The Mathematics of Moving Contact Lines in Thin Liquid Films

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Thin Films and Moving Contact Lines

The motion of a liquid under the influence of surface tension is a phenomenon we experience every day when we take a shower, drink a cup of coffee, or turn on the windshield wipers. All of these real-world situations involve not only the motion of the liquid and surrounding air but also their interaction with adjacent hard surfaces. As we know from waxing our cars and cooking with nonstick cookware, the dynamics of a fluid coating a solid surface depend heavily on the surface chemistry. Many industrial processes, ranging from spin coating of microchips to de-icing of airplane wings, rely on the ability to control these interactions.

An ongoing challenge is to explain the underlying physics of the motion of a *contact line*, a triple juncture of the solid/air, solid/liquid, and liquid/air interfaces. When the system is at rest, the three interfacial energies, determined by the energy per unit area γ_S ($S = sa$, sl, or la) on each surface, are in balance, and an equilibrium contact angle θ satisfying

$$\gamma_{sa} - \gamma_{sl} - \gamma_{la} \cos\theta = 0 \tag{1}$$

results. (See Figure 1. A derivation appears in [13].) However, the dynamically evolving contact line requires much more subtle modeling involving the interaction among multiple-length scales; the reason for this is born in the underlying fluid dynamics.

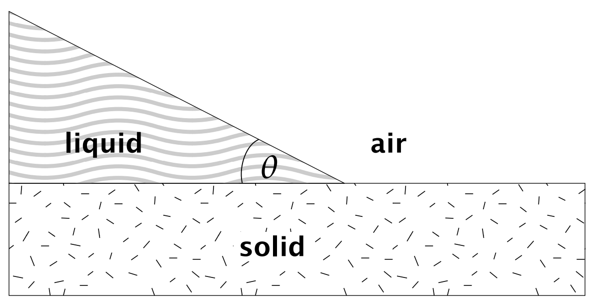

Figure 1: Simple trigonometry is all that is needed to derive Young's law (1), which is the equation for the equilibrium contact angle. However, in cases like complete wetting or driven contact lines a dynamic model is required. Physicists have been fascinated by this problem for decades.

The classical theory of fluids [1] tells us that when a viscous fluid meets a solid boundary, the correct model for the boundary is a "no-slip" condition on the solid/liquid interface.[1] Mathematically this requires setting the fluid velocity to be zero on the solid boundary. While this makes sense for the *Navier-Stokes equations* (describing the motion of an incompressible fluid) in bounded domains, its relevance to the moving contact line problem is dubious. The problem is that a moving contact line coupled with a no-slip condition on the liquid/solid interface results in a multivalued velocity field. This means that the velocity field is not

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[1] *See [15], pp. 676–680, for a comprehensive discussion of the history of the "no-slip" boundary condition.*

well defined at the contact line because the limit along the surface is zero, while the limit along the liquid/air interface (which is moving) is nonzero. Regardless of the liquid/air interface model, the tangential component of force exerted by the fluid on the solid diverges whenever the velocity is multivalued at the contact line [14, 18].

The fact that such a paradox exists is hardly surprising. We should not expect to find a self-consistent *universal* hydrodynamic model that does not incorporate the surface chemistry. Several models have been proposed to study the motion of moving contact lines. All of them involve adding an additional effect on a microscopic length-scale. The two that we discuss in the next paragraphs are (1) weakening the no-slip boundary condition via a slip condition effective at small scales and (2) incorporating the effect of long-range "Van der Waals forces" between the liquid and solid.

Perhaps the simplest context in which to test these theories is that of thin viscous coating flows. For such problems a lubrication approximation simplifies bulk flow fluid dynamics to a single equation, relating the depth-averaged horizontal fluid velocity to the shape and thickness of the liquid/air interface. The *Navier slip* condition[2] near the liquid/solid interface demands that the velocity at the interface be proportional to its normal derivative:

$$u = \frac{\partial u}{\partial z} k(h) \quad \text{at} \quad z = 0. \tag{2}$$

Here u is the vector-valued horizontal fluid velocity and z is the variable in the direction normal to the solid surface. The parameter $k(h)$ is a slip parameter and can depend on the thickness h of the film. We can think of condition (2) as a generalization of the standard no-slip condition, which corresponds to $k \equiv 0$ in (2).

Another choice for removing the singularity due to no slip is to include microscopic scale forces, in the form of long-range *Van der Waals* (VW) interactions between the liquid and solid substances, near the contact line. The most systematic way to do this is via an additional body force in the fluid of the form[3]

$$\Pi(h) = A_D h^{D-5}, \tag{3}$$

where D is the dimension of the substrate.[4] Here A_D is the Hamaker constant, depending on the dimension of space and also on the strength of the interaction between the liquid and solid particles. The sign of A_D depends on whether the VW forces are attractive or repulsive. The particular power in (3) comes from assuming the particles in the fluid interact with particles in the solid substrate via a "nonretarded" potential. The references [13] and [20] and the references therein provide more discussion of this and other potentials.

The lubrication approximation can be derived from a systematic rescaling and asymptotic expansion of the Navier-Stokes equations in the limit of vanishing *capillary number* C_a and *Reynolds number* R_e, two dimensionless parameters given by

$$Ca = \frac{3\nu V}{\gamma}, \quad R_e = \frac{\rho V h_0}{\nu}, \tag{4}$$

where ν is viscosity, γ is surface tension, and V is the characteristic velocity of the film. The result is the dimensionless lubrication equation

$$\begin{gathered} h_t + \nabla \cdot (f(h)(\nabla \Delta h - \nabla g(h))) = 0, \\ f(h) = h^3 + b^{3-p} h^p, \\ g(h) = (Ca)^{1/2} h + C\Pi(h). \end{gathered} \tag{5}$$

Here b represents a dimensionless slip length, and C is a dimensionless parameter that depends on the Hamaker constant and the characteristic height h_0 of the film.

Typically only a subset of the terms in the equation appear in any one given paper. For example, Greenspan [16] derives (5) with $b > 0$, "singular slip" $p = 1 > 0$, and $\Pi(h) = 0$. Haley and Miksis [17] consider this same model with different integer values of $p = 0, 1, 2$. Williams and Davis [24] study film rupture due to Van der Waals interactions via an equation of the type (5) with $b = 0$ (no slip) and the incorporation of Van der Waals forces (with $\Pi < 0$). In all cases the highest-order term in the model describes fourth-order degenerate diffusion, a phenomenon we discuss in more detail in the next section.

The engineering and applied mathematics literature has had much discussion of the most appropriate boundary conditions for an equation of the form (5) near the vicinity of a contact line, especially in the context of a slip model.[5] During the past eight years mathematicians working in the field of nonlinear PDEs have become interested in this problem from a more analytical point of view.

In this article we explain some of the fundamental mathematics problems associated with such equations as well as some of the rigorous machinery and numerical methods that have been developed recently to attack these problems.

Fourth-Order Degenerate Diffusion

Diffusion equations arise in models of any physical problem in which some quantity spreads or smears out. The classical example is the heat equation $h_t = \nabla \cdot k \nabla h$ where the diffusion coefficient k controls the rate at which heat "diffuses" through

[2] *A generalization of the no-slip condition in which the fluid is allowed to slip tangentially along the solid boundary.*

[3] *As in §II.D of [13] and in §II.E of [20].*

[4] *That is, $D = 2$ for a film on a two-dimensional surface and $D = 1$ for a flow in the plane, bounded by a line.*

[5] *See §§II.B and V of [20] and the references therein. See also Hocking, J. Fluid Mech.* **239** *(1992).*

the medium. In order to understand the models proposed in equation (5) we need to understand something about *degenerate diffusion equations*, where the constant k depends on the solution u in a degenerate way, so that $k \to 0$ as $u \to 0$. A family of second-order degenerate diffusion equations is known as the *porous media equations* [21]:

$$h_t - \Delta(\Phi(h)) = 0, \tag{6}$$

where $\Phi'(h) > 0$ for $h > 0$ and $\Phi(h) \sim h^m$ as $h \to 0$. Here $m > 1$ makes the equation degenerate.

The Laplacian operator Δ endows the evolution equation (6) with some well-known special properties:

1. *Instantaneous smoothing* of the solution in regions of positive h, since the equation is uniformly parabolic (i.e., the "diffusion coefficient" is bounded away from zero) where the solution is bounded away from zero.
2. *Maximum principle.* The solution is bounded from above and below by its initial data. This is true regardless of whether or not $m = 1$ (heat equation) or $m > 1$.
3. *Well-posed weak solutions* for smooth nonnegative initial data.
4. *Finite speed of propagation* of the support of the solution.

The last property is special to *degenerate* diffusion ($m > 1$). The heat equation ($m = 1$) has infinite speed of propagation of the support.

Consider now the fourth-order analogue of (6),

$$h_t + \nabla \cdot (f(h)\nabla\Delta h) = 0. \tag{7}$$

In the context of thin film dynamics we are interested in questions of existence, uniqueness, and finite speed of propagation of the support of weak solutions of equations of the form (7). The important difference from the case (6) is that (7) is fourth order as opposed to second order. It is diffusive, so we have property (1), instantaneous smoothing where the solution is positive; but property (2), the maximum principle, is far from guaranteed. Indeed, if we take the nondegenerate case $f(h) = 1$, then solutions can change sign. This can be seen by simply examining the heat kernel for fourth-order diffusion in $\mathbf{R}^D$ and noting that unlike the well-known second-order heat kernel, the fourth-order heat kernel has an oscillatory exponentially decaying tail that changes sign. This behavior is illustrated in the color image shown on the cover of this issue. It is not immediately apparent why the nonlinear problem (7) should have solutions that preserve their sign.

What is remarkable is that the nonlinear structure of (7) can endow it with a positivity-preserving property. In particular, one can show for one space dimension for $f(h) = h^n$ with $n \geq 3.5$ on a periodic spatial domain that if the initial condition h_0 is positive, then the solution $h(x,t)$ is guaranteed to stay positive. In fact, one can derive an a priori pointwise lower bound depending only on the H^1 norm and minimum value of the initial data. This form of a weak maximum principle is due to the nonlinear structure of (7), not the structure of the fourth-order diffusion operator. It is noteworthy that other fourth-order degenerate diffusion equations with different nonlinear structure have weak solutions that change sign (F. Bernis, *Nonlinear analysis and applications*, 1987). Despite the positivity-preserving property for large n, solutions of (7) with smaller values of n computationally exhibit finite-time singularities of the form $h \to 0$. We discuss this phenomenon in more detail in the next section. The fact that such singularities may occur makes the development of a weak solution theory, analogous to that of the porous media equation, all the more difficult. Over the past few years, mathematical machinery, largely involving energy estimates and nonlinear entropies, have been developed to address these problems. Such methods have been used to prove weak maximum principles, to derive existence results for weak (nonnegative) solutions, and to prove results concerning the finite speed of propagation of the support of nonnegative solutions (F. Bernis, 1996 articles in *Adv. Differential Equations* and *C. R. Acad. Sci. Paris*).

Finite-Time Singularities and Similarity Solutions of Lubrication Equations

The study of finite-time singularities and similarity solutions of (7) began in the early 1990s by a group at the University of Chicago. The original project addressed the breakup of a thin neck in the "Hele-Shaw cell" when forced by external pressures. The experiment, performed by Goldstein at Princeton [11], can be modeled, via lubrication theory, by a fourth-order degenerate diffusion equation in one space dimension:

$$h_t + (h^n h_{xxx})_x = 0 \tag{8}$$

with "pressure" boundary conditions $h(\pm 1) = 1$, $h_{xx}(\pm 1) = -p$, and $n = 1$. Carefully resolved numerical computations revealed that this problem yields both finite and infinite time singularities for various initial data.

What is unusual about the structure of these singularities is that, while they locally have self-similar structure of the form

$$h(x,t) \sim \tau(t) H\left(\frac{x - a(t)}{l(t)}\right), \tag{9}$$

the time dependences τ, $l(t)$, and $a(t)$ are not determined by dimensional analysis of the PDE. Such anomalous "second type" scaling [3] arises in problems like the focusing solution of the porous media equation (Aronson and Graveleau, European J. Appl. Math. (1993)), where one solves a nonlinear eigenvalue problem to determine the profile H and the relationship between scales τ and $l(t)$.

However, in the case of the lubrication singularities above, the scaling relations are typically found by asymptotic matching involving the boundary conditions or matching to an intermediate length-scale.

The original work on the Hele-Shaw problem was subsequently generalized to the case of variable nonlinearity (other values of n) with other boundary conditions [10, 2] and to different fourth-order degenerate PDEs (SIAM J. Appl. Math (1996), by the author). The similarity solutions observed were found using careful numerical computations involving adaptive mesh refinement near the singularity. Scaling was observed for many decades in h_{min}. All of these papers make the following observations:

- All observed finite-time singularities of the form $h \to 0$ as $t \to t_c$ involve second type scaling behavior in which the similarity solution described in (9) satisfies the quasi-static equation $(f(h)h_{xxx})_x = 0$.
- Sometimes several kinds of similarity solutions can occur for different initial conditions within the same equation. The far field dynamics of the structure may cause the similarity solution to destabilize, at arbitrarily small length-scales, from one type of similarity solution to another [2].

As an example, consider equation (8) with $n = 1/2$, periodic boundary conditions on $[-1, 1]$, and initial condition

$$h_0(x) = 0.8 - \cos(\pi x) + 0.25\cos(2\pi x). \tag{10}$$

The solution develops a finite-time "pinching" singularity with a simultaneous blowup in the fourth derivative. The third derivative forms a step function (see Figure 2). Near the pinch point the solution has a leading order asymptotic form

$$h(x,t) \approx c(t_c - t) + \frac{p(x - x_c)^2}{2},$$

where t_c is the time of pinch-off and x_c is the pinch point and the constant p is the curvature of the interface at the time of pinch. The blowup in higher derivatives can be seen only in higher-order terms:

$$h_{xxx} \approx \frac{cx}{\sqrt{c(t_c - t) + p(x - x_c)^2/2}},$$

so that the local curvature h_{xx} has the form

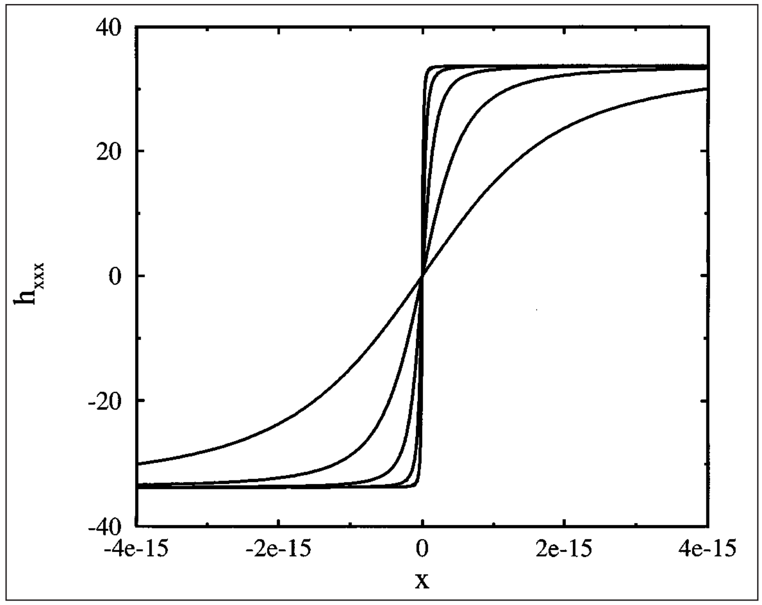

Figure 2: Onset of initial singularity in solution of (8) with $n = 1/2$ and initial data (10). Formation of a jump discontinuity in the third derivative. The solution can be continued after the initial pinch-off singularity. We discuss the continuation of this particular example later in this paper (see Figures 3–5).

$$p + \frac{c}{p}\sqrt{c(t_c - t) + p(x - x_c)^2/2}.$$

This scaling structure of the singularity was confirmed via numerical simulations using a self-similar adaptive mesh refinement code that resolved the singularity over thirty orders of magnitude in $h(x_c, t)$. The solution can be continued after the initial pinch-off singularity. We discuss the continuation of this particular example later in this paper (see Figures 3–5).

The fact that we can rigorously prove that finite-time singularities cannot occur for $n \geq 3.5$ yet they are observed for certain $n < 2$ suggests the existence of a *critical exponent*. This is a value of $n_* > 0$ for which solutions to (8) stay positive whenever $n > n_*$ and where finite-time singularities are possible for $n \leq n_*$. To date no such n_* has been established, but numerical simulations suggest that $1 < n_* < 3.5$. It is also not clear whether n_* depends on boundary conditions. Since singularities appear to be localized, it is reasonable to expect that n_* might be independent of boundary conditions. It is an interesting open question whether this behavior persists in higher space dimensions ($D > 1$).

Entropies, the Weak Maximum Principle, and Weak Solutions

In the previous section we discussed the open problem of finding a "critical exponent" associated with strictly positive initial data: equations with exponent larger than n_* have solutions that remain strictly positive, while ones with exponents less than n_* allow for the possibility of finite-time singularities. Critical exponents are also relevant for the weak solutions that continue the evolution after a "touch down" singularity or that evolve nonnegative initial data. Here the critical exponent n_{crit} separates equations for which the solution has increasing support from equations for which the support of the solution cannot increase. For the porous media equation (6), the support of the solution is always monotonically increasing, regardless of the size of $m > 1$. For the lubrication equation (8) with $D = 1$, the support of the solution cannot increase whenever $n \geq 4$, as is shown in [6]. On the other hand, there are solutions with support that eventually increase to fill the entire domain for all $n < 3$. It has been conjectured that the critical exponent for increasing support is $n_{crit} = 3$, but this remains to be proved.

The exact value of the critical exponent has important ramifications for the moving contact line problem. If indeed $n_{crit} = 3$, it tells us that there are no solutions of (5) with $b = 0$ (no slip) that describe a moving contact line. Such a result would not be surprising. It is consistent with the fact that such a scenario introduces a multivalued velocity field that is known to produce infinities in the physics (hence the introduction of the slip terms that give $n < 3$).

Examples of known exact solutions support the conjecture that $n_{crit} = 3$ in both one and two space dimensions. One class of examples is known as the "source type solutions", solutions that start as a delta function at the origin and spread out in a self-similar way while conserving their mass. Starov [22] looked for such solutions to (7) with $f(h) = h^3$ in two space dimensions. He was trying to find a similarity solution to describe spreading drops under the influence of surface tension. What he discovered was that the resulting ODE for the similarity solution did not have any solutions of compact support. That is, there are no similarity solutions describing spreading drops with no-slip on the solid/liquid interface. Bernis and collaborators[6] showed that in all space dimensions source type solutions ($f(h) = h^n$) exist for $n < 3$ and they cease to exist for $n \geq 3$. What is interesting is that this critical exponent cannot be predicted from dimensional analysis of the equation; it is determined by properties of the ODE for the shape of the similarity solution. Traveling wave (i.e., advancing front) solutions also change behavior at the critical exponent[7] of 3.

We now discuss some of the key ideas used to prove results about the PDE (7). A seminal paper in the mathematical development of the theory of weak solutions for lubrication-type equations is the work [7] by Bernis and Friedman. There they showed that, in addition to conservation of mass,

$$\frac{\partial}{\partial t}\int h(x)dx = 0, \tag{11}$$

and surface tension energy dissipation,

$$\frac{\partial}{\partial t}\int |\nabla h|^2 = -\int f(h)|\nabla \Delta h|^2 dx, \tag{12}$$

equations of the type (7) possess a nonlinear *entropy* dissipation of the form

$$\frac{\partial}{\partial t}\int G(h) = -\int |\Delta h|^2 dx. \tag{13}$$

Here $G(h)$ is a convex function satisfying $G''(h) = 1/f(h)$. For the case $f(h) = h$ (e.g., Hele-Shaw) the entropy $\int G(h)$ is of the form $\int h \log h$; hence the name "entropy" was born [9] to describe this object. Using the entropy (13), Bernis and Friedman proved that in one space dimension the critical exponent n_*, above which singularity formation is forbidden, satisfies $n_* < 4$. The proof uses the fact that (12) and conservation of mass imply an a priori bound on the $C^{1/2}$ norm of the solution while (13) insures a bound on $\int h^{2-n}$. This gives an a priori pointwise lower bound for the solution.

It turns out that the integral $\int G(h)dx$ above is not the only dissipative entropy. In one dimension we also have a family of entropies satisfying

$$\frac{\partial}{\partial t}\int G^s(h) \leq 0, \quad (G^s)'' = \frac{h^s}{f(h)}, \tag{14}$$

where $\frac{1}{2} \leq s \leq 1$. Taking $s \to \frac{1}{2}$ gave the upper bound $n_* \leq 3.5$ proved in [10].

The generalized entropy plays an important role in the development of a weak existence theory for nonnegative solutions from nonnegative initial data and for proving results on finite speed of propagation of the support. Uniqueness of weak solutions still remains an open problem. Later in this paper we see how entropies have also been used recently to design numerical methods for solving these equations.

Weak Solutions versus Constitutive Laws for Moving Contact Lines

The recent results on weak solutions of (7) have interesting ramifications for the moving contact line problem. Consider, for example, equation (5) with $f(h)$ as given in (2) with $b > 0$, $0 < p < 3$, and $g(h) = 0$. This particular model has been used many times to describe motion of a moving contact line in either a partial wetting (where there exists an equilibrium configuration that locally solves Young's law (1)) or complete wetting context (where the liquid energetically prefers to wet the solid). Greenspan and McKay considered this model with "singular slip" ($p = 1$) and made an argument that an additional boundary condition at the contact

[6] *In Nonlinear Anal., TMA (1992), and European J. Appl. Math. (1997).*

[7] *Boatto et al., Phys. Rev. E.* **48** *(6) (1993).*

line, in the form of a constitutive law, was required to obtain a well-posed model. Such conditions make sense for nondegenerate fourth-order equations, but these arguments do not directly carry over to the general case where $f(h) \to 0$ as $h \to 0$.

On a more physical level, we see that the constitutive law and fixed contact angle models may make sense locally at a contact line, but they do not address things such as topological transition, i.e., what happens when two contact lines collide, or when a film ruptures and a new contact line forms.

Recent progress has been made at constructing more robust models for certain specific cases. For example, in the case of complete wetting we would like to construct a solution that has a zero contact angle and will eventually spread to cover the entire surface. It was proved in [6, 9] that such a solution does exist (for $D = 1$) for all slip conditions (2) with $0 < p < 3$. The solution is for general H^1 initial data and includes such phenomena as film rupture and droplet merger (see the computational example in the next section). The method of construction is to use the weak maximum principle for such problems and to construct a positive solution of a regularized problem (see, e.g., equation (18) below) and then pass to the limit in the regularization parameter. These results have recently been extended to higher space dimensions.[8] The higher-dimensional proof does not directly use the regularization (18), since it does not guarantee positive approximations in more than one dimension. However, the recent existence results are derived using higher-dimensional forms of the generalized entropies (14).

Another recent manuscript by F. Otto proves the existence of a fixed contact angle solution in one space dimension of (7) with $f(h) = h$. An interesting open problem is to try to extend this result to prove existence of fixed contact angle solutions for other slip models.

Van der Waals Forces and Superdiffusion

The Van der Waals model with $b = 0$ and $g(h) = C\Pi(h)$ also yields an interesting set of mathematical problems. Here we consider models of the type

$$\frac{\partial h}{\partial t} = -\mathrm{div}(h^3(\nabla(\Delta h - \Pi(h)))). \tag{15}$$

The singularity in $\Pi(h)$ (from (3)) yields an evolution equation (15) that has fourth-order *degenerate* diffusion and second-order superdiffusion. The latter refers to cases where the diffusion coefficient blows up as $h \to 0$. Superdiffusive problems are known from [12] and the references therein to have some strange behavior, including infinite speed of propagation of the support (as in the case of regular, nondegenerate diffusion) as well as the possibility of extinguishing of the solution in finite time.

In the case where $\Pi(h)$ is positive (attractive forces) this could lead to a model where the superdiffusive term leads to some unphysical behavior for the solution. However, it turns out that the model (3) for long-range Van der Waals interactions is valid only on a mesoscopic length-scale, that of 100–1000 Ångstroms. The model breaks down when the film reaches a molecular-scale thickness. There are two ways of dealing with this breakdown of continuum theory: one is to use a modified continuum model with a cutoff of the singularity in (3) on a molecular scale. The other is to use a molecular model on this scale. In a 1994 article in *Nonlinearity*, the author and Mary Pugh considered the former approach for the case of solutions of (3) that depend on only one space coordinate. We showed that if one uses a "porous media" type cutoff of (3), where the effective second-order diffusion coefficient behaves like the nonlinear term in (6) with $1 < m < 2$, then there exists a solution to (15) with support that eventually increases to fill the domain and has, almost every time, a zero contact angle at the edge of the support. Numerical simulations of the model show that the "porous media" cutoff dominates the behavior of the solution at the edge of its support.

A number of authors have performed simulations of molecular dynamics models of moving contact lines (see, e.g., [25, 23, 19]). However, the problem with a purely molecular model is that it is impossible to put enough particles in the system in order to see the interaction of the molecular scale with macroscopic structures several orders of magnitude larger than the molecular scale. An interesting and difficult problem is the understanding of the interactions between these microscopic effects and the large-scale dynamics such as surface tension.

Numerical Methods for Solving Lubrication Equations

The complex structure of the fourth-order PDE poses a challenging problem for the design of numerical methods for solving these problems. For the computation of nonnegative weak solutions, a nonnegativity-preserving "finite element method" was proposed in [5]. This method allows for solutions with positive initial data to lose positivity; a variational problem involving a Lagrange multiplier must then be solved to advance the nonnegative solution.

Even when the analytical solution is strictly positive, the solution of a generic scheme may become negative, especially when the grid is underresolved. And once the numerical solution becomes negative it cannot always be continued in time in

[8] *In Dal Passo et al., SIAM J. Math. Anal.* **29** *(2) (1998), and references therein.*

a unique or stable way. When a positive approximation of the solution is desired, it has been necessary to do computationally expensive local mesh refinement near the minimum of the solution in order to avoid such premature or "false" singularities [10]. Other examples include flow down an inclined plane,[9] where resolution was required at the apparent contact line, and the approximation of nonnegative weak solutions via strong solutions [8].

Recent work of L. Zhornitskaya and the author [26] shows that it is possible to use the entropy ideas above for smooth solutions of the PDE to construct numerical schemes that preserve positivity of the solution and hence have global solutions.

For example, consider a one-dimensional periodic domain divided up into N equally spaced intervals of size Δx, with nodes $x_0, \ldots, x_N$. Let y_i approximate $h(x_i)$, and denote by

$$y_{x,i} = \frac{y_{i+1} - y_i}{\Delta x}, \qquad y_{\bar{x},i} = \frac{y_i - y_{i-1}}{\Delta x},$$
$$y_{\bar{x}x,i} = \frac{y_{\bar{x},i+1} - y_{\bar{x},i}}{\Delta x}, \quad y_{\bar{x}x\bar{x},i} = \frac{y_{\bar{x}x,i} - y_{\bar{x}x,i-1}}{\Delta x}$$

the finite differences in space.

The coupled system of ODEs

$$\begin{aligned} &\partial_t y_i + (a(y_{i-1}, y_i) y_{\bar{x}x\bar{x},i})_x = 0, \\ &i = 0, 1, \ldots, N-1, \\ &y_i(0) = h_0(x_i), \end{aligned} \tag{16}$$

is a continuous-time discrete-space approximation of the PDE

$$\partial_t h + \partial_x (f(h) \partial_x^3 h) = 0$$

provided $a(y_{i-1}, y_i)$ approximates $f(h(x))$ (again, let $f(h) \sim h^n$ as $h \to 0$) on the interval $[x_{i-1}, x_i]$. One example of a choice of a is $a(s_1, s_2) = 0.5(f(s_1) + f(s_2))$.

While any choice of $a(s_1, s_2)$ yields a scheme that satisfies the discrete form of conservation of mass (11) and surface tension energy dissipation (12), only the special choice of

$$a(s_1, s_2) = \begin{cases} \frac{s_1 - s_2}{G'(s_1) - G'(s_2)} & \text{if } s_1 \neq s_2, \\ f(s_1) & \text{if } s_1 = s_2, \end{cases} \tag{17}$$

yields a scheme that dissipates a discrete form of the entropy (13) and preserves positivity of the numerical solutions for all $n \geq 2$. The lower bound on the solution depends on the grid size for $2 \leq n < 3.5$ and is independent of the grid size for $n \geq 3.5$. This special choice of discretization yields a scheme that, for all $n \geq 2$, has global solutions for arbitrary grid size and converges to a positive solution of the PDE as $O((\Delta x)^2)$.

[9] *As in Bertozzi and Brenner, Phys. Fluids* **9** *(3) (1997).*

This idea can be generalized to an abstract finite-element setting. For positive solutions the "entropy-dissipating" (EDS) finite-element method discussed in [26] differs from the one proposed in [5] only in that for the EDS scheme a nonlinear function of the solution $G'(z)$ is assumed to be in the element space instead of the solution z itself and an additional numerical integration rule is imposed. For solutions that lose positivity the scheme in [5] requires solving a variational problem, while EDS schemes are guaranteed not to lose positivity. We expect that the best choice of scheme will depend on the specific problem of interest.

We now present a computational example from [26] that illustrates the effectiveness of using a positivity-preserving (EDS) scheme over a generic one. Consider the example discussed earlier with initial condition (10) and $n = 1/2$. We discussed the formation of a finite-time singularity that exhibited a discontinuiuty in third derivative as $h \to 0$. From [7, 6, 9] we know that the solution can be continued in time as the limit of a sequence of positive approximations. That is, consider the regularization

$$\begin{aligned} &h_{\epsilon t} + (f_\epsilon(h_\epsilon) h_{\epsilon xxx})_x = 0, \\ &f_\epsilon(h_\epsilon) = \frac{h_\epsilon^4 f(h_\epsilon)}{\epsilon f(h_\epsilon) + h_\epsilon^4}. \end{aligned} \tag{18}$$

Coarse Grid Computation. Generic Scheme.

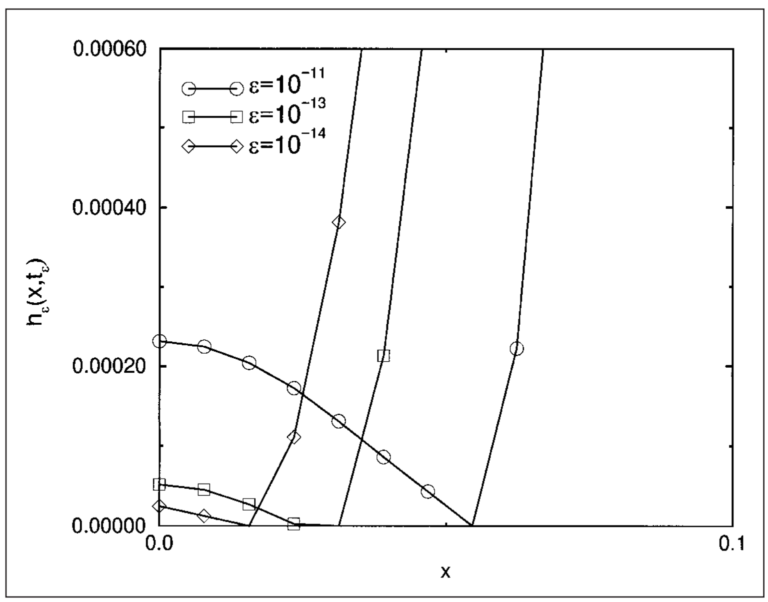

Figure 3: Failed attempt to compute, using a generic difference scheme on a coarse grid, the positive approximations of the weak continuation after the initial singularity described in Figure 2. Final times $t \approx$ 0.00086, 0.00076 and 0.00074 correspond to $\epsilon = 10^{-11}$, 10^{-13}, and 10^{-14}; 128 grid points on [0,1]; $\log_{10}$(min Δt) = −14. We could not continue computing beyond these times, since the numerical solution becomes negative.

Coarse Grid Computation. Entropy Dissipating Scheme.

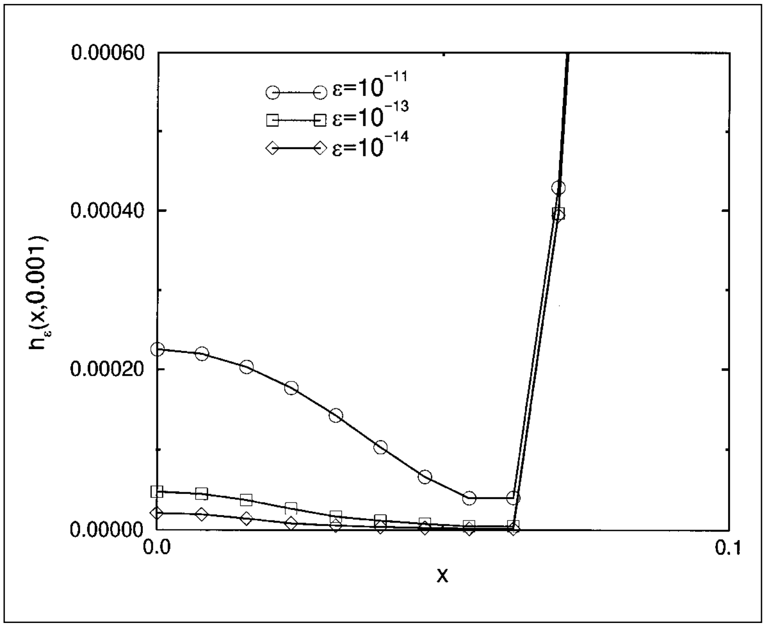

Figure 4: Successful attempt to compute, using an entropy dissipating scheme on a coarse grid, the numerical solution at fixed time $t = 0.001$, $\epsilon = 10^{-11}$, $\epsilon = 10^{-13}$, and $\epsilon = 10^{-14}$; 128 grid points on [0,1]; $\log_{10}(\min \Delta t) = -6.6$ for $\epsilon = 10^{-11}$, -7.2 for $\epsilon = 10^{-13}$, and -7.4 for $\epsilon = 10^{-14}$.

Fine Grid Computation. Entropy Dissipating Scheme.

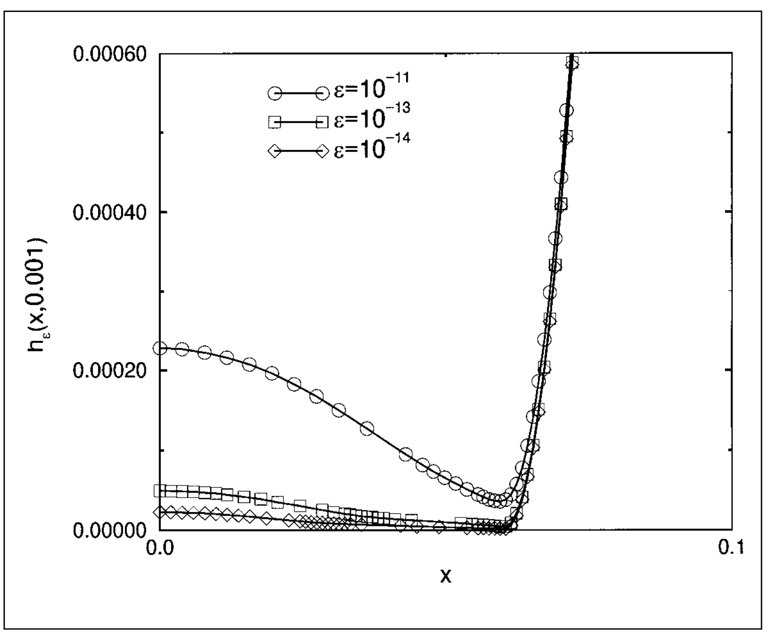

Figure 5: Comparison of computation in Figure 4 with numerical solution on a fine grid. Same fixed time $t = 0.001$, $\epsilon = 10^{-11}$, $\epsilon = 10^{-13}$, and $\epsilon = 10^{-14}$; 1,024 grid points on [0,1]; $\log_{10}(\min \Delta t) = -6.7$ for $\epsilon = 10^{-11}$, -7.0 for $\epsilon = 10^{-13}$, and -7.3 for $\epsilon = 10^{-14}$.

Since

$$f_\epsilon(h_\epsilon) \sim \frac{h_\epsilon^4}{\epsilon} \quad \text{as } h_\epsilon \to 0$$

we know that for all $\epsilon > 0$ the analytical solution of the regularized problem is positive. In [8] a nonnegative weak solution was computed numerically by taking successively smaller values of ϵ in the above. That paper used a scheme of the type (16) with $a(s_1, s_2) = f(0.5(s_1 + s_2))$. A fine grid was required to resolve the spatial structure and keep the numerical solution positive in order to continue the computation. Here we show that an entropy-dissipating scheme does a much better job at computing this problem without requiring excessive spatial resolution.

Figure 3 shows the computational results obtained by the generic scheme for three values of the regularization parameter $\epsilon = 10^{-11}, 10^{-13}$, and 10^{-14} on the grid that had 128 points on $[0, 1]$. In all of those cases we prescribed the final time to be 10^{-3}. However, the generic scheme developed a singularity earlier, which made us unable to compute the solution at the time prescribed.

Figure 4 shows the results that the entropy-dissipating scheme gave for the same input. In this case we did successfully compute the numerical solution at $t = 10^{-3}$. Note that in both cases we used the same purely implicit method for time integration, choosing the time step Δt small enough to ensure that the discrete-time system shows the same behavior as a continuous-time one.

Figure 5 shows the results obtained by the entropy-dissipating scheme on a much finer grid, namely, on the one that had 1,024 points on [0,1]. Note that even though the graphs look much smoother now, they show very good agreement with those shown in Figure 2.

Remarks

The contact line problem has generated some very interesting and difficult mathematical problems associated with the model equations discussed in this paper. In particular, questions of uniqueness of weak solutions and the precise value of critical exponents remain rigorously unresolved. In the case of critical exponents for finite-time pinch-off, it is difficult even to conjecture what the correct value might be. Much of the work on this particular aspect of the thin film equations is numerical, and this work has shown what is probably just a small subset of the kind of behavior that is possible for solutions of higher-order degenerate diffusion equations.

We find that the dynamics of the moving contact line models can lead to complicated structure of the solution in a neighborhood of the contact line. Indeed, the complications associated with the models described here have led applied mathematicians to look at new formulations for removing the singularity at the contact line [4].

It is the hope of the author that this article will spark more interest in these problems within the mathematical community which could lead to fruitful interactions with physicists and engineers working in this field.

Acknowledgments

The author thanks Michael Brenner, Anthony Knapp, and Mary Pugh for useful comments regarding this article. This work is supported by a PECASE award from the Office of Naval Research and by a Sloan research fellowship.

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About the Cover

Fourth-order diffusion (in R^2)of an initially nonnegative function with compact support. The top figure shows a surface plot of the positive part of the solution for the case of linear diffusion, $h_t = -\Delta^2 h$. The pattern of rings is due to the oscillatory behavior in the tail of the fourth-order heat kernel (behavior not present in second-order diffusion, like the heat equation). Fourth-order degenerate diffusion can remove the change in sign, as shown in the bottom surface. Here we start with the same initial data but evolve according to $h_t = -\nabla \cdot (h^2 \nabla \Delta h)$. Such degenerate diffusion equations arise in models for moving contact lines, as discussed in this article, starting on page 689.