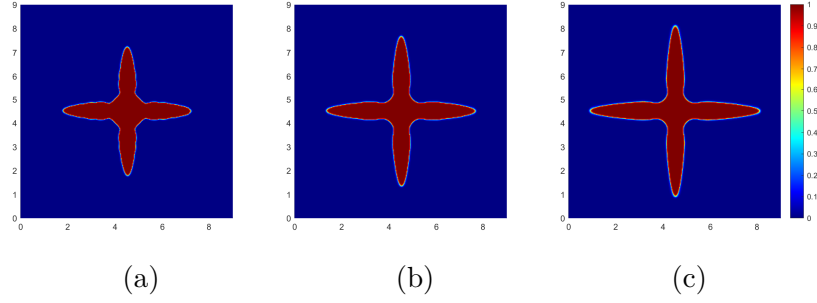


Figure 4.10: Crystal growth with (a) $\bar{\varepsilon} = 0.008$, (b) $\bar{\varepsilon} = 0.009$, and (c) $\bar{\varepsilon} = 0.010$.

Figure 4.10 shows the effect of the interface width parameter $\bar{\varepsilon}$ on the morphology of dendritic crystal growth. The parameter is shown for three values: $\bar{\varepsilon} = 0.008$, $\bar{\varepsilon} = 0.009$, and $\bar{\varepsilon} = 0.010$. For $\bar{\varepsilon} = 0.008$ (a), the crystal arms are shorter and thicker, forming a more compact shape. As $\bar{\varepsilon}$ increases to 0.009 (b), the arms become slightly longer and thinner. At $\bar{\varepsilon} = 0.010$ (c), the arms are significantly longer, thinner, and more defined. This shows that increasing the interface width leads to smoother and more extended growth, while smaller interface widths produce more compact crystals.

CHAPTER 5

CONCLUSION

5.1 Summary of Findings

This thesis has presented a curvilinear phase-field model for dendritic crystal growth, employing an algebraic transformation to generate a non-uniform grid. Through this approach, we aimed to improve computational efficiency and accuracy in capturing the critical regions of anisotropic growth. Our results demonstrated that simulations conducted on this non-uniform grid is consistent with those obtained on a uniform grid, validating the reliability of this method for modeling dendritic growth.

We also performed a comprehensive analysis of the factors influencing dendritic crystal growth within this two-dimensional phase-field model. By varying key parameters, such as latent heat, relaxation time, and interface width, we investigated how each of these parameters controls the morphology, growth rate, and stability of dendritic structures. The findings highlight the critical role of these parameters in defining the anisotropic growth patterns characteristic of dendritic crystals, providing deeper insight into how growth dynamics can be modulated within a non-uniform grid

framework.

These contributions advance the field of crystal growth modeling by offering new insights into the effects of specific parameter adjustments on dendritic morphology within a non-uniform grid domain. This work highlights the potential of using curvilinear grid adaptations in phase-field modeling to more accurately simulate anisotropic phenomena in dendritic solidification. However, this study is limited by its assumptions of two-dimensional modeling and a fixed fourfold anisotropy, which may not capture the full complexity of real-world crystal growth in three-dimensional or variable anisotropy settings.

5.2 Suggestion for Future Work

There are several directions for future work that could expand upon the findings in this research. First, extending the model to three dimensions would allow for more realistic simulations of dendritic growth, capturing phenomena that are inherently three-dimensional.

Additionally, implementing adaptive grid refinement could significantly improve computational efficiency by focusing resolution in regions of rapid growth, such as dendrite tips and high-curvature areas.

Furthermore, the integration of machine learning for parameter optimization and high-performance computing for large-scale simulations could greatly enhance the model’s capabilities. Using high-performance computing resources could further support these simulations.

Experimental validation of these simulations against real-world data would provide essential calibration, ensuring that the insights gained from this research have practical relevance in materials science. Comparisons with experimental results could help fine-tune model parameters and verify predicted growth patterns, making the model more applicable to industrial processes, such as alloy solidification, where precise control over dendritic morphology is essential.

APPENDIX A

A.1 MATLAB Codes

```
1      % CURVILINEAR DENDRITIC CRYSTAL GROWTH
2      % PHASE-FIELD MODEL BY KOBAYASHI
3      % CURVILINEAR COORDINATES MODEL AND CODES BY HABIBURRAHMAN
4      % Consider the transformation  $x = x(\xi)$  and  $y = y(\eta)$ 
5      %  $(x,y)$  the physical domain (nonuniform)
6      %  $(\xi,\eta)$  the computational domain (uniform)
7      % Central Difference in space
8      % Forward Euler in time
9
10     % Parameters
11     tau = 0.0003;
12     alpha = 0.9;
13     gamma = 10;
14     eps_bar = 0.01;
15     delta = 0.02;
16     aniso = 4;
17     Te = 1;
18     K = 1.8;
19     lambda = 0.01;
20     a = 0;
21     b = 9;
22     n = 300;
23     h = (b-a)/n;
24     dt = 0.0002;
25     tmax = 0.4;
26     ntime = tmax/dt;
27     nt = 0.001;
28     r0 = 0.005;
29     x0 = b/2;
30     y0 = b/2;
```

```

31     e0 = 0.0005;
32
33     % Initialization
34     p = zeros(n+1);
35     T = zeros(n+1);
36     p_xi = zeros(n+1);
37     p_eta = zeros(n+1);
38     T_xi = zeros(n+1);
39     T_eta = zeros(n+1);
40     p_xi2 = zeros(n+1);
41     p_eta2 = zeros(n+1);
42     T_xi2 = zeros(n+1);
43     T_eta2 = zeros(n+1);
44     epsilon2 = zeros(n+1);
45     a = zeros(n+1);
46     f = zeros(n+1);
47     x = zeros(1,n+1);
48     y = zeros(1,n+1);
49     x_xi = zeros(n+1);
50     y_eta = zeros(n+1);
51     x_xi2 = zeros(n+1);
52     y_eta2 = zeros(n+1);
53     J = zeros(n+1);
54     E = zeros(1,tmax/nt);
55     M = zeros(1,tmax/nt);
56     xi = a:h:b;
57     eta = a:h:b;
58     [XI,ETA] = meshgrid(xi,eta);
59     n1 = 0;
60     t = 0;
61
62     % Transforming coordinates
63     for i=1:n+1
64         x(i) = xi(i) + b*lambda/pi*sin(2*pi*xi(i)/b);
65         y(i) = eta(i) + b*lambda/pi*sin(2*pi*eta(i)/b);
66         for j=1:n+1
67             x_xi(i,j) = 1 + 2*lambda*cos(2*pi*XI(i,j)/b);
68             y_eta(i,j) = 1 + 2*lambda*cos(2*pi*ETA(i,j)/b);
69             x_xi2(i,j) = -4*lambda*pi/b*sin(2*pi*XI(i,j)/b);
70             y_eta2(i,j) = -4*lambda*pi/b*sin(2*pi*ETA(i,j)/b);
71             J(i,j) = x_xi(i,j)*y_eta(i,j);
72         end
73     end
74     [X,Y] = meshgrid(x,y);
75
76     % Initial condition

```

```

77     for i=1:n+1
78         for j=1:n+1
79             p(i,j) = (tanh((r0 - ((x(i)-x0)^2 + (y(j)-y0)^2))/e0)
80                 + 1)/2;
81             T(i,j) = 0;
82         end
83     end
84     % save the data files
85     save_data(sprintf('p and T at t = %.3f.dat',t*dt),X,Y,[],p,T)
86
87     for t=1:ntime
88         energy = 0;
89         for i=1:n+1
90             for j=1:n+1
91                 ip = mod(i,n)+1;
92                 im = mod(i-2,n)+1;
93                 jp = mod(j,n)+1;
94                 jm = mod(j-2,n)+1;
95                 p_xi(i,j) = (p(ip,j) - p(im,j))/(2*h);
96                 p_eta(i,j) = (p(i,jp) - p(i,jm))/(2*h);
97                 p_xi2(i,j) = (p(ip,j) - 2*p(i,j) + p(im,j))/(h^2);
98                 p_eta2(i,j) = (p(i,jp) - 2*p(i,j) + p(i,jm))/(h^2)
99                 ;
100                 T_xi(i,j) = (T(ip,j) - T(im,j))/(2*h);
101                 T_eta(i,j) = (T(i,jp) - T(i,jm))/(2*h);
102                 T_xi2(i,j) = (T(ip,j) - 2*T(i,j) + T(im,j))/(h^2);
103                 T_eta2(i,j) = (T(i,jp) - 2*T(i,j) + T(i,jm))/(h^2)
104                 ;
105                 theta = atan2(p_eta(i,j),p_xi(i,j));
106                 epsilon = eps_bar*(1 + delta*cos(aniso*theta));
107                 epsilon_prime = -eps_bar*delta*aniso*sin(aniso*
108                     theta);
109                 epsilon2(i,j) = epsilon^2;
110                 a(i,j) = epsilon*epsilon_prime;
111                 p1 = p(i,j);
112                 T1 = T(i,j);
113                 m = alpha/pi*atan(gamma*(Te - T1));
114                 f(i,j) = p1*(p1 - 1)*(p1 - 0.5 + m);
115             end
116         end
117     for i=1:n+1
118         for j=1:n+1
119             ip = mod(i,n)+1;
120             im = mod(i-2,n)+1;
121             jp = mod(j,n)+1;

```

```

119         jm = mod(j-2,n)+1;
120         epsilon2_xi = (epsilon2(ip,j) - epsilon2(im,j))
            /(2*h);
121         epsilon2_eta = (epsilon2(i,jp) - epsilon2(i,jm))
            /(2*h);
122         a_xi = (a(ip,j) - a(im,j))/(2*h);
123         a_eta = (a(i,jp) - a(i,jm))/(2*h);
124         term1p = epsilon2(i,j)*(y_eta(i,j)^2*p_xi2(i,j) +
            x_xi(i,j)^2*p_eta2(i,j))/(J(i,j)^2);
125         term2p = (epsilon2_xi^2*(y_eta(i,j)^2)/(J(i,j)^2)
            + a_eta/J(i,j) - epsilon2(i,j)*x_xi2(i,j)*(
            y_eta(i,j)^3)/(J(i,j)^3))*p_xi(i,j);
126         term3p = (epsilon2_eta^2*(x_xi(i,j)^2)/(J(i,j)^2)
            - a_xi/J(i,j) - epsilon2(i,j)*(x_xi(i,j)^3)*
            y_eta2(i,j)/(J(i,j)^3))*p_eta(i,j);
127         term1T = ((y_eta(i,j)^2)*T_xi2(i,j)+(x_xi(i,j)^2)*
            T_eta2(i,j))/(J(i,j)^2);
128         term2T = -x_xi2(i,j)*(y_eta(i,j)^3)*T_xi(i,j)/(J(i
            ,j)^3);
129         term3T = -(x_xi(i,j)^3)*y_eta2(i,j)*T_eta(i,j)/(J(
            i,j)^3);
130         p1 = p(i,j);
131         T1 = T(i,j);
132         p(i,j) = p1 + (term1p + term2p + term3p - f(i,j))*
            dt/tau;
133         T(i,j) = T1 + (term1T + term2T + term3T)*dt + K*(p
            (i,j) - p1);
134     end
135 end
136 if mod(t*dt,0.05)==0
137     % save the data files
138     save_data(sprintf('p and T at t = %.3f.dat',t*dt),X,Y
        ,[],p,T)
139 end
140 end
141
142 function save_data(filename, x, y, z, values1, values2)
143 % Open file for writing
144 fid = fopen(filename, 'w');
145
146 % Tecplot file header
147 fprintf(fid, sprintf('TITLE = "Phase Field and Temperature
        Field"\n'));
148 fprintf(fid, 'VARIABLES = "X", "Y"');
149 if ~isempty(z)
150     fprintf(fid, ', "Z"');

```

```

151     end
152     fprintf(fid, ', "Phase-Field", "Temperature"\n');
153
154     % Get the grid dimensions
155     [nx, ny, nz] = size(values1);
156
157     % Specify zone and dimensions
158     fprintf(fid, 'ZONE T="Zone 1", I=%d, J=%d', nx, ny);
159     if ~isempty(z)
160         fprintf(fid, ', K=%d', nz);
161     end
162     fprintf(fid, ', F=POINT\n');
163
164     % Write the data: x, y, (z if 3D), values1, values2 at each
        point
165     for k = 1:nz
166         for j = 1:ny
167             for i = 1:nx
168                 if isempty(z)
169                     fprintf(fid, '%f %f %f %f\n', x(i, j), y(i, j)
                        , values1(i, j, k), values2(i, j, k));
170                 else
171                     fprintf(fid, '%f %f %f %f %f\n', x(i, j, k), y
                        (i, j, k), z(i, j, k), values1(i, j, k),
                        values2(i, j, k));
172                 end
173             end
174         end
175     end
176
177     % Close the file
178     fclose(fid);
179     end

```

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