Level Set Methods, with an Application to Modeling the Growth of Thin Films

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Abstract

The level set method was devised in 1987 by S. Osher and J.A. Sethian [OSe] as a versatile and useful tool for analyzing the motion of fronts. It has proven to be phenomenally successful as both a theoretical and computational device.

In this paper we review its properties, discuss the advances in level set technology since the original paper, highlight some of the application areas, and present a new application to the modeling of epitaxial growth of thin film semiconductor devices (see also [Ca, Me, CGMORVZ]).

1 Introduction

The idea behind the level set method is a simple one. Given an interface Γ in R^n of co-dimension one, bounding a (perhaps multiply connected) open region Ω, we wish to analyze and compute its subsequent motion under a velocity field $\vec{v}$. This velocity can depend on position, time, the geometry of the interface (its normal, mean curvature...) and the external physics. The idea, as devised in 1987 by S. Osher and J.A. Sethian, is merely to define a smooth (at least Lipschitz continuous)

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function $\varphi(x,t)$, that represents the interface as the set where $\varphi(x,t) = 0$. Here $x = (x_1, \ldots, x_n)\ \varepsilon\ R^n$.

The level set function φ has the following properties

$$\begin{aligned} \varphi(x,t) &> 0 \quad \text{for } x\ \varepsilon\ \Omega \\ \varphi(x,t) &< 0 \quad \text{for } x\ \not\varepsilon\ \bar{\Omega} \\ \varphi(x,t) &= 0 \quad \text{for } x\ \varepsilon\ \partial\Omega = \Gamma(t) \end{aligned}$$

Thus, the interface is to be captured for all later time, by merely locating the set $\Gamma(t)$ for which φ vanishes. This deceptively trivial statement is of great significance for numerical computation, primarily because topological changes such as breaking and merging are well defined and performed "without emotional involvement".

The motion is analyzed by convecting the φ values (levels) with the velocity field $\vec{v}$. This elementary equation is

$$\frac{\partial \varphi}{\partial t} + \vec{v} \cdot \nabla \varphi = 0. \tag{1}$$

Here $\vec{v}$ is the desired velocity on the interface, and is arbitrary elsewhere.

Actually, only the normal component of v is needed: $v_n = \vec{v} \cdot \frac{\vec{\nabla}\varphi}{|\nabla\varphi|}$, so (1) becomes

$$\frac{\partial \varphi}{\partial t} + v_n |\nabla \varphi| = 0. \tag{2}$$

In the next section we give simple and computationally fast prescriptions for (1) reinitializing the function φ to be signed distance to Γ, at least near the boundary [SSO] (2) smoothly extending the velocity field v_n off of the front Γ [CMOS] and (3) solving (2) only locally near the interface Γ, thus lowering the complexity of this calculation by an order of magnitude [PMZOK]. This makes the cost of level set methods competitive with boundary integral methods, in cases when the latter are applicable [HLOZ].

We emphasize that all this is easy to implement in the presence of boundary singularities, topological changes, and in 2 or 3 dimensions. Moreover, in the case which v_n is a function of the direction of the unit normal, as in crystalline motion [OM], then equation (2) becomes the first order Hamilton-Jacobi equation

$$\frac{\partial \varphi}{\partial t} + |\nabla \varphi| \gamma \left(\frac{\nabla \varphi}{|\nabla \varphi|} \right) = 0 \tag{3}$$

for $\gamma = \gamma(\vec{n})$ a given function of the normal.

High order accurate, essentially non-oscillatory discretizations to general Hamilton-Jacobi equations including (3) were obtained in [OSh], see also [OSe,BO].

Theoretical justification of this method for geometric based motion came through the theory of viscosity solutions for scalar time dependent partial differential equations [CGG,ES]. The notion of viscosity solution—which applies to a very wide class of these equations, including those derived from geometric based motions—enables a user to have confidence that their computer simulations give accurate, unique solutions. A particularly interesting result is in [ESS] where motion by mean curvature as defined by Osher and Sethian in [OSe], is shown to be essentially the same motion as is obtained from the asymptotics in the phase field reaction diffusion equation. The motion in the level set method involves no superfluous stiffness as is required in phase field models. As was proven in [MBO2], this stiffness due to a singular perturbation involving a small parameter ϵ will lead to incorrect answers as in [Ko] without the use of adaptive grids [NPV]. This is unnecessary in order for the level set model to function.

An interesting variant of the level set method for geometry based motion was introduced in [MBO1] as diffusion generated motion, and has now been generalized to forms known as convolution generated motion or threshold dynamics. This method splits the reaction diffusion model into two highly simplified steps. For an overview of this approach, see [RM].

2 The Level Set Dictionary and Technology

We list key terms and advances in technology and define them by their level set representation.

1. The interface boundary $\Gamma(t)$ is defined by: $\{x|\varphi(x,t) = 0\}$. The region $\Omega(t)$ bounded by $\Gamma(t)$: $\{x|\varphi(x,t) > 0\}$.

2. The unit normal $\vec{n}$ to $\Gamma(t)$ is given by

$$\hat{n} = -\frac{\nabla\varphi}{|\nabla\varphi|}.$$

3. The mean curvature k is defined by

$$k = -\nabla \cdot \left(\frac{\nabla\varphi}{|\nabla\varphi|}\right).$$

4. The Dirac delta function concentrated on an interface is:

$$\delta(\varphi)|\nabla\varphi|,$$

where $\delta(x)$ is a one dimensional delta function.

5. The characteristic function χ of a region $\Omega(t)$:

$$\chi = H(\varphi)$$

where

$$\begin{aligned} H(x) &\equiv 1 \text{ if } x > 0 \\ H(x) &\equiv 0 \text{ if } x < 0. \end{aligned}$$

6. The surface (or line) integral of a quantity $p(x,t)$ over Γ:

$$\int_{R^n} p(x,t)\delta(\varphi)|\nabla\varphi|dx.$$

7. The volume (or area) integral of $p(x,t)$ over Ω

$$\int_{R^n} p(x,t)H(\varphi)dx.$$

8. The distance reinitialization procedure:
Let $d(x,t)$, be signed distance of x to the closest point on Γ. The quantity $d(x,t)$ satisfies $|\nabla d| = 1,\ d > 0$ in $\Omega, d < 0$ in $(\bar{\Omega})^c$ and is the steady state solution (as $\tau \to \infty$) to

$$\begin{aligned} \frac{\partial\psi}{\partial\tau} + \text{sgn}(\varphi)(|\nabla\psi| - 1) &= 0 \\ \psi(x,0) &= \varphi(x,t). \end{aligned} \tag{4}$$

where $\text{sgn}(x) = 2H(x) - 1$ is the signum function.

Note: in recent work [PMOZK] it was found that degeneracies in the initial data φ for (4)—such as extreme flatness/steepness (vanishing/infinite $\partial\varphi/\partial n$)—can be removed by preconditioning it via:

$$\begin{aligned} \varphi^{(1)}(x,0) &= \frac{\varphi(x,t)}{|\nabla\varphi(\bar{x},t)|} \\ \varphi^{(2)}(x,0) &= \frac{\varphi^{(1)}(x,0)}{|\nabla\varphi^{(1)}(x,0)|} \\ \psi(x,0) &= \varphi^{(2)}(x,0) \end{aligned}$$

Moreover, in order to define d in a band of width ϵ around Γ, we need only solve (4) for $\tau = 0(\epsilon)$. Thus the computational complexity of this construction is minimal.

9. Smooth extension of a quantity, e.g. v_n on Γ off of Γ. Let the quantity be $p(x,t)$. Solve to steady state, $\tau \to \infty$

$$\begin{aligned} \frac{\partial q}{\partial \tau} &+ \operatorname{sgn}(\varphi)\left(\frac{\nabla\varphi}{|\nabla\varphi|}\cdot\nabla q\right) = 0 \\ q(x,0) &= p(x,t). \end{aligned}$$

Again, we need only solve this for $\tau = 0(\epsilon)$ in order to extend p to be constant in the direction normal to the interface in a tube of width ϵ. See, e.g. [PMOZK,CMOS].

10. Local level set method [PMOZK]. We may solve (2) in a neighborhood of Γ of width $m\Delta x$, where m is typically 5 or 6. Points outside of this neighborhood need not be updated by this motion. This algorithm works in "φ" space – so no intricate computer science is used. For details see [PMOZK]. Thus this local method works easily in the presence of topological changes and for the multi-phase problems described below.

    Additionally, this method may be used to compute distance to Γ, with any order of accuracy, with computational complexity which is of order N, the total number of points updated. In fact, the same is true for the solution of general geometric based motion such as a curvature regularization of a first order Hamilton-Jacobi equation. In contrast, the fast marching algorithm introduced in [Se] applies to much more restricted class of equations, those where the speed function is given à priori and does not change sign. It is also only first order accurate, with no simple extension to higher order. High accuracy is important if we are computing a distance function which must have accurate gradients and second derivatives for the purpose of computing interface normals and curvature. Also, fast marching actually has greater formal complexity ($N \log N$) than the above PDE based method, though in actual implementation it can be faster—especially for problems where the propagation speed varies by orders of magnitude over the domain.

11. Coupling to external physics in two-phase Navier-Stokes flow: [SSO,CHMO]

$$\begin{aligned} \vec{u}_t &= -\vec{u}\cdot\nabla\vec{u} - \frac{\nabla p}{\rho(\varphi)} + \vec{g} + \frac{1}{R_e}\nabla\cdot\left(\frac{(2\mu D)}{\rho(\varphi)}\right) && (5) \\ &- \left(\frac{1}{Bd}\right)\left(\nabla\left(\frac{\nabla\varphi}{|\nabla\varphi|}\right)\right)\nabla H(\varphi), && (6) \\ \nabla\cdot\vec{u} &= 0 \end{aligned}$$

where $\vec{u} = (u, v)$ is the fluid velocity, $\rho = \rho(\varphi)$ and $\mu = \mu(\varphi)$ are the piecewise constant fluid densities and viscosities, D is the viscous stress tensor, $\bar{g}$ is the gravitational force, k is the curvature of the interface, H is the Heaviside function and $R_e; Bd, \frac{\rho_1}{\rho_2}$, and $\frac{\mu_1}{\mu_2}$ are the parameters defining a given flow.

This equation is coupled to the front motion through the level set evolution equation (1) with $\vec{v} = \vec{u}$. This involves defining the interface numerically as having the width of the approximation to the jump in the approximate Heaviside function, which is approximately $3\Delta x$ in [SSO].

12. Coupling to the external physics in Stefan problems [CMOS]. Solve:

$$\begin{aligned} \frac{\partial T}{\partial t} &= \nabla^2 T, \quad x \not\in \partial\Omega = \Gamma(t) \\ v_n &= [\frac{\partial T}{\partial n}], \quad \bar{x} \in \Gamma(t) \end{aligned} \tag{7}$$

where $[\cdot]$ denotes the jump across the boundary, and

$$T = -\bar{\varepsilon}_c k(1 - A\cos(k_A\theta + \theta_0)) + \bar{\varepsilon}_v v_n(1 - A\cos(k_A\theta + \theta_0))$$

on $\Gamma(t)$, and where k is the curvature, $\theta = \cos^{-1}\frac{\varphi_x}{|\nabla\varphi|}$, and the constants $A, k_A, \varphi_0, \bar{\varepsilon}_c$, and $\bar{\varepsilon}_v$ depend upon the material being modeled.

We directly discretize the boundary conditions at Γ: To update T at grid nodes near the boundary, if the stencil for the heat equation would cross Γ (as indicated by nodal sign change in φ), we merely use dimension by dimension one sided interpolation and the given boundary T value at a ghost node placed at $\varphi = 0$ (found by interpolation on φ) to compute T_{xx} and or T_{yy}, (never interpolating across the interface) rather than the usual three point central stencils. The level set function φ is updated, after reinitialization to be distance, by (1), using the extension off the interface of v_n as defined in (7).

13. Multi-phase flow using exactly as many level set functions as there are phases, with applications to drops and bubbles [ZCMO,ZMOW]; a variational level set approach.

Define an energy function involving the area (length) of each interface, the volume (area) of each phase (using $\delta(\varphi_i), H(\varphi_i)$). Apply gradient descent to this energy using time as the descent variable. Enforce a no-vacuum, no-overlap constraint: This leads to slightly coupled system of geometrically driven motion perturbed by the constraints [ZCMO]. Additional constraints such as volume preservation may also be enforced in order to compute falling drops and bubble motion [ZMOW]. Finally, inertial forces are added in [KMOS].

14. Topological regularization of ill posed problems with applications to vortex motion in incompressible flow.

In [HOS] we computed two and three dimensional unstable vortex motion without regularization other than that in the discrete approximation to $\delta(\varphi)$ – this is done over a few grid points. The key observation, first made in [HO] is that viewing a curve or surface as the level set of a function, and then evolving it with a perhaps unstable velocity field, prevents certain types of blow up from occuring. This is denoted "topological regularization". For example a tracked curve can develop a figure 8 pattern, but a level set captured curve will pinchoff and stabilize before this happens. For the set up (involving two functions), see [HO], where we perform calculations involving the Cauchy-Riemann equations. The motions agree until pinchoff, when the topological stabilization develops.

As an example, we consider the two dimensional incompressible Euler equations, which may be written as

$$\begin{aligned} \omega_t + \vec{u} \cdot \nabla \omega &= 0 \\ \nabla \times \vec{u} &= \omega \\ \nabla \cdot \vec{u} &= 0 \end{aligned}$$

We are interested in situations in which the vorticity is initially concentrated on a set characterized by the level set function φ as follows

$$\begin{gathered} \text{Vortex patch: } \omega = H(\varphi) \\ \text{Vortex sheet: } \omega = \delta(\varphi) \text{ (strength of sheet is } \tfrac{1}{|\nabla \varphi|}) \\ \text{Vortex sheet dipole: } \omega = \tfrac{d}{d\varphi}\delta(\varphi) = \delta'(\varphi). \end{gathered}$$

The key observation is that φ also satisfies (8) and ω can be recovered from (8).

For example, for the vortex sheet case we solve

$$\begin{aligned} \varphi_t + \vec{u} \cdot \nabla \varphi &= 0 \\ \vec{u} &= \begin{pmatrix} -\partial y \\ \partial x \end{pmatrix} \Delta^{-1} \delta(\varphi). \end{aligned}$$

Off the shelf Laplace solvers may be used. See [HOS] for results involving two and three dimensional flows.

15. The Wulff shape as the asymptotic limit of a growing crystalline interface [OM].

For an initial state consisting of any number of growing crystals in R^n, n arbitrary, moving outward with normal velocity $\gamma > 0$ which depends on the angle

of the unit normal, the asymptotic growth shape is a Wulff crystal, appropriately scaled in time. This shape minimizes the surface energy, i.e. the surface integral of γ, for a given volume. The proof uses the level set idea and then analyzes the solution to (3) using the Hopf-Bellman formulas [BE]. This result was first conjectured by Gross in (1918) [Gr].

Additionally, with the help of the Brunn-Minkowski inequality, we show that if we evolve a convex surface under the motion described in (3), that the ratio to be minimized monotonically decreases to its minimum as time increases. Thus there is a new link between this hyperbolic surface evolution and this (generally nonconvex) energy minimization.

16. Other applications of the level set method include Hele-Shaw flow (slow flow through porous media) [HLOZ], generalized interpolation of curves and surfaces [ZOMK], the construction of (Wulff) minimal surfaces [CMO], generalized ray tracing [FEO], computer vision [CCCD], computer aided design [KB], and combustion [ABS].

3 The Island Dynamics Model for Epitaxial Growth

We have developed a new continuum model for the epitaxial growth of thin films [Ca,Me,CGMORVZ]. Since our model describes hundreds of moving and merging interfaces, the level set method is essential for practical calculation. Here we will briefly outline the model and the novel level set techniques for the computations. We also show representative numerical results.

3.1 Epitaxial Growth

Molecular Beam Epitaxy (MBE) is is a method for growing extremely thin films of material. The essential aspects of this growth process are as follows: under vacuum conditions a flux of atoms is deposited on a substrate material, typically at a rate that grows one atomic monolayer every several seconds. When deposition flux atoms hit the surface, they bond weakly rather than bounce off. These surface "adatoms" are relatively free to hop from lattice site to site on a flat (atomic) planar surface. However, when they hop to a site at which there are neighbors at the same level, they form additional bonds which hold them in place. This bonding could occur at the "step edge" of a partially formed atomic monolayer, which contributes the growth of that monolayer. Or, it could occur when two adatoms collide with each other. If the

critical cluster size is one, the colliding adatoms nucleate a new partial monolayer "island" that will grow by trapping other adatoms at its step edges.

By these means, the deposited atoms become incorporated into the growing thin film. Each atomic layer is formed by the nucleation of many isolated monolayer islands, which then grow in area, merge with nearby islands, and ultimately fill in to complete the layer. Because the deposition flux is continually raining down on the entire surface, including the tops of the islands, a new monolayer can start growing before the previous layer is completely filled. Thus islands can form on top of islands in a "wedding cake" fashion, and the surface morphology during growth can become quite complicated.

The process has traditionally been modeled using Kinetic Monte Carlo methods and Molecular Dynamics methods. These follow the trajectories of adatoms hopping on the surface, with varying degrees of accuracy. Such direct simulation methods provide a wealth of insight into the growth process, but they are computationally expensive. Also, the focus on single atoms makes it difficult to capture the behavior at the longer lengths scales that are important for the performance of integrated circuit devices grown via MBE.

For example, Resonant Tunneling Diodes (RTDs) are a very fast switching component grown with MBE and used in satellite communications electronics. The active region in these devices is a thin film on the order of 50 monolayers thick, with a lateral dimensions of tens of thousands of atoms. The performance characteristics of the RTD depend extremely sensitively on the thickness, roughness, and general morphology of this film. For practical device growth, it is important to achieve a high degree of repeatability and controllability of these film properties. For device design, it is further important to develop an understanding of how they relate to the device characteristics.

3.2 The Island Dynamics Model

The Island Dynamics model is a continuum model designed to capture the longer length scale features that are likely to be important for the analysis and control of monolayer thin film growth. It is also intended to model the physics relevant to studying basic issues of surface morphology, such as the effects of noise on growth, the long time evolution of islands, and the scaling relations ships between surface features (mean island area, step edge length, etc) in various growth regimes (precoalescence, coalescence). Refer to the classic work of [BCF] for useful background on the modeling of the growth of material surfaces.

In the Island Dynamics model, we treat each of the islands present as having a unit height, but a continuous (step edge) boundary on the surface. This represents

the idea that the films are atomic monolayers, so that height is discrete, but they cover relatively large regions on the substrate, so x-y are continuum dimensions. The adatoms are modeled by a continuous adatom density function on the surface. This represents the idea that they are very mobile, and so they effectively occupy a given site for some fraction of the time, with statistical continuity, rather than discretely.

Thus, the domain for the model is the x–y region originally defined by the substrate, and the fundamental dynamical variables for this model are:

- The island boundary curves $\Gamma_i(t), i = 1, 2, \ldots, N$
- The adatom density on the surface $\rho(x, y, t)$

The adatom density ρ obeys a surface diffusive transport equation, with a source term for the deposition flux

$$\frac{\partial \rho}{\partial t} = \nabla \cdot (D \nabla \rho) + F,$$

where $F = F(x, y, t)$ is specified. During most phases of the growth, it is simply a constant. This equation may also include additional small loss terms reflecting adatoms lost to the nucleation of new islands, or lost to de-absorption off the surface. This equation must be supplemented with boundary conditions at the island boundaries. In the simplest model of Irreversible Aggregation, the binding of adatoms to step edges leaves the adatom population totally depleted near island boundaries, and the boundary condition is

$$\rho|_\Gamma = 0$$

More generally, the effects of adatom detachment from boundaries, as well as the energy barriers present at the boundary, lead to boundary conditions of the form

$$\left[A\rho + B \frac{\partial \rho}{\partial n} \right] = C$$

where C is given and $[\cdot]$ denotes the local jump across the boundary. In particular, note that ρ itself can have a jump across the boundary, even though it satisfies a diffusive transport equation. This simply reflects that fact that the adatoms on top of the island are much more likely to incorporate into the step edge than to hop across it and mix with the adatoms on the lower terrace, and vice versa.

The islands boundaries Γ_i move with velocities $\vec{v} = v_n \vec{n}$, where the normal velocity v_n reflects the island growth. This is determined simply by local conservation of atoms: the total flux of atoms to the boundary from both sides times the effective area per atom, a^2, must equal the local rate of growth of the boundary, v_n:

$$v_n = -a^2 [\vec{q} \cdot \vec{n}]$$

(this assumes there is no particle transport along the boundary; more generally, there is a contribution from this as well) where $\vec{q}$ is the surface flux of adatoms to the island boundary and $\vec{n}$ is the local outward normal. In general, the net atom flux $\vec{q}$ can be expressed in terms of the the diffusive transport, as well as attachment and detachment probabilities, all of which can be directly related to the parameters of Kinetic Monte Carlo models. In the special case of Irreversible Aggregation, $\vec{q}$ is simply the surface diffusive flux of adatoms

$$\vec{q} = -D\nabla\rho$$

To complete the model we include a mechanism for the nucleation of new islands. If islands nucleate by random binary collisions between adatoms (and if the critical cluster size is one), we expect the probability that an island is nucleated at a time t, at a site (x, y), scales like

$$P[dx, dy, dt] = \epsilon\rho(x, y, t)^2 dt\, dx\, dy.$$

This model describes nucleation as a site-by-site, time step-by-time step random process. A simplifying alternative is to assume the nucleation occurs at the continuous rate obtained by averaging together the probabilistic rates at each site. In this case, if we let $n(t)$ denote the total number of islands nucleated prior to time t, we have the deterministic rate equation

$$\frac{dn}{dt} = < \epsilon\rho^2 >$$

where $< \cdot >$ denotes the spatial average. In this formulation, at each time when $n(t)$ reaches an new integer value, we nucleate a new island in space. This is carried out by placing it randomly on the surface with a probability weighted by ρ^2, so that the effect of random binary collisions is retained.

This basic model also has natural extensions to handle more complex thin film models. For example, additional continuum equations can be added to model the dynamics of the density of kink sites on the island boundaries, which is a micro-structural property that significantly influences the local adatom attachment rates (see [CGMORVZ]). Also, we can couple this model to equations for the elastic stress that results from the "lattice mismatch" between the size of the atoms in the growing layers and the size of the atoms in the substrate.

Conversely, the above model has a particularly interesting extreme simplification. We can go to the limit where the adatoms are so mobile on the surface ($D \to \infty$) that the adatom density is spatially uniform, $\rho(x, y, t) = \rho(t)$. In this case, the loss of adatoms due to the absorbing boundaries is assumed to take on a limiting form proportional to the adatom density and the total length L of all the island boundaries,

which can be written as a simple sink term

$$\frac{d\rho}{dt} = F - \lambda L \rho.$$

(This equation can be derived systematicaly from the conservation law for the total number of adatoms, $\int \rho$, that follows from the adatom diffusion equation. The above loss term is just a simplified model for the net loss of adatoms to the island boundaries.) Further, it is assumed the velocity takes on a given normal dependent limiting form, $v_n = v_n(\vec{n})$ (which implies that growing islands will rapidly assume the associated "Wulff shape" for this function $v_n(\vec{n})$ (as in [OM])). We have used this "Uniform Density" model to prototype the numerical methods, and to develop an understanding of how the island dynamics models are related to the continuum "rate equation" models that describe island size distribution evolution while using no information at all about the spatial interactions of the islands.

3.3 Level Set Methods for Island Dynamics

Much of the above model is formally a Stefan problem and many of the level set techniques required for this were developed in [CMOS] and can similarly be applied here. For example, the internal boundary condition discretization of the adatom diffusion equation, and the the procedure for extending the interface velocity v_n to a velocity defined on all of space. Here we will only highlight the aspects of the level set method were newly developed for the island dynamics model.

Representation Islands can only merge if they are part of the same monolayer, and the islands on monolayer j must be on top of a larger island in monolayer $j-1$. Since there is no overhang at step edges, it is also true that the boundaries of islands on different layers j, k will never cross. We can capture all this behavior conveniently in a level set representation by letting the $\phi = 0$ level represent the island boundaries of the first monolayer, the $\phi = 1$ level represent the island boundaries of the second monolayer, and in general the $\phi = j - 1$ level represent the boundaries of islands in the jth monolayer, where ϕ is a smooth function (The 2 level case of this was introduced in [CHMO] to handle immiscible fluids.) In this regard, ϕ is just a smooth version of the surface height function $h(x, y)$, which is integer valued and jumps at the boundaries Γ_i. Indeed, $h = (\phi)$, where (z) denotes the least integer greater than z. The advantage of computing with ϕ is that its smoothness allows us to solve the level set advection equation and compute normals, curvature, etc of island boundaries much more accurately. However, note that there is no longer a simple

canonical choice for such a smooth ϕ. In practice, we simply allow ϕ to evolve from the trivial initial $\phi = -0.5$, through the processes of nucleation an growth. But it is no longer convenient to reinitialize ϕ during the calculation.

Nucleation Island nucleation is modeled simply by selecting a nucleation site on the grid, and increasing the ϕ values at this point (and a few neighboring points) by $+1$, which automatically introduces a new $\phi = j$ level, consisting of the smallest loop that is representable on the grid. Such an island is born with a small, grid dependent area, and in order to better conserve the total number of atoms, we include a loss term in the adatom transport equation proportional to the nucleation rate dn/dt and the area of this small newly seeded island. This is a small $O(dx^2)$ correction to the ideal equations, for the sake of better discrete conservation of atoms.

Connected Components Gathering statistics in the island dynamics model requires counting the number of islands, and determining their individual areas, boundary lengths, etc. Individual islands are precisely the connected components of the $\phi = 0, 1, 2, \ldots$ levels. Thus we require an algorithm for identifying connected components of level sets. In contrast, many level set applications never require such distinctions.

A practical and fast algorithm can be based on the iterative propagation of an arbitrary component label on the grid, as follows: the goal is to label every connected component, and also label each grid point as being in a certain connected component. Starting from an arbitrary node, it is labeled as being in component 1. At each iteration, every labeled node passes its label to its neighbors that are (a) unlabeled and (b) are not separated from it by a $\phi = 0, 1, 2, \ldots$ boundary. Whenever there are no such neighbors found for any of the labeled nodes, we select any remaining unlabeled node and give it the label 2, and continue in this fashion. This process terminates when all nodes have been labeled. The connected component j simply consists of all nodes with the label j, and the total number of connected components N equals the highest value of the label used. This arbitrary labeling allows us to count and locate each of the $j = 1, 2, \ldots, N$ islands in the domain. Combined with the subgrid representation of the component boundaries implicit in ϕ, we can accurately compute all the individual island properties without ever having to apply any complicated decision procedures to locate components.

Penalty Formulation of Internal Boundary Conditions In [CMOS], the internal boundary conditions for the Stefan problem were implemented in direct fashion, which was relatively simple in the level set formulation. However, it required the use of spatial difference stencils for the Laplacian that are one-sided, irregular, and include

small cut cells (and hence require implicit timestepping to avoid CFL limitations) near the interface. It is desirable to have an even simpler level-set based method for Stefan problems that avoids all these complications due to irregular discretization.

To achieve this, we have implemented the $\rho|_\Gamma = 0$ condition of the Irreversible Aggregation model via a penalty formulation. In order to keep ρ near zero on Γ we simply add a strong spatial sink term, proportional to ρ and concentrated only on Γ. I.e., the sink is proportional to a delta function concentrated on Γ. Thus the diffusion equation with internal boundary conditions is replace by the diffusion-sink equation

$$\frac{\partial \rho}{\partial t} = \nabla(D\nabla\rho) + F - K\rho\delta_\Gamma$$

with no added internal boundary conditions. Here δ_Γ is a delta function on the island boundaries, which is represented by the usual level set means ([CHMO], [SSO]). K is a large penalty constant, which should scale like D/ϵ, where ϵ is the width of the smoothed out delta function used in practice. This formulation is similar to the delta function source term formulations used to treat surface tension forces (which otherwise would be internal boundary jump conditions on the PDEs) in two-phase flow, [CHMO], [SSO]. The advantage is that this form can be discretized using standard stencils, and solved using standard diffusion equation solvers (in particular, explicit timestepping can be used for the evolution, if we want the simplest possible implementation).

In the context of Stefan problems, this form can be derived more abstractly by viewing dynamics of ρ as a constrained steepest descent on the gradient energy of ρ, $E[\rho] = \int D|\nabla\rho|^2$, and then including the constraint $\rho_\Gamma = 0$ into the energy as a penalty term of the form $\int K\rho^2\delta_\Gamma$. Using this energy formulation, it is also possible to conveniently express more general Γ-boundary conditions as well, in terms of other penalties or as changes in D (diffusion barriers, mimicking the physics that yields such conditions) that are concentrated only the island boundaries.

One nice side effect of this formulation is that if atoms attaching to the boundary are counted by integrating the local sink term—instead of the local gradient flux of ρ—we get this simple asymptotic expression for the boundary velocity

$$v_n \approx K\rho$$

on the island boundary. This is a pointwise evaluation rather than the less local $[\partial\rho/\partial n]$ from the internal boundary condition formulation. Note that ρ is nearly 0, but this is balanced by fact that K is very large. In the $K \to \infty$ limit, the correct and well-defined v_n is obtained.

3.4 Computational Results

Figure 1 shows the island boundary evolution for the simple Uniform Density model, in the case where the specified normal velocity is isotropic. The figures shows the view one would have looking directly down at the surface, at coverages (ratio of number of atoms deposited on the surface to the number of lattice sites on the surface) of 10%, 50% , 100% and 130%. Islands on the first monolayer are shown with solid line boundaries, while those on the second monolayer have dashed line boundaries and those on the third (one such island is shown in the 130% coverage case) have dot-dashed line boundaries. These calculations were done on a 128×128 numerical grid.

Figure 2 shows a similar evolution (computed on a 256×256 grid), except the specified normal velocity now has a three-fold anisotropy, which causes the islands to naturally assume an asymptotically triangular ("Wulff") shape as they grow. We emphasize that this shape is not imposed on the growth—it is simply the asymptotic shape that results from a particular simple normal velocity specification $v_n(\vec{n})$, as proven in [OM].

These results from the simple Uniform Density model illustrates the ability of our numerical method to capture the types of growing and merging anisotropic shapes that are observed in real epitaxial growth conditions. For example, certain metals grown on certain silicon substrates produce very precise triangular island shapes.

Figure 3 shows results from the Irreversible Aggregation model, using realistic physical parameters for D, F and the size of the system ($D/F = 10^6$, the growth is on a lattice of 400×400 atoms). The island boundaries are shown at coverages of 10% and 50%, and the corresponding adatom density $\rho(x, y_0)$ profiles along a cross section $y = y_0$ through the middle of the spatial domain are also show. Note how the adatom density dips towards zero at island boundaries, as desired in this model. (Note: it does not vanish exactly due to the penalty formulation of the boundary condition used here.) The two density plots illustrate how the adatom density is lower when there are a large amount of step edges on the surface to soak up adatoms. The calculations were done on a 128×128 numerical grid. A total of 56 islands were nucleated during the growth of one complete layer in this simulation, which implies that a similar number of merger events took place curing the course of filling in the layer.

3.5 Conclusion

Our recent results, as illustrated here, demonstrate that the Island Dynamics models include the desired physical features, and that the level set numerical methods can effectively solve these models. Together, they provide a promising new framework for

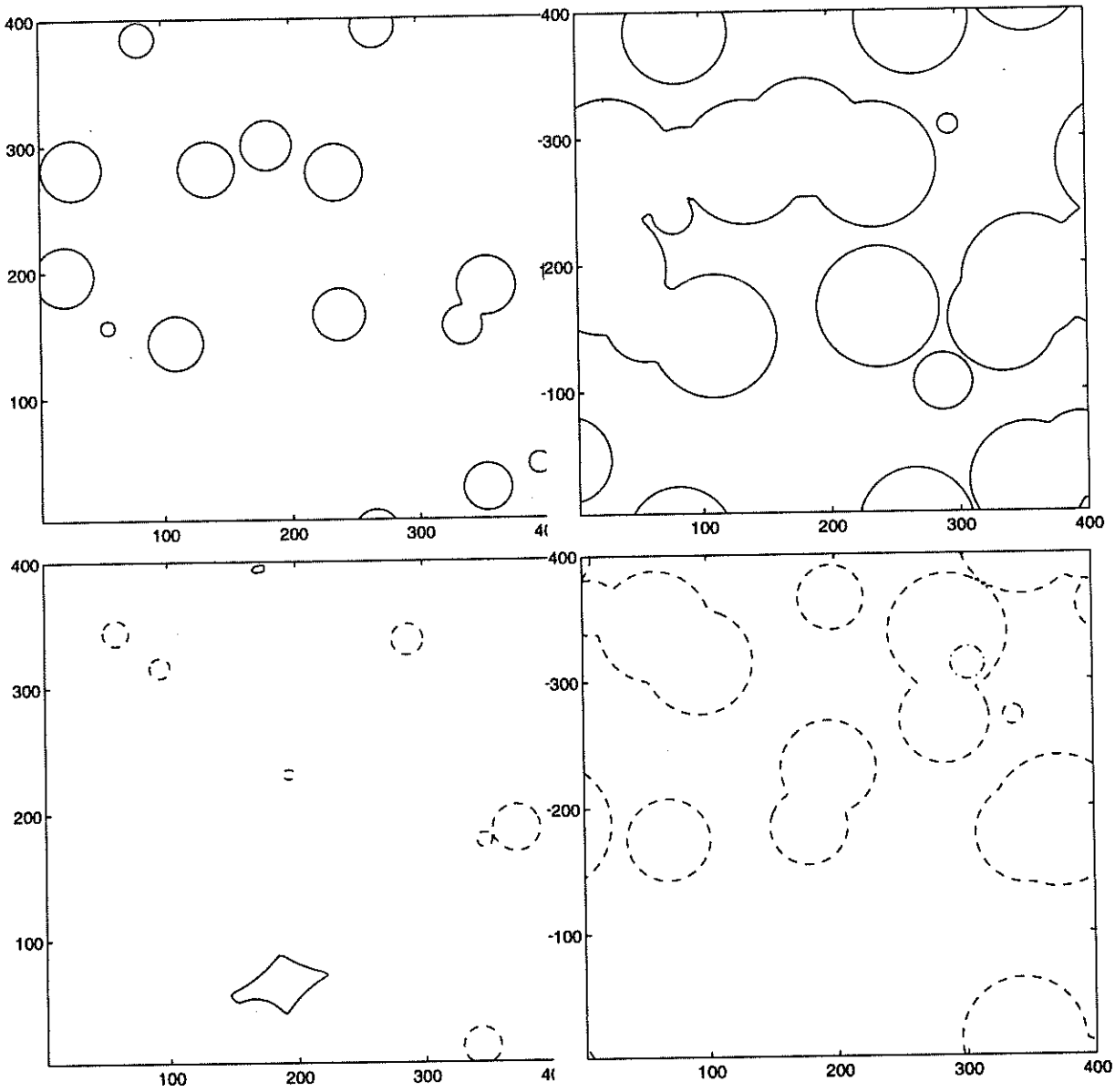

Figure 1: Island boundaries during growth in the simplified Uniform Density model, with isotropic normal velocity, at coverages of 10%, 50%, 100% and 130%. Islands on the first, second and third monolayers are shown with solid, dashed, and dot-dashed lines, respectively.

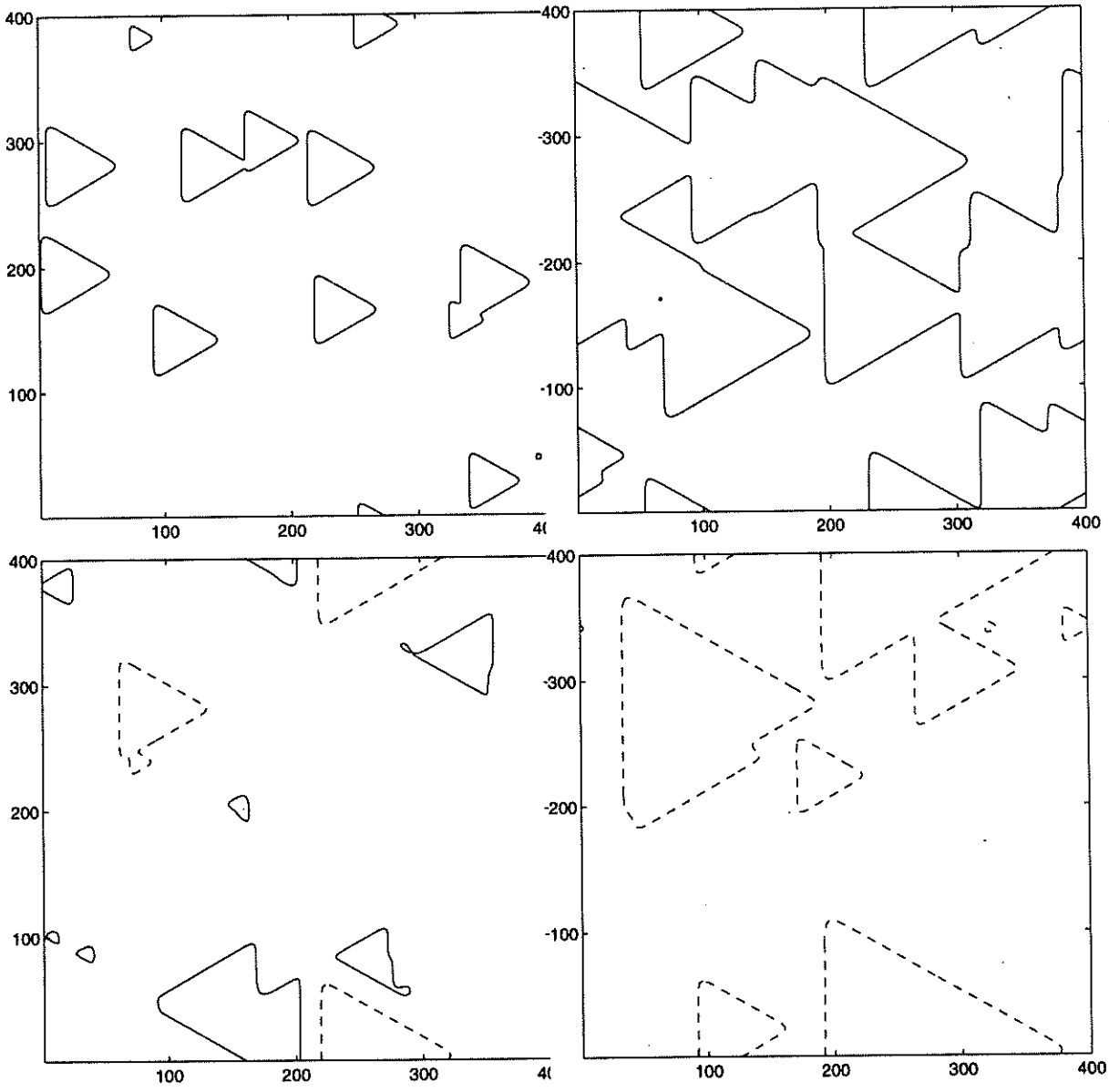

Figure 2: Island boundaries during growth in the simplified Uniform Density model, with anisotropic normal velocity, at coverages of 10%, 50%, 100% and 130%; line dashing indicates different monolayers. The islands are nucleated circular, but rapidly assume the triangular Wulff shape associated with their anisotropic velocity v_n.

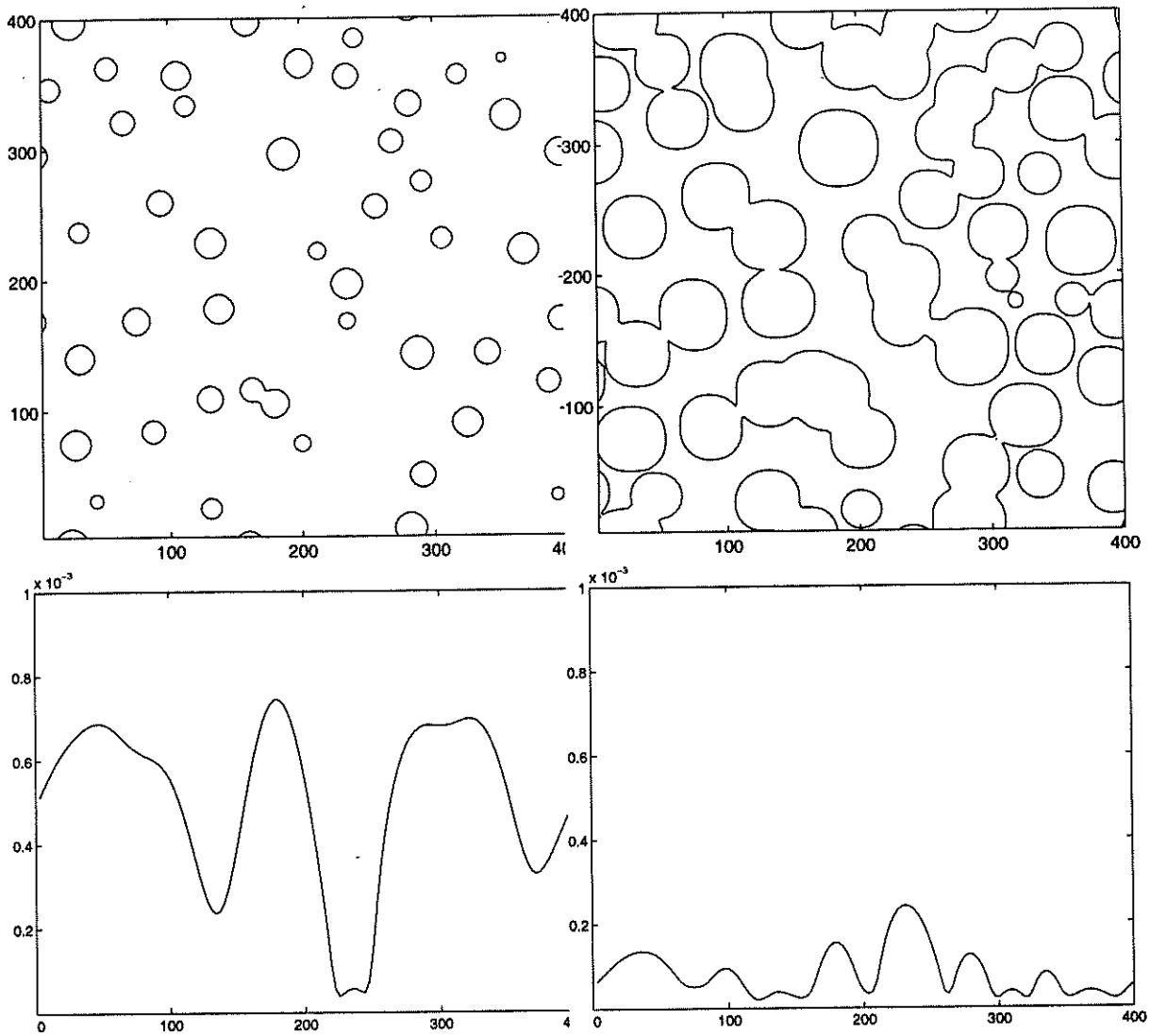

Figure 3: Island and adatom density evolution in the Irreversible Aggregation model. The surface is shown at 10% and 50% coverages; associated adatom densities are shown along the horizontal midline through the domain. Note the much lower mean density at 50% coverage, due to greater absorption at the many island boundaries.

doing analysis and control of thin film epitaxial growth.

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