Retrieving topological information from the phase-field description of geometric evolution

Qiang Du*

Department of Mathematics, Pennsylvania State University, University Park, PA 16802, USA.

Phase field and diffuse interface are popular methods for the modeling and simulations of evolving interfaces. They do not track the interface explicitly, and are insensitive to topological events. In some areas of applications, detecting and controlling topological change may be important. In this talk, we discuss some recent works with current and former colleagues at Penn State (C. Liu, R. Ryham, and X. Wang) on the development of effective formula for retrieving topological information within the phase field framework.

1 Phase Field/Diffuse Interface Methods

In the multi–scale modeling and simulation of multi-component alloys, large scale numerical simulation of the micro-structures in the material plays an important step [6]. Phase field methods employ diffusive interface representations of the micro-structures. In contrast to the sharp interface approach, they are very effective in handling complex evolutions in the morphology and are insensitive to topological events. While working on the integration of the phase field modelling with other simulation tools ranging from first principle calculations, phase diagram computation and the computation of micro-mechanical effect, it becomes important to be able to efficiently collect useful statistics on the underlying microstructure such as particle numbers, average grain sizes, etc, from the computed data or images.

In [2], we studied the phase field model but from a different, and perhaps also very novel, point of view. We were motivated by the fact that in many engineering and biological applications, topological information can be part of the very interesting and useful statistics. Though the insensitivity to the appearance of topological event is regarded as an advantage of the phase field simulation, it becomes very fascinating to see if such events can in fact be effectively detected and possibly even controlled. This has many obvious applications such as collecting statistics during the microstructure evolution. In the modeling of blood cells in vascular systems and in the design of bilayer liposome as drug delivery vehicles, topological information of the vesicle membranes are also of critical value. Thus, how to detect and control the topological change of the interface in the phase field modeling and numerical simulation becomes an important issue. Partly due to the nature of the phase field method (and all other level set methods) in their standard formulation, there is no mechanism preventing the topological change of the membranes or other interfaces. In fact, some of the topological changes are due purely to the formulations, instead of the underlined physics. To our knowledge, there has not been any discussion in the literature on how to recover relevant topological information from the phase field simulations, nor to address further control mechanisms.

2 Retrieving topological information

As the phase field model is based on the diffuse interface approximation of the surface curvature, it becomes then natural for us to employ the Gauss-Bonnet formula, so that useful topological information, in particular, the Euler-Poincare index, can be determined through the computation of the Gaussian curvature. This in turn leads to statistics of practical interests.

Briefly, let a phase function $\phi = \phi(x)$ be defined on the physical (computational) domain Ω. ϕ is used to label the inside and the outside of the vesicle Γ. We visualize that the level set $\{x : \phi(x) = 0\}$ gives the interface of interests, while $\{x : \phi(x) > 0\}$ represents the interior of the interface and $\{x : \phi(x) \leq 0\}$ the outside. In a typical phase field formulation, we may assume that ϕ is nearly ± 1 except in a small transition layer around the interface, typically with thickness characterized by a parameter ϵ [1]. Given such a phase field function ϕ, we define the 3×3 matrix

$$M_{ij}(\phi) = \frac{1}{2\sqrt{\pi(a-b)|\nabla\phi|}}(\nabla^2\phi - \frac{\nabla|\nabla\phi|^2 \cdot \nabla\phi}{2|\nabla\phi|^4}\nabla_i\phi\nabla_j\phi) \ , \tag{1}$$

where the constant parameters maybe properly chosen. Let F denote the coefficient of the linear term of the characteristic polynomial of $M = (M_{ij})$, i.e. $F(M) = M_{11}M_{22} + M_{11}M_{33} + M_{22}M_{33} - M_{12}^2 - M_{13}^2 - M_{23}^2$. The Euler number can then be calculated by

$$\frac{\chi}{2} \sim \int_{b\leq\phi(x)\leq a} F(x)\, dx \ . \tag{2}$$

* Corresponding author: e-mail: qdu@math.psu.edu, Phone: +1 814 865 3674, http://www.math.psu.edu/qdu

A particular choice of a and b is given by $a = 0.5$ and $b = -0.5$.

In [2], simplifications have also been considered, based on the asymptotic profiles of the phase function ϕ which minimized the bending elastic energy. For instance, the modified matrix with entries

$$\tilde{M}_{ij}(\phi) = \sqrt{\frac{35\epsilon}{64\sqrt{2}\pi}} \left((1-\phi^2)\nabla^2\phi + 2\phi\nabla_i\phi\nabla_j\phi\right) \ , \tag{3}$$

can be used to give the Euler number [2]:

Theorem 2.1 *The Euler number χ of the zero level set of ϕ satisfies:*

$$\frac{\chi}{2} \ = \int_\Omega F(\tilde{M}(x))\, dx \ + o(1) \ , \quad as \quad \epsilon \to 0 \tag{4}$$

for the $\tilde{M}$ and F given above. In the 2d case, it simplifies to

$$\chi = \lim_{\epsilon\to 0} \frac{1}{4\pi} \int_\Omega \left(-\triangle\phi + \frac{1}{\varepsilon^2}(\phi^2-1)\phi \right) \ dx \ + o(1) \ , \quad as \quad \epsilon \to 0 \ . \tag{5}$$

Applications of these formulae as well as the generalized interpretation for the phase field representation of singular and self-intersecting surfaces can be found in [2, 3]

3 Regularization and Normalization

In [4], a set of new interfacial energies was introduced for the approximation of the Euler number of level surfaces in the phase field (diffuse-interface) representation. These new formulae have simpler forms than those studied earlier in [2] and do not contain higher order derivatives of the phase field function. For example, functionals of the following form can be used:

$$\frac{\chi_\epsilon(\phi)}{2} = -\frac{1}{4\pi c_0 \epsilon} \int_\Omega \left(\Delta\phi - \frac{1}{\epsilon^2} W'(\phi) \right) p(\phi)\, dx. \tag{6}$$

For simplicity, we may take W as the double welled potential, $W(t) = (t^2-1)^2/4$, but more general W may also be applicable. the weight function p of the form $p(t) = d((1-t^2)^n)/dt = -2n(1-t^2)^{n-1}t$ for $n \geq 1$. Let $P(t) = (1-t^2)^n$ so that $p(t) = dP(t)/dt$. The constant $c_0 = 2\int_{-\infty}^{\infty} P(q(s))\, ds$. The new formulae are particularly accurate for phase field functions of the form $\phi(x) = q(d(x)/\epsilon)$ where q is a typical tanh profile, that is $q(t) = \tanh(t/\sqrt{2})$. $d = d(x)$ is the distance function to the interface. Theoretical justifications are provided via formal asymptotic analysis, and practical validations are performed through numerical experiments. To minimize the errors encountered when the phase field variables deviates away from the ideal tanh profile, relaxation and renormalization schemes are also developed to improve the robustness of the new energy functionals.

Acknowledgements The works reported here were carried out jointly with Chun Liu of Pennsylvania State University, Xiaoqiang Wang of Florida State University, and Rolf Ryham of Rice University. The research was partially supported by NSF-DMS 0712744 and NSF-DMR (ITR) 0205232. The speaker would like to thank Xiaobing Feng (University of Tennessee, USA) and Andreas Prohl (Eberhard Karls Universitat Tubingen, Germany) for their kind invitation to the stimulating minisymposium on the *Applications and numerical approximations of geometric partial differential equations*.

References

[1] Q. Du, C. Liu and X. Wang, *A Phase Field Approach in the Numerical Study of the Elastic Bending Energy for Vesicle Membranes*, J. Comp. Phy., **198**, 450-468 (2004).

[2] Q. Du, C. Liu and X. Wang, *Retrieving topological information for phase field models*, SIAM J Appl Math, **65**,1913-1932 (2005).

[3] Q. Du, C. Liu and X. Wang, *Simulating the Deformation of Vesicle Membranes under Elastic Bending Energy in Three Dimensions*, J. Comp. Phys., **212**, 757-777 (2005).

[4] Q. Du, C. Liu, R. Ryham and X. Wang, *Diffuse Interface Energies Capturing the Euler Number: Relaxation and Renomalization*, Comm. Math. Sci, **5**, 233-242, (2007).

[5] P. Yu, S. Hu, Q. Du and L.-Q. Chen, *An Iterative-Perturbation Scheme for Treating Inhomogeneous Elasticity in Phase-Field Models*, J. Comput. Phys., **208**, 34-50 (2005)

[6] Z. Liu, L. Chen, P. Raghavan, Q. Du, J. Sofo, S. Langer and C. Wolverton, *An integrated Framework for multi-scale materials simulation and design*, J. Computer Aided Material Design, **11**, 183-199 (2004).