RGC Ref.: N_HKBU204/12 NSFC Ref.: 11261160486
(please insert ref. above)

The Research Grants Council of Hong Kong
NSFC/RGC Joint Research Scheme
Joint Completion Report

(Please attach a copy of the completion report submitted to the NSFC by the Mainland researcher)

Part A: The Project and Investigator(s)

1. Project Title

Mathematical Modeling and High Performance Computing of Complex Fluids

2. Investigator(s) and Academic Department/Units Involved

	Hong Kong Team	Mainland Team
Name of Principal Investigator *(with title)*	Prof. TANG Tao	Prof. YUAN Li
Post	Honorary Chair Professor	Professor
Unit / Department / Institution	Department of Mathematics, Hong Kong Baptist University	Institute of Computational Mathematics and Scientific/Engineering Computing, Chinese Academy of Sciences
Contact Information	ttang@lsec.cc.ac.cn	lyuan@lsec.cc.ac.cn
Co-investigator(s) *(with title and institution)*	Zhonghua Qiao (Associate Professor) Department of Applied Mathematics, The Hong Kong Polytechnic University	Hui Zhang (Professor) School of Mathematical Sciences, Beijing Normal University

3. Project Duration

	Original	Revised	Date of RGC/ Institution Approval *(must be quoted)*
Project Start date	1-1-2013		
Project Completion date	31-12-2016		
Duration *(in month)*	48		

Deadline for Submission of Completion Report	31-12-2017		

Part B: The Completion Report

5. Project Objectives

5.1 Objectives as per original application

1. Further explore the energy law and other conservative properties of the existing phase transition models, liquid crystal models and two-phase flow models.
2. Develop new mathematical models that describe complicated phase separation and fluids dynamics, based on the density functional theory.

3. Investigate efficient numerical schemes which can preserve the discrete energy law and other conservative properties of the existing and newly developed phase field type models. In particular, we will study the so-called gradient-stable schemes which have been shown very useful for large time simulations.

4. Develop adaptive time-stepping algorithms which can resolve not only the steady state but also the dynamics of several physical models. The adaptive time-stepping strategy may provide useful tools for large time simulations aiming at reliable statistical data collection.

5.2 Revised Objectives

Date of approval from the RGC: ____________________

Reasons for the change: ____

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1.
2.
3. ....

6. Research Outcome

Major findings and research outcome
(maximum 1 page; please make reference to Part C where necessary)

On the modeling side, we obtain many kinds of micro-structures by virtue of the mean self-consistent field theory. We present not only the micro-structures which are consistent with the experiments, but also some new micro-structures which are not found by the experiments. For the dynamic mechanics of the MMC hydrogel, we can set up the phase transition model (named as MMC-TDGL model) by using the gradient flow approach based on the new free energy through the Boltzmann entropy theorem and the lattice theory.

On the numerical side, this project develops high stability and accurate numerical methods for phase transition models, liquid crystal models and two-phase flow models. The main difficulty for developing a numerical method for phase field equations is a severe stability restriction on the time step due to nonlinearity and high order differential terms. It is known that the phase field models satisfy a nonlinear stability relationship called gradient stability, usually expressed as a time-decreasing free-energy functional. This property has been used recently to derive numerical schemes that inherit the gradient stability. Part of this project studies the implicit-explicit time discretizations which satisfy the energy stability. The second part is to discuss time-adaptive strategies for solving the phase-field problems, which is motivated by the observation that the energy functionals decay with time smoothly except at a few critical time levels. The classical operator-splitting method is a useful tool in time discretization. In the final part, we have provided some preliminary results using operator-splitting approach.

Potential for further development of the research and the proposed course of action
(maximum half a page)

For the mathematical models and numerical methods to the complex fluids, several good approaches for the modeling and schemes have been developed in this project. However, more systemetic analysis, in particular well-posedness and convergence analysis, is required.

These deep theoretical analyses are challenging, as existing tools seem not working for these newly developed models and schemes. Some preliminary efforts have been made recently, and it is expected some more relevant results can be obtained.

7. The Layman's Summary

(describe <u>in layman's language</u> the nature, significance and value of the research project, in no more than 200 words)

This project is focused on modeling and computation of complex fluids with applications in multi-phase fluids and biomaterials. It aims at the development and analysis of mathematical models and the cutting-edge simulation tools, which will help us to better understand the properties of the complex fluids. The key issues will include development of multiscale modeling and computations, simulation of flows of the complex fluids in complex geometries, high performance computing and parallel computing for complex systems. There have been considerable recent interests in developing highly stable and efficient numerical schemes for solving phase-field models. In this project, we studied three classes of effective time discretization schemes. The efficiency and theoretical analysis of these methods have been extensively investigated.

<u>Part C: Research Output</u>

8. Peer-reviewed journal publication(s) arising <u>directly</u> from this research project

(Please attach a copy of each publication and/or the letter of acceptance if not yet submitted in the previous progress report(s). All listed publications must acknowledge RGC's funding support by quoting the specific grant reference.)

The Latest Status of Publications				Author(s) (***bold** the authors belonging to the project teams and denote the corresponding author with an asterisk**)	Title and Journal/ Book *(with the volume, pages and other necessary publishing details specified)*	Submitted to RGC *(indicate the year ending of the relevant progress report)*	Attached to this report *(Yes or No)*	Acknowledged the support of this Joint Research Scheme *(Yes or No)*	Accessible from the institutional repository *(Yes or No)*
Year of publication	Year of Acceptance *(For paper accepted but not yet published)*	Under Review	Under Preparation *(optional)*						
2015				Yuanzhen Cheng, Alexandar Kurganov*, Zhuolin Qu and **Tao Tang**	Fast and stable explicit operator splitting methods for phase-field models, J. Comput. Phys. 303 (2015), 45-65.		Yes	Yes	No

2015				**Zhonghua Qiao**, **Tao Tang** and Hehu Xie	Error analysis of a mixed finite element method for the molecular beam epitaxy model, SIAM J. Numer. Anal. 53 (2015), 184-205.		Yes	Yes	No
2015				Xinlong Feng, **Tao Tang** and Jiang Yang	Long time numerical simulations for phase-field problems using p-adaptive spectral deferred correction methods, SIAM J. Sci. Comput. 37 (2015), A271-A294.		Yes	Yes	No
2017				Dong Li, **Zhonghua Qiao*** and **Tao Tang**	Gradient bounds for a thin film epitaxy equation, Journal of Differential Equations, 262 (2017), 1720-1746.		Yes	Yes	No

2016				Dong Li, **Zhonghua Qiao** and **Tao Tang**	Characterizing the stabilization size for semi-implicit Fourier-spectral method to phase field equations, SIAM Journal on Numerical Analysis, 54 (2016), 1653-1681.		Yes	Yes	No
2016				**Hui Zhang**	Strain-stress relation in macromolecular microsphere composite hydrogel, Applied Mathematics and Mechanics, 37 (2016), 1539.		Yes	Yes	No
2015				Qiao Tang and **Hui Zhang**	Nonlinear continuum theory of smectic-C liquid crystals, Commun. Math. Sci., 13 (2015)1787-1891.		Yes	Yes	No

2015				Rui Chen, Guanghua Ji, Xiaofeng Yang and **Hui Zhang***	Decoupled energy stable schemes for phase-field vesicle membrane model, Journal of Computational Physics, 302 (2015), 509-523.		Yes	Yes	No
2015				Xiao Li, Guanghua Ji and **Hui Zhang***	Phase transitions of macromolecular microsphere composite hydrogels based on the stochastic Cahn-Hilliard equation, Journal of Computational Physics, 283 (2015), 81-97.		Yes	Yes	No

2016				Xiao Li, **Zhonghua Qiao*** and **Hui Zhang**	An unconditionally energy stable finite difference scheme for a stochastic Cahn-Hilliard equation, Science China Mathematics, 59 (2016), 1815-1834.		Yes	Yes	No

9. Recognized international conference(s) in which paper(s) related to this research project was/were delivered *(Please attach a copy of each delivered paper. All listed papers must acknowledge RGC's funding support by quoting the specific grant reference.)*

Month/Year/ Place	Title	Conference Name	Submitted to RGC *(indicate the year ending of the relevant progress report)*	Attached to this report *(Yes or No)*	Acknowledged the support of this Joint Research Scheme *(Yes or No)*	Accessible from the institutional repository *(Yes or No)*
April/2014 /Bethesda, MD	Hermite spectral methods and discrete least square projection with random evaluations	Modern Perspective s in Applied Mathematics: Theory and Numerics of PDEs		Yes	Yes	No
May/2015/Suwon, Korea	Stablized and Adaptive Time-Stepping Methods for Phase-Field Models	KSIAM 2015 Spring Conference		Yes	Yes	No
May/2015/ Wuhan, China	Hermite Spectral Method and its Applications	International Conference on Numerical Partial Differential Equations and Their Applications		Yes	Yes	No

10. Student(s) trained *(Please attach a copy of the title page of the thesis.)*

Name	Degree registered for	Date of registration	Date of thesis submission/ graduation
Jiang Yang	Doctor of Philosophy	2011-07-01	2014-07-31
Bo Gong	Doctor of Philosophy	2013-09-01	2017-08-31

11. Other impact *(e.g. award of patents or prizes, collaboration with other research institutions, technology transfer, etc.)*

N/A