

## DOCTORAL THESIS

### Numerical analysis and simulations for phase-field equations

Yang, Jiang

*Date of Award:*  
2014

[Link to publication](#)

#### General rights

Copyright and intellectual property rights for the publications made accessible in HKBU Scholars are retained by the authors and/or other copyright owners. In addition to the restrictions prescribed by the Copyright Ordinance of Hong Kong, all users and readers must also observe the following terms of use:

- Users may download and print one copy of any publication from HKBU Scholars for the purpose of private study or research
- Users cannot further distribute the material or use it for any profit-making activity or commercial gain
- To share publications in HKBU Scholars with others, users are welcome to freely distribute the permanent URL assigned to the publication

# Abstract

Research on interfacial phenomena has a long history, which has attracted tremendous interest in recent years. One of the most successful tools is the phase-field approach. As phase-field models usually involve very complex dynamics and it is nontrivial to obtain analytical solutions, numerical methods have played an important role in various simulations. This thesis is mainly devoted to developing accurate, efficient and robust numerical methods and the related numerical analysis for three representative phase-field models, namely the Allen-Cahn equation, the Cahn-Hilliard equation and the thin film models.

The first part of this thesis is mainly concentrated on the stability analysis for these three models, with particular attention to the Allen-Cahn equation. We have established three stability criterion, i.e., nonlinear energy stability,  $L^\infty$ -stability and  $L^2$ -stability.

As shared by most phase-field models, one of the intrinsic properties of the Allen-Cahn and the Cahn-Hilliard equations is that they satisfy a nonlinear stability relationship, usually expressed as a time-decreasing free energy functional. We have studied several stabilized temporal discretization for both the Allen-Cahn and the Cahn-Hilliard equations so that the relevant nonlinear energy stability can be preserved. The corresponding temporal discretization schemes are linear and are of second-order accuracy. We also apply multi-step implicit-explicit methods to approximate the Allen-Cahn equation. We demonstrate that by suitably choosing the parameters in multi-step implicit-explicit methods the nonlinear energy stability can be preserved.

Apart from studying the energy stability for the Allen-Cahn equation, we also establish the numerical maximum principle for some fully discretized schemes. We further extend our analysis technique to the fractional-in-space Allen-Cahn equation. A more general Allen-Cahn-type equation with a nonlinear degenerate mobility and a logarithmic free energy is also considered.

The third stability under investigation is the  $L^2$ -stability. We prove that the continuum Allen-Cahn equation satisfies a uniform  $L^p$ -stability. Furthermore, we show that both semi-discretized Fourier Galerkin and Fourier collocation methods can inherit this stability for  $p = 2$ , i.e.,  $L^2$ -stability. Based on the established  $L^2$ -stability, we accomplish the spectral convergence estimate for the Fourier Galerkin methods. We adopt the second-order Strang splitting schemes in the temporal direction with Fourier collocation methods to demonstrate the uniform  $L^2$ -stability in the fully discretized scheme.

Another contribution of this thesis is to propose a  $p$ -adaptive spectral deferred correction methods for the long time simulations for all three models. We develop a high-order accurate and energy stable scheme to simulate the phase-field models by combining the semi-implicit spectral deferred correction method and first-order stabilized semi-implicit schemes. It is found that the accuracy improvement may affect the overall energy stability. To compromise the accuracy and stability, a local  $p$ -adaptive strategy is proposed to enhance the accuracy by sacrificing some local energy stability in an acceptable level. Numerical results demonstrate the high effectiveness of our proposed numerical strategy.

**Keywords:** Phase-field models, Allen-Cahn equations, Cahn-Hilliard equations, thin film models, nonlinear energy stability, maximum principle,  $L^2$ -stability, adaptive simulations, stabilized semi-implicit schemes, finite difference, Fourier spectral methods, spectral deferred correction methods, convex splitting.

## Acknowledgements

First I would like to express my deep gratitude to my principal supervisor Prof. Tao Tang. His meticulous attitude in scholarship and modest manner in discussions will benefit me lifetime. He always gives me the maximum freedom in research, which make me enjoy doing research. I would also like to thank my co-supervisor Dr. Zhonghua Qiao and Dr. Leevan Ling for their support and help.

Thanks are due to Prof. Jie Shen for offering me an opportunity to visit Purdue University and for his support and guidance during the visit. Thanks are also due to Prof. Ming-Chih Lai, Dr. Heyu Wang, Dr. Hehu Xie and Dr. Fusheng Luo for their discussions during their visiting to Hong Kong Baptist University. My thanks extends to my collaborators Dr. Xinlong Feng, Dr. Tianliang Hou and Dr. Huailing Song. I am also grateful to Dr. Zhengru Zhang, Dr. Guanghui Hu and Dr. Tao Zhou for their useful advices in research.

I would like to give my special thanks to my fellow students, Mr. Chuan Chen, Miss Liyuan Chen, Mr. Bo Gong, Dr. Hongwei Li, Miss Xinxin Li, Mr. Mutong Qiao, Mr. Chenyang Shen, Mr. Wenyi Tian, Dr. Qiong Wu, Dr. Hongwei Yue and Miss Wei Zhang for their friendship in the three unforgotten years in Hong Kong.

I am grateful to Hong Kong Baptist University and Hong Kong Research Grant Council (via Prof. Tang's grants). I also like to thank secretaries and technicians in the Department of Mathematics for their professional and kind assistances.

Finally, I would like to thank my family for their selfless love and unconditional support accompanying these years, which is the essential motivation of what I achieve today.

# Table of Contents

<b>Declaration</b>	<b>i</b>
<b>Abstract</b>	<b>ii</b>
<b>Acknowledgements</b>	<b>iv</b>
<b>Table of Contents</b>	<b>v</b>
<b>List of Tables</b>	<b>ix</b>
<b>List of Figures</b>	<b>x</b>
<b>Chapter 1 Introduction</b>	<b>1</b>
1.1 Phase-field models . . . . .	1
1.2 Allen-Cahn equations . . . . .	2
1.3 Cahn-Hilliard equations . . . . .	4
1.4 Thin film models . . . . .	6
1.5 Numerical schemes and challenges . . . . .	8
1.5.1 Some existing numerical schemes . . . . .	8
1.5.2 Numerical challenges . . . . .	10
<b>Chapter 2 Nonlinear energy stability for temporal discretizations</b>	<b>12</b>
2.1 Introduction . . . . .	12
2.2 Stabilized Crank-Nicolson/ Adams-Bashforth schemes . . . . .	14
2.2.1 Stabilized schemes for the Allen-Cahn equation . . . . .	15
2.2.2 Stabilized schemes for the Cahn-Hilliard equation . . . . .	19
2.2.3 Numerical tests for convergence rate . . . . .	22
2.3 Multi-step implicit-explicit Methods for the Allen-Cahn equation . . . . .	25

2.3.1	General linear multi-step implicit-explicit schemes . . . . .	26
2.3.2	First-order IMEX schemes . . . . .	29
2.3.3	Second-order IMEX schemes . . . . .	30
2.3.4	Numerical experiments . . . . .	32
2.4	Concluding remarks . . . . .	37
<b>Chapter 3 Maximum principle for the Allen-Cahn-type equations</b>		<b>38</b>
3.1	Preliminaries . . . . .	38
3.2	Discrete maximum principle for the Allen-Cahn equation . . . . .	44
3.2.1	Discrete maximum principle and discrete energy stability . . .	45
3.2.2	Stabilized semi-implicit schemes . . . . .	47
3.2.3	Error analysis . . . . .	48
3.2.4	Numerical tests . . . . .	49
3.3	Discrete maximum principle for the generalized Allen-Cahn equation	52
3.3.1	The semi-discrete semi-implicit scheme . . . . .	53
3.3.2	The fully discrete semi-implicit scheme . . . . .	55
3.3.3	Logarithmic free energy with nonlinear degenerate mobility . .	58
3.3.4	Error analysis . . . . .	61
3.3.5	Numerical tests . . . . .	64
3.4	Discrete maximum principle for the fractional-in-space Allen-Cahn equa- tion . . . . .	71
3.4.1	Introduction . . . . .	71
3.4.2	The discrete maximum principle . . . . .	73
3.4.3	The discrete energy stability . . . . .	75
3.4.4	Numerical examples . . . . .	77
3.5	Concluding remarks . . . . .	80
<b>Chapter 4 <math>L^2</math>-stability of spectral methods for the Allen-Cahn equation</b>		<b>83</b>
4.1	Introduction . . . . .	83

4.2	$L^p$ -stability for continuum equations . . . . .	84
4.3	Fourier-Galerkin methods and $L^2$ -stability . . . . .	87
4.3.1	Stability analysis . . . . .	87
4.3.2	Spectral convergence rate . . . . .	90
4.3.3	A numerical example . . . . .	93
4.4	Fourier-Collocation methods and $L^2$ -stability . . . . .	94
4.4.1	Semi-discrete equations and $L^2$ -stability . . . . .	94
4.4.2	Operator splitting methods . . . . .	96
4.4.3	Fully discretized schemes using second-order splitting . . . . .	98
4.4.4	Numerical tests . . . . .	100
4.5	Concluding remarks . . . . .	104
<b>Chapter 5 Long time simulations with <math>p</math>-adaptivity</b>		<b>105</b>
5.1	Introduction . . . . .	105
5.2	Energy stability . . . . .	109
5.2.1	Allen-Cahn equations . . . . .	110
5.2.2	Cahn-Hilliard equations . . . . .	112
5.2.3	Thin film models . . . . .	113
5.3	SDC schemes and Semi-implicit SDC schemes . . . . .	115
5.3.1	SDC methods based on Euler methods . . . . .	116
5.3.2	Semi-implicit SDC Methods . . . . .	118
5.4	Spatial discretization and a fast solver . . . . .	119
5.5	Efficiency enhancement with $p$ -adaptivity . . . . .	121
5.6	Numerical experiments . . . . .	124
5.6.1	Convergence tests . . . . .	124
5.6.2	SDC allows large time step . . . . .	124
5.6.3	Long time simulations . . . . .	127
5.7	Concluding remarks . . . . .	134

<b>Chapter 6 Summary and future work</b>	<b>136</b>
6.1 Summary of the thesis . . . . .	136
6.2 Future research . . . . .	137
<b>Bibliography</b>	<b>139</b>
<b>Curriculum Vitae</b>	<b>149</b>