The Heterogeneous Multi-Scale Method for Interface Dynamics

Li-Tien Cheng *
Weinan E †

December 14, 2002

Dedicated with admiration and gratitude to Stan Osher on the occasion of his 60th birthday.

Abstract

We apply the framework of the heterogeneous multi-scale method (HMM) to develop numerical methods for the study of macroscale interfacial motion in situations where the dynamics of the system are only specified at the microscopic level. The level set method is employed on the macroscopic level to capture the evolution of the desired interface while the nature of that evolution is determined on the microscopic level. Applications to interfaces and front propagation in strongly heterogeneous media are presented.

1 Introduction

The heterogeneous multi-scale method (HMM) developed in [8] provides a general framework for designing numerical methods for problems with multiple scales. In cases when the macroscale model is not explicitly given and has to be inferred from a given microscale model, it provides a simple and efficient methodology for capturing the macroscale behavior of the system without having to resolve all details on the microscopic level. Preliminary results on several classes of problems have demonstrated the potential of HMM [1, 9, 14, 27].

Suppose we have selected a correct set of macroscale variables, denoted by U, for which there should in principle exist a closed model describing

*Deparment of Mathematics, University of California San Diego, La Jolla, California 92093

†Department of Mathematics and PACM, Princeton University, Princeton, NJ 08544

its dynamics or equilibrium properties. For the sake of concreteness, let us assume the macroscale model is of the form

$$U_t = F(U, \nabla U, \nabla^2 U, \ldots), \tag{1}$$

or comes from a minimization problem

$$\min_U F(U, \nabla U, \nabla^2 U, \ldots). \tag{2}$$

Suppose the specific form of F is not completely known, however, we do have at our disposal a model for the microscale behavior of the system in terms of the microscale state variable u. The philosophy of HMM is to proceed as if the macroscale model is known and solve (1) or (2) using a standard macroscale numerical method where, in the implementation, unknown quantities are measured through numerical experiments on the microscale model. Compared with the traditional approach in which the explicit form of F is assumed to be given through constitutive relations with parameters measured by physical experiments, the key idea in HMM is the replacement of these physical experiments by numerical ones. The advantage is that it is no longer necessary to specify a particular form of the constitutive relation. Furthermore, feasibility and efficiency arise out of the separation of the macroscopic and microscopic scales of the system.

HMM thus has the potential to be useful in a very large class of multiscale problems. However, it also takes into account the unique characteristics of each specific application. For each of these applications, there are non-trivial issues that need to be effectively dealt with. This mirrors the issues found in physical experiments where questions on how to set up the experiment and how to process the experimental data in order to extract the quantities of interest are of concern. There are also choices to be made in selecting a good macroscale solver as some fit better in the HMM framework than others.

In this paper, we apply the HMM philosophy to the study of interface motion in a multi-scale setting. Our main interest is to capture the dynamics of the interface at the macroscopic level in the case where the velocity is not explicitly specified by the geometry of the macroscale interface. Instead, available to us is a microscale model to help determine those dynamics. Some examples of such microscale models include:

1. Microscale interface dynamics with normal interfacial velocity of the form
$$v_n(x) = c^\epsilon(x, \gamma) = c\left(x, \frac{x}{\epsilon}, \gamma\right). \tag{3}$$

Here $\epsilon \ll 1$ is the ratio between the microscale and macroscale and γ denotes the microscale interface. Note the dependence of c on γ may result in curvature effects. Such models arise in the study of interface propagation in strongly heterogeneous media such as composite materials, polycrystals, materials with impurities, and porous media, to name a few.

The problem is a homogenization problem. In this subject, there exists interesting research in the direction of deriving the homogenized equation for the dynamics of the macroscale interface (see [6, 7, 26]). These equations are usually not explicit in form since they involve solutions to "cell problems". They are also restricted in applications to situations where the microstructure is periodic. Hence this approach has limited value as a numerical tool, however, it does give hints as to the form of the macroscale model.

2. Front propagation in phase-field models. Consider, for example, the Allen-Cahn equation

$$u_t = \epsilon \Delta u + \frac{1}{\epsilon} u(1 - u^2). \tag{4}$$

It is well-known [19] that for small ϵ, (4) describes the propagation of a front whose inward normal velocity is the mean curvature of the front. In this case, an equation for mean curvature flow can be solved in place of (4) to capture the large scale dynamics of the front. Indeed, this has been done in many different ways (see, e.g., [17]).

However, if the phase field model takes a more complex form or if non-trivial chemical reactions occur at the front, deriving analytically the effective dynamic laws for the front becomes a difficult task. In this direction, we mention the related work of R. Klein et al. [13].

3. Discrete microscale models such as kinetic Monte Carlo or molecular dynamics. Examples include the dynamics of step edges on the surface of an epitaxially grown crystal and grain boundaries in solids, to name a few. Treatment of this case will be postponed to a later work.

2 The Level Set Method as Macroscopic Solver

We now look at the construction of HMM for our interface problems of interest. The HMM framework consists of two or possibly more components,

depending on the number of scales in the problem. At the macroscopic level, a solver is needed to move the interface once the correct velocity for the motion is determined. This velocity is calculated at the microscopic levels through numerical experiments using the microscale models. Conventional methods for interface dynamics in the frameworks of the level set method [17], front tracking [10], or the segment projection method [22, 23] can be used to produce the macroscale solver. In this work, we use the level set method in this capacity.

In the framework of the level set method, an interface is described as the zero level set of a globally defined function Φ, called the level set function. All operations, in particular evolution, are then performed on this function in place of the interface of interest. For example, motion of the interface in a globally defined velocity field translates to a transport PDE on the level set function. The advantages of working on the level set function instead of directly on the interface of interest are in the opportunity to use fixed, uniform grids for both computations and resolution and the ability to automatically handle topological changes. This has allowed the level set method to be successfully applied to numerous interface problems in both two and three dimensions.

The PDE for evolution of an interface described by the level set function Φ in a globally defined velocity field v takes the form

$$\Phi_t + v \cdot \nabla \Phi = 0.$$

Since the normal vectors to the interface, and in fact to any of the level sets of Φ, can be written as $\pm \nabla \Phi / |\nabla \Phi|$, motion under a globally defined normal velocity field v_n is described by

$$\Phi_t \pm v_n |\nabla \Phi| = 0. \tag{5}$$

In many problems, though, the velocity is only naturally specified at the interface. An extension of these values off the interface to the rest of points in space is thus required [3, 4, 28]. A general approach for this involves extending the values constant in the normal direction and can be accomplished, for example, through application of fast marching [11, 20, 25] and fast sweeping [24] techniques. The level set equation (5) can then be handled by overlooking any dependence of v_n on Φ and solving the resulting Hamilton-Jacobi equation using standard discretization techniques (see, e.g., [12, 21]).

Efficiency of the approach can be retained through use of local level set techniques [2, 18], which include limiting computations and storage to those grid points contained in a small tubular neighborhood about the interface

of interest and employing reinitialization techniques to avoid adverse effects arising from the tube boundaries. As this procedure can be added on without difficulty, we concentrate our attention in this paper on obtaining the correct interfacial motion in the clearer global level set setting. For more on the level set method, see [15, 16].

Henceforth, Φ takes the place of U for the macroscale variable.

3 Measuring the Macroscale Interface Velocity

What remains is determining the normal velocities necessary for evolution of Φ at the macroscale grid points from the microscale model. This can be accomplished by first calculating the velocities at a selection of points lying on the macroscale interface and then extending these values off the interface to the rest of space. A selection of points commonly taken are the intersections between the interface and grid lines. Note, following the spirit of the level set method, the selection can also be the set of grid points neighboring the front. Normal velocity at such a grid point, which may not lie on the interface, is then translated as that of the particular level set of Φ passing through the point. We now detail the calculation of normal velocities at the selected points for the front propagation problems of interest.

If the normal velocity of the macroscale interface is known to only depend on the orientation of the local tangent plane of the interface then we may approximate the interface locally by a hyperplane. On the other hand, if the normal velocity is also known to depend on the local curvature, a quadratic approximation such as a circular arc in two dimensions or an ellipsoid in three dimensions is needed.

We first consider the homogenization problem. The level set representation of the microscale model, using the microscale level set variable ϕ, in this case takes the form

$$\phi_t + c\left(x, \frac{x}{\epsilon}\right)|\nabla\phi| = 0, \tag{6}$$

which describes motion in the normal direction at speed c. Note we may use the hyperplane approximation, with ϕ representing it as its zero level set, initially. At later times, the zero level set of ϕ will, in general, deviate from being a straight line.

Furthermore, it is convenient to perform a change of variables so that this hyperplane coincides with the $\{x_n = 0\}$-plane. We then solve (6) in a rectangular domain Δ with sides orthogonal to the coordinate axes (see Figure 1).

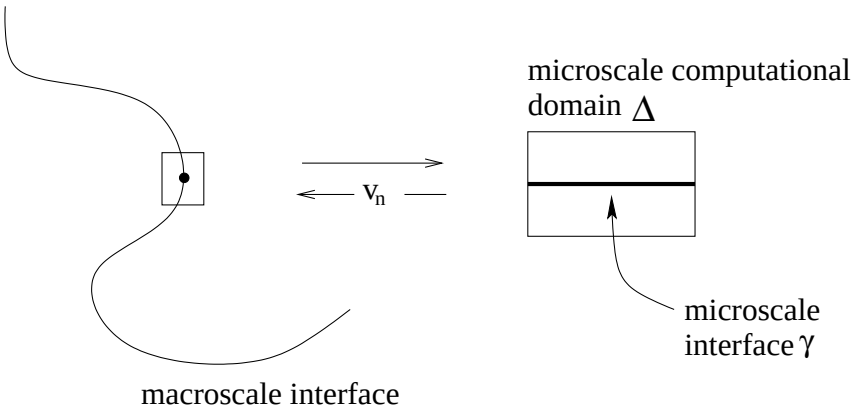

Figure 1: A pictorial description of our setup showing the link between the macroscopic and microscopic levels.

This domain should be, generally, a few times larger than the size of the periodic cell or the correlation length of c. Lastly, periodic boundary conditions are imposed in the $x_1, x_2, \ldots, x_{n-1}$-directions. In the x_n-direction, periodicity is imposed after subtracting out the background, or initial, configuration. These periodic boundary conditions are valid since the microstructure is locally homogeneous, with the size of the domain Δ larger than the microscale length ϵ. An underlying grid that resolves the microscale length ϵ can then be placed over Δ, allowing for the numerical discretization and solution of the microscale equation in the microscale computational domain.

To extract the quantity of interest, at each microscale time step, the microscale Hamiltonian $c(x, x/\epsilon)|\nabla\phi|$ is averaged in the central region $\tilde{\Delta}$ of the domain to reduce spurious effects that may arise from the boundary and the chosen boundary conditions. Denote this value by $h^\epsilon(t)$ (see Figure 2). This signal is then processed, as in [5], by time averaging to obtain

$$\frac{1}{t^*}\int_0^{t^*} h^\epsilon(t) K\left(\frac{t}{t^*}\right)\, dt,$$

where t^* is chosen so that this quantity has converged (see Figure 3). Note, due to a separation of scales, the convergence time, a relaxation time, is much shorter than the macroscopic time scale. The normal velocity for evolution of the front is thus calculcated at the chosen location from

$$v_n = \frac{1}{t^*|\nabla\phi|}\int_0^{t^*} h^\epsilon(t) K\left(\frac{t}{t^*}\right)\, dt. \tag{7}$$

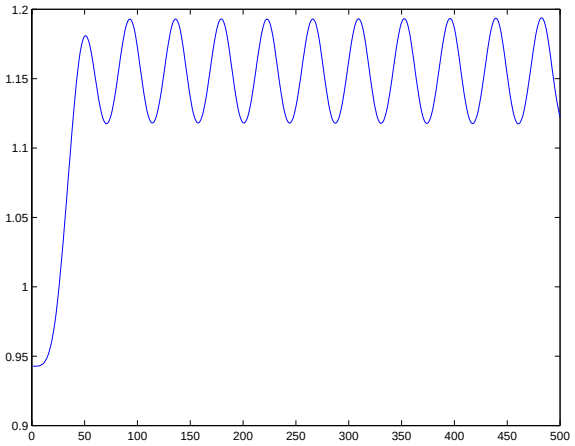

Figure 2: Typical flux values calculated at the time steps during the solve of the microscale equation in the homogenization problem with periodic microstructure. Note the initial transient followed by periodic behavior.

We note that the rate of convergence for the processed flux data, as well as the computational cost of this part of the algorithm, depends on factors such as the size of Δ, the number of grid points resolving Δ, and the number of experiments run, if ensemble averaging is used. However, the optimal desired balance of these is problem dependent and, as of yet, not particularly well understood. Some basic information is known, for example, the importance of smoothness in the averaging kernel. Furthermore, a general idea can be obtained from viewing the behavior of acquired data for the specific problem being considered.

After v_n is calculated at the selected points, a global normal velocity can be constructed through extension of v_n to all macroscale grid points following the ideas mentioned previously. The evolution equation for the level set function can then be evolved for a macroscale time step using this velocity and the process then repeated. Note the time stepping procedure used here can be replaced for better accuracy. This altogether gives the HMM for this front propagation problem.

Next we consider the case where the microscale model is described by a phase-field equation. Specifically, we study the model

$$u_t = \epsilon \nabla \cdot \left(a\left(x, \frac{x}{\epsilon}\right) \nabla u \right) + \nabla \cdot \left(b\left(x, \frac{x}{\epsilon}\right) u \right) - \frac{1}{\epsilon} \frac{\partial V}{\partial u}(u), \tag{8}$$

where $a(x, y) > 0$ and $b(x, y)$ are smooth functions that are either periodic

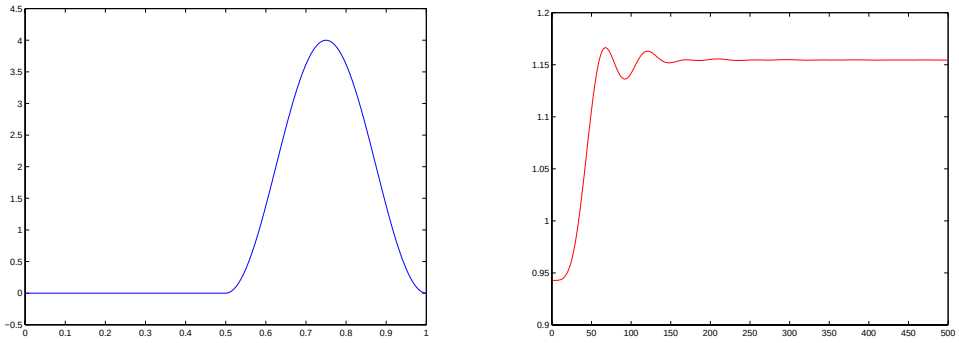

Figure 3: Profile of the kernel K used in the time averaging (left) and the results of this averaging on the flux shown in Figure 2 (right). The bias in K to the end of the interval removes the effect of the initial transient. This allows for the averaged flux to converge in a few number of steps.

in y or stationary random in y with rapidly decaying correlation at large distances and V is a double well potential with minima at $u = \alpha, \beta$.

In the case $V(\alpha) \neq V(\beta)$, then to leading order, the normal velocity of the macroscale interface depends only on the local tangent. Therefore we can once again take a hyperplane approximation for the initial form in the microscale. Let $\tilde{u}_0$ be a function defined as $\tilde{u}_0 = \alpha$ on one side of the hyperplane, $\tilde{u}_0 = \beta$ on the other side, and $u_0 = \tilde{u}_0 * \eta_\epsilon$, where $\eta_\epsilon = \frac{1}{\epsilon^n}\eta\left(\frac{x}{\epsilon}\right)$ is a mollifier of scale ϵ. We can then use a procedure similar to that in the homogenization problem to solve the microscale problem (8) in the domain Δ with periodic boundary conditions in the $x_1, x_2, \ldots, x_{n-1}$-directions and Dirichlet boundary conditions $\phi = \alpha, \beta$ in the x_n-direction.

As for the normal velocity, integrating (8) over the possibly smaller domain $\tilde{\Delta}$ gives on the left hand side, approximately, $(\alpha - \beta)L(\tilde{\Delta}, n)v_n$, where $L(\tilde{\Delta}, n)$ denotes the length of the domain $\tilde{\Delta}$ in the x_n-direction. Thus v_n can be approximated through the expression

$$v_n = \frac{1}{(\alpha-\beta)L(\tilde{\Delta},n)} \cdot \int_{\tilde{\Delta}} \left[\epsilon\nabla\cdot\left(a\left(x,\frac{x}{\epsilon}\right)\nabla u\right) + \nabla\cdot\left(b\left(x,\frac{x}{\epsilon}\right)u\right) - \frac{1}{\epsilon}\frac{\partial V}{\partial u}(u)\right] dx. \tag{9}$$

The typical behavior of v_n calculated at the microscale time steps in random media is shown in Figure 4. Time or ensemble averaging can be considered to obtain a better converged value, however, even without these techniques, v_n is only slightly oscillating after a few steps. Note that the figure also

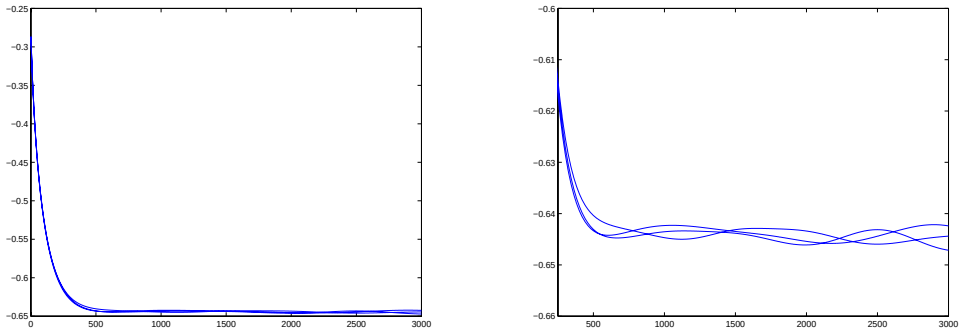

Figure 4: Typical normal velocity values calculated at the time steps during the solve of the microscale equation for front propagation problems with a phase-field model for the microscale equation (left). A zoom of the result is also shown (right). The small oscillations seen at the tail end are due to randomness in the medium and can be removed with time or ensemble averaging.

shows that the formula for v_n makes sense at each microscale time step even though the microscale interface location may not have changed much from one step to the other. Especially, the convergence of the values allows us to accept the final v_n.

In the case where $V(\alpha) = V(\beta)$, local curvature matters and we instead make a quadratic approximation of the front. The procedure then follows the same principles, with the quadratic approximation mapped to $\{x_n = 0\}$, and the normal velocity v_n can once again be determined for use in the level set macroscale solver.

As a summary, we detail the steps of the our HMM approach to front propagation:

1. The initial macroscale front location represented by the level set function Φ_0 is given.

2. Select a set of points on or near the interface in the macroscopic level, for example, where the interface intersects grid lines. For each of these points, create the microscale domain Δ and solve the microscale equation (6) or (8) in this domain with the previously described boundary conditions until the value for v_n, from equation (7) or (9), converges. Time or ensemble averaging may be needed to better enforce this convergence.

3. Extend the calculated values for v_n at the selected points to all grid points using fast marching or fast sweeping techniques.

4. Solve the level set evolution equation (5) in the macroscopic level for one macroscale time step using this globally defined normal velocity.

5. Stop and output if the desired time is reached in the macroscale solve. Otherwise, repeat from step 2 using the newly evolved level set function Φ and its corresponding interface.

Note since microscale computations are not performed everywhere, the algorithm is fast. In fact, the complexity of the algorithm is independent of ϵ and so great gains can be made when ϵ is very small.

4 Numerical Results

We first look at the homogenization problem where the microstructure is periodic. In this case, the microstructure may induce anisotropy in the macroscale interface motion [7]. Figure 5 shows the anisotropic effects of the macroscopic dynamics for an initially growing circle along with the normal velocities calculated and used in the algorithm when the microstructure is composed of square tiles. Figure 6 shows an example of anisotropic dynamics along with the calculated normal velocities when the microstructure is banded. In this case, two initial circles expand and a topological change eventually develops. The ease with which the level set method handles topological changes is one of the main reasons for using it as the macroscale solver in these interface problems.

For the case of the phase-field microscale model and random media, Figure 7 shows the results of our algorithm for a certain choice of a and b and with $\alpha = 1, \beta = -2$. An initial ellipse translates and shrinks and the normal velocities calculated for this flow are displayed. Figure 8 shows another result with different choices of a and b. The normal velocities for this case are also displayed, along with a zoomed image of part of the velocity plot. Note there is some scattering of the calculated normal velocities in this case, though this does not affect the stability of the solution.

5 Conclusion

We conclude by commenting that the example we considered of a microscale phase-field model provides a natural compromise between the level set and

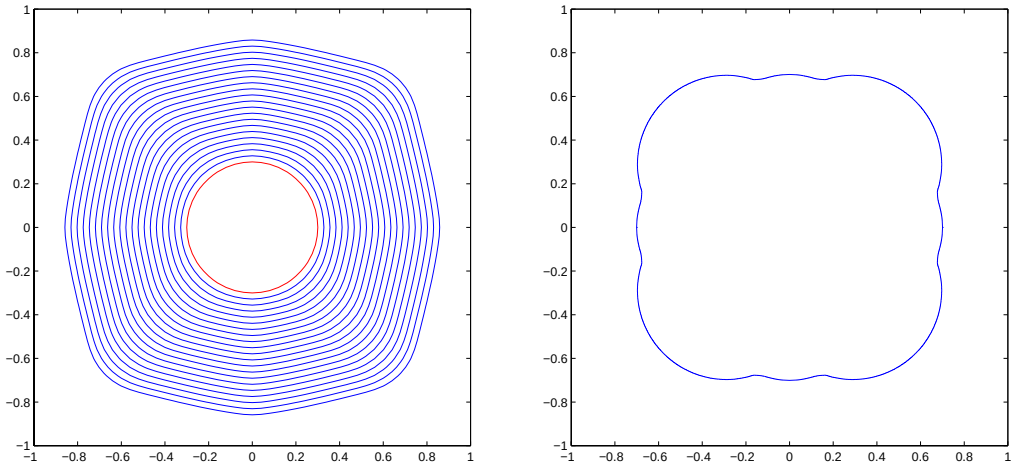

Figure 5: Anisotropic effects for an initial circle growing over a periodic microstructure for the homogenization problem (left). The computed normal velocities are shown in a polar plot (right).

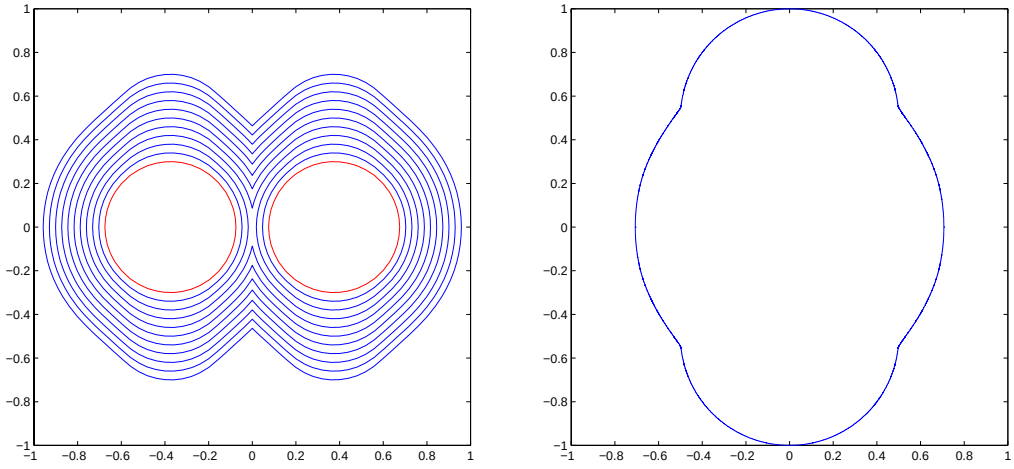

Figure 6: Anisotropic effects for two initial circles growing over a periodic microstructure for the homogenization problem (left). Note a topological change occurs during the flow. The computed normal velocities are shown in a polar plot (right).

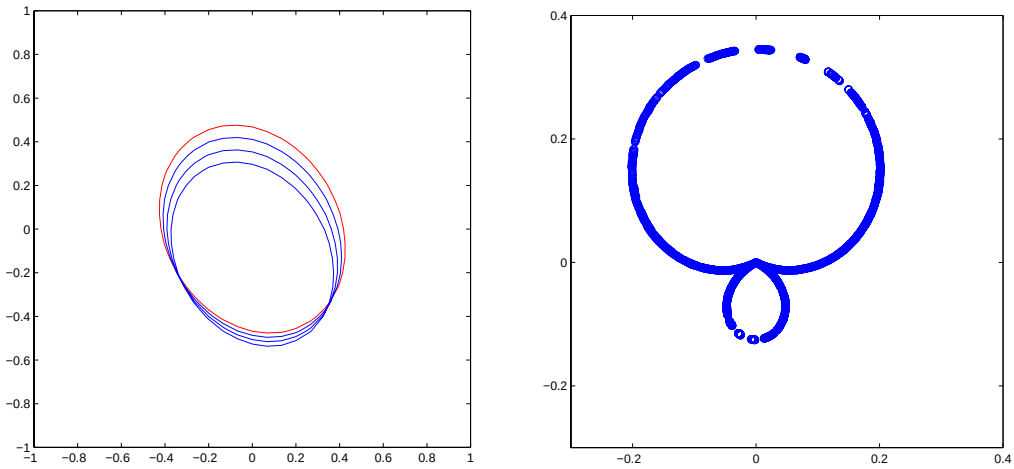

Figure 7: Shrinking and translating ellipse computed using the microscale phase-field model in a random medium (left). Magnitudes of the normal velocity calculated during the solve are shown in a polar plot (right).

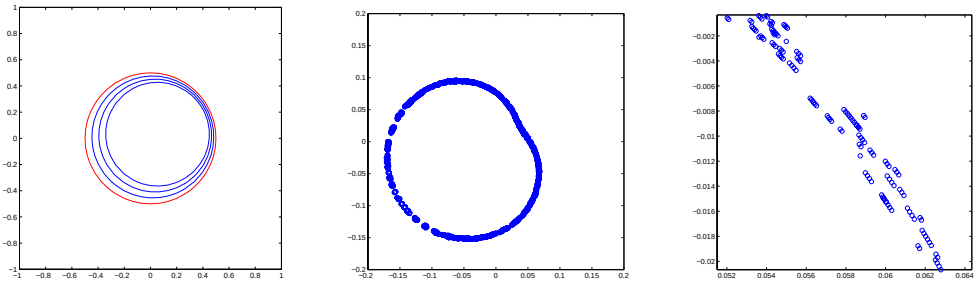

Figure 8: Shrinking and translating circle computed using the microscale phase-field model in a random medium (left). Magnitudes of the normal velocity calculated during the solve (middle) and a zoomed portion (right) are shown in polar plots. Note the slight scattering in the values in this case.

phase-field approaches. This HMM retains the flavor of the level set method, especially in topological changes, but without the need for an explicit interface dynamics model. Furthermore, it can be thought of as an adaptive mesh refinement procedure for the phase-field model, though the refinement is only performed for the purpose of accurately obtaining the macroscale interface dynamics in contrast to the microscopic details of the phase-field model that is usually sought. This fits into the general spirit of the HMM framework.

6 Acknowledgements

The authors would like to thank Bjorn Engquist, Xiantao Li, Yen-Hsi Richard Tsai, Eric Vanden-Eijnden, and Jack Xin for various helpful discussions. The work of Cheng is supported by NSF grant #0208449 and ONR grant #N00014-01-1-0674. The work of E is supported by ONR grant #N00014-01-1-0674.

References

[1] A. Abdulle and W. E. Finite Difference HMM for Homogenization Problems. In preparation.

[2] D. Adalsteinsson and J.A. Sethian. A Fast Level Set Method for Propagating Interfaces. *J. Comput. Phys.*, 118:269–277, 1995.

[3] D. Adalsteinsson and J.A. Sethian. The Fast Construction of Extension Velocities in Level Set Methods. *J. Comput. Phys.*, 148:2–22, 1999.

[4] S. Chen, B. Merriman, S. Osher, and P. Smereka. A Simple Level Set Method for Solving Stefan Problems. *J. Comput. Phys.*, 135:8–29, 1997.

[5] L.-T. Cheng and W. E. Numerical Homogenization of Hamilton-Jacobi Equations. In preparation.

[6] B. Craciun and K. Bhattacharya. Effective Motion of a Curvature-Sensitive Interface Through a Heterogeneous Medium. Preprint, 2002.

[7] B. Craciun and K. Bhattacharya. Homogenization of a Hamilton-Jacobi Equation Associated With the Geometric Motion of an Interface. Preprint, 2002.

[8] W. E and B. Engquist. The Heterogeneous Multi-Scale Methods. To appear in Comm. Math. Sci.

[9] W. E and B. Engquist. The HMM for Homogenization Problems. Submitted to MMS.

[10] J. Glimm, O. McBryan, R. Menikoff, and D.H. Sharp. Front Tracking Applied to Rayleigh-Taylor Instability. *SIAM J. Sci. Statist. Comput.*, 7(1):230–251, 1986.

[11] J. Helmsen, E. Puckett, P. Colella, and M. Dorr. Two New Methods for Simulating Photolithography Development in 3D. *Proc. SPIE*, 2726:253–261, 1996.

[12] G.S. Jiang and D. Peng. Weighted ENO Schemes for Hamilton Jacobi Equations. *SIAM J. Scient. Comput.*, 21(6):2126–2143, 2000.

[13] R. Klein. Private communications.

[14] T. Li, E. Vanden-Eijnden, P. Zhang, and W. E. Stochastic Models of Polymeric Fluids at Small Deborach Number. Preprint.

[15] S. Osher and R. Fedkiw. Level Set Methods: An Overview and Some Recent Results. *J. Comput. Phys.*, 169:463–502, 2001.

[16] S. Osher and R. Fedkiw. *Level Sets and Dynamic Implicit Surfaces.* Springer-Verlag, 2002.

[17] S. Osher and J.A. Sethian. Fronts Propagating with Curvature Dependent Speed: Algorithms Based on Hamilton-Jacobi Formulations. *J. Comput. Phys.*, 169(1):12–49, 1988.

[18] D. Peng, B. Merriman, S. Osher, H.K. Zhao, and M. Kang. A PDE-Based Fast Local Level Set Method. *J. Comput. Phys.*, 155(2):410–438, 1999.

[19] J. Rubinstein, P. Sternberg, and J.B. Keller. Fast Reaction, Slow Diffusion, and Curve Shortening. *SIAM J. Appl. Math.*, 49(1):116–133, 1989.

[20] J.A. Sethian. Fast Marching Level Set Methods for Three Dimensional Photolithography Development. *Proc. SPIE*, 2726:261–272, 1996.

[21] C.-W. Shu and S. Osher. Efficient Implementation of Essentially Nonoscillatory Shock-Capturing Schemes. *J. Comput. Phys.*, 77(2):439–471, 1988.

[22] A.-K. Tornberg and B. Engquist. The Segment Projection Method for Interface Tracking. To appear in CPAM.

[23] A.-K. Tornberg and B. Engquist. Interface Tracking in Multiphase Flows. In *Multifield Problems*, pages 58–65. Springer, Berlin, 2000.

[24] Y.-H. Tsai, L.-T. Cheng, S. Osher, and H.K. Zhao. Fast Sweeping Algorithms for a Class of Hamilton-Jacobi Equations. CAM Report 01-27, UCLA, 2001. Accepted by SINUM.

[25] J.N. Tsitsiklis. Efficient Algorithms for Globally Optimal Trajectories. *IEEE Transactions on Automatic Control*, 50:1528–1538, 1995.

[26] J. Xin. Front Propagation in Heterogeneous Media. *SIAM Rev.*, 42(2):161–230, 2000.

[27] X. Yue. Comparison of Some Multi-Scale Methods for Homogenization Problems. Preprint.

[28] H.K. Zhao, T.F. Chan, B. Merriman, and S. Osher. A Variational Level Set Approach to Multiphase Motion. *J. Comput. Phys.*, 127:179–195, 1996.