

Adaptive algorithms for phase field models of some interface problems

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We present our on-going works with current and former colleagues at Penn State (L.Q. Chen, W.M. Feng, S. Hu, Z.K. Liu, P. Yu, X. Wang and J. Zhang) on the numerical algorithms for the phase field simulations of some interface problems, ranging from microstructure evolution in multicomponent alloy to multicomponent lipid vesicles. We discuss recent development of highly adaptive computational algorithms for large scale phase field simulations.

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1 Adaptive methods for phase field models

Phase field method has been extensively applied to many physical and biological processes such as the modeling microstructure evolution for various materials processes including solidification, solid state phase transformations, grain or phase coarsening, and the modeling of vesicle membrane deformation and interaction with external fields. It is an attractive and popular approach since the evolution of different microstructural features can be predicted by means of a single set of equations, and there are no explicit boundary conditions defined at interfaces. However, full three-dimensional computer simulations using the phase field method are still computationally challenging in both memory and computational time. Adaptive methods have been used in many phase field simulations, see, for example, [3, 18, 19, 21]. In this talk, we present recent works on both adaptive finite element element and adaptive Fourier spectral methods

2 Adaptive finite element methods

Vesicle membranes, formed by bilayers of lipid molecules, are simple forms of biological membranes which exist everywhere in life, and compartmentalize living matter into cells and sub-cellular structures and are essential for many biological functions. The equilibrium shapes of bilayer vesicle membranes have been successfully modeled via the minimization of certain shape energy. Phase field formulations of the bending elasticity model has been developed recently [10]. More studies on such a model and its various generalizations, analysis and simulations can be found in [5, 6, 7, 8, 9, 11, 12, 13, 15]. In [14], a three dimensional adaptive finite element method is developed for the resulting variational phase field bending elasticity model of vesicle membrane deformations. The adaptivity is implemented through a local mesh refinement and coarsening strategy for isotropic finite elements based on a posteriori error estimators [1, 20]. In the adaptive method studied in [14], a mixed finite element method (FEM) is used to discretize the associated nonlinear system of equations of the phase field bending elasticity model. The convergence and a priori error estimate have been given in [13, 15]. A residual type *a posteriori* error estimate is derived in [14] which is then used in a marking strategy to guide the local mesh refinement and coarsening. Effectively, the nodes of the adaptive mesh are concentrated near the interface (the membrane surface) so that the number of nodes is significantly reduced, comparing with the number of nodes in the uniform mesh cases, while the high level resolution gets maintained in the adaptive FEM solution. The resulting mesh adaptivity significantly improves the efficiency of the phase field simulation of vesicle membranes and enhances its capability in handling complex shape and topological changes. The effectiveness of the adaptive method is further demonstrated through numerical examples.

3 Adaptive Fourier spectral methods

In recent years, Fourier spectral methods have emerged as competitive numerical methods for large-scale phase field simulations of microstructures in computational materials sciences [2]. While the Fourier spectral approximation offers much faster computational speed and high resolution for many problems where the phase field methods have been applied to, with conventional implementation, they suffer from limitations of working with problems defined on a regular geometry and with rigid Cartesian grid structure. For nucleation of new phase particles [23] and microstructures involving both dislocations and precipitates, local mesh refinement and grid adaptation in space are not only highly desirable but necessary, in order to provide more accurate resolution of the interface. In this regard, novel and adaptive techniques for spatial spectral approximations are of great interest.

We recently developed a new adaptive Fourier-spectral semi-implicit method (AFSIM) for solving the phase field equation by combining an adaptive moving mesh method and the semi-implicit Fourier spectral algorithm. A major progress has

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been made in making grid points spatially adaptive in the physical domain via a moving mesh strategy, while maintaining a uniform grid in the computational domain for the spectral implementation. By introducing a suitable mapping between the physical domain and the computational domain, more mesh points become clustered in regions near the actual microstructure interfaces, yielding better resolution and less computational cost. A particular novelty in the new algorithm is the use of spatially varying physical domains [22].

In this talk, we present the application of AFSIM to the Allen-Cahn equation [16] and the Cahn-Hilliard equation with inhomogeneous, anisotropic elasticity [17]. Numerical implementations and test examples in both two and three dimensions are considered with a particular illustration using the well-studied example of mis-fitting particles in a solid as they approach to their equilibrium shapes. It is shown that significant savings in memory and computational time is achieved while accurate solutions are preserved.

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References

- [1] I. Babuska and T. Strouboulis, *The Finite Element Method and Its Reliability*, Oxford University Press, London, (2001).
- [2] L.Q. Chen and J. Shen, Applications of semi-implicit Fourier-spectral method to phase field equations, *Computer Physics Communications*, **108**, 147-158 (1998).
- [3] Z. Chen, R. Nochetto and A. Schmidt, *Error control and adaptivity for a phase relaxation model*, *M2AN*, **34**, 775-797 (2000).
- [4] Q. Du, M. Gunzburger and J. Peterson, *Analysis and Approximation of the Ginzburg-Landau Model of Superconductivity*, *SIAM Review*, **34**, 54-81 (1992).
- [5] Q. Du, M. Li and C. Liu, *Analysis of a Phase Field Navier-Stokes Vesicle-Fluid Interaction Model*, *Disc. Cont. Dyn. Sys. B*, **8**, 539-556 (2007).
- [6] Q. Du, C. Liu, R. Ryham and X. Wang, *Modeling vesicle deformations in flow fields via energetic variational approaches*, (2006).
- [7] Q. Du, C. Liu, R. Ryham and X. Wang, *A phase field formulation of the Willmore problem*, *Nonlinearity*, **18**, 1249-1267 (2005).
- [8] Q. Du, C. Liu, R. Ryham and X. Wang, *Modeling the spontaneous curvature effects in static cell membrane deformations by a phase field formulation*, *Comm Pure Appl Anal*, **4**, 537-548 (2005).
- [9] Q. Du, C. Liu, R. Ryham and X. Wang, *Diffuse Interface Energies Capturing the Euler Number: Relaxation and Renormalization*, *Comm. Math. Sci*, **5**, 233-242 (2007).
- [10] Q. Du, C. Liu and X. Wang, *A phase field approach in the numerical study of the elastic bending energy for vesical membranes*, *J. Computational Physics*, **198**, 450-468 (2004).
- [11] Q. Du, C. Liu and X. Wang, *Simulating the deformation of Vesicle Membranes under Elastic Bending Energy in Three Dimensions*, *J. Computational Physics*, **212**, 757-777 (2005).
- [12] Q. Du, C. Liu and X. Wang, *Retrieving Topological Information for Phase Field Models*, *SIAM J. Appl. Math*, **65**, 1913-1932 (2005).
- [13] Q. Du and X. Wang, *Convergence of numerical approximations to a phase field bending elasticity model of membrane deformations*, *Inter J. Numer. Anal. Modeling*, **4**, 441-459 (2006).
- [14] Q. DU AND J. ZHANG, *Adaptive Finite Element Method for a Phase Field Bending Elasticity Model of Vesicle Membrane Deformations*, submitted to *SIAM J. Sci. Comp.*, (2006).
- [15] Q. Du and L. Zhu, *Analysis of a Mixed Finite Element Method for a Phase Field Elastic Bending Energy Model of Vesicle Membrane Deformation*, *J. Comp. Math.*, **24**, 265-280 (2006).
- [16] W.M. Feng, P. Yu, S.Y. Hu, Z.K. Liu, Q. Du and L.Q. Chen, *Spectral Implementation of An Adaptive Moving Mesh Method for Phase-field Equations*, **220**, 498-510 (2006).
- [17] W.M. Feng, P. Yu, S.Y. Hu, Z.K. Liu, Q. Du and L.Q. Che, *A Fourier Spectral Moving Mesh Method for the Cahn-Hilliard Equation with Elasticity*, submitted to *Comm. Comp. Phys.*, (2007).
- [18] J. A. Mackenzie and M. L. Robertson, *A moving mesh method for the solution of the one-dimensional phase-field equations*, *J. Computational Physics*, **181**, 526-544 (2002).
- [19] N. Provatas, N. Goldenfeld and J. Dantzig, *Efficient Computation of Dendritic Microstructures Using Adaptive Mesh Refinement*, *Phys. Rev. Lett.*, **80**, 3308-3311 (1998).
- [20] R. Verfurth, *A review of a posteriori error estimation and adaptive mesh-refinement techniques*, Wiley, Chichester, (1996).
- [21] S.M. Wise, J.S. Lowengrub, J.S. Kim and W.C. Johnson, *Efficient phase-field simulation of quantum dot formation in a strained heteroepitaxial film*, *Superlattices and Microstructures*, **36**, 293-304 (2004).
- [22] P. Yu, L. Chen and Q. Du, *Applications of Moving Mesh Methods to the Fourier Spectral Approximations of Phase-Field Equations*, in *Recent Advances in Computational Sciences: Selected Papers from the International Workshop on Computational Sciences and Its Education*, edited by Jorgensen et. al., World Scientific, (2007).
- [23] L. Zhang, L.-Q. Chen and Q. Du, *Morphology of critical nuclei in solid state phase transformations*, *Physical Review Letters*, **98**, 265703 (2007).