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Numerics of contact line motion for thin films

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Abstract: We introduce an algorithm for the explicit treatment of contact line motion for thin-film problems and compare its solutions with exact source-type solutions and their asymptotic behavior near the contact line. The algorithm uses a variational formulation and avoids dealing with singularities near the contact line.

Keywords: thin fluid films, free boundary problems, numerical algorithms, self-similar solutions

1. MODEL AND ALGORITHM

The spreading of a viscous liquid droplet of height $h(t,x)$ over a solid substrate by surface tension is governed by a partial differential equation of the type

$$\dot{h} + (|h|^n h_{xxx})_x = 0, \tag{1a}$$
$$h(0,x) = h_0(x), \tag{1b}$$

where we use the notation $\dot{h} = h_t$ for time derivatives. For illustration of the geometry see fig. 1. The mobility exponent n depends on the type of friction with the substrate, where usually one has $0 < n \leq 3$ as it is discussed by Eggers (2004). Additionally we assume that the initial support is an interval $(x_-, x_+) := \operatorname{supp} h_0$, where $x_\pm$ evolve with time. As boundary conditions we consider a zero contact angle and specify a kinematic condition, so that for $t > 0$

$$h_x(t, x_\pm) = 0, \tag{1c}$$
$$\dot{x}_\pm = \lim_{x \to x_\pm} \left(|h|^{n-1} h_{xxx} \right). \tag{1d}$$

Solutions of (1) conserve the volume $v(t) = \int h \, \mathrm{d}x \equiv v(0)$ and it is known that the support moves with finite speed, see Hulshof et al. (1998). For $n > 1$ the kinematic condition (1d) implies $h_{xxx} \to \infty$ as $x \to x_\pm$ for the contact line to move with a finite velocity. This singularity with the fact that $h \to 0$ as $x \to x_\pm$ is one major difficulty in using (1d) to evaluate the velocity of the boundary.

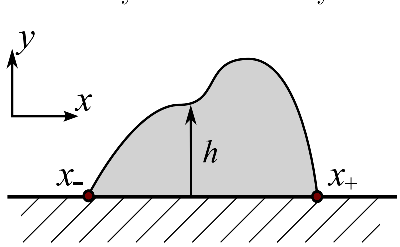

Fig. 1. droplet parametrized by h on a solid substate

The thin-film problem is known already for quite some time, i.e. existence of weak solutions was shown by Bernis and Friedman (1990). In the context the free-boundary problem above existence of solutions in weighted Hölder spaces was shown by Giacomelli and Knüpfer (2010). In general one can not guarantee that after starting with an interval (x_-, x_+) the solution will always stay strictly positive inside $(x_-(t), x_+(t))$ and no topological transitions occur.

Numerical algorithms for this problem mainly rely on global solutions for this problem, i.e. algorithms which solve for $h(t,x)$ for $x \in \mathbb{R}$ and preserve non-negativity outside (x_-, x_+) in a sense, see e.g. the works by Zhornitskaya and Bertozzi (1999); Grün and Rumpf (2000). Here we go a different route and do *not* look for global solutions but rather seek solutions of the free-boundary problem (1). Such an approach is certainly not feasible to treat topological transitions. Our proposed method is to first solve (1a) using the space and time-discrete variational formulation using finite elements just on the support (x_-, x_+). Here we seek piecewise linear functions $\dot{h}, \pi$ that satisfy

$$\int_{x_-}^{x_+} (\dot{h}\phi + |h|^n \pi_x \phi_x) \, \mathrm{d}x = 0, \tag{2a}$$
$$\int_{x_-}^{x_+} (\pi\varphi - \tau \dot{h}_x \varphi_x) \, \mathrm{d}x = \int_{x_-}^{x_+} h_x \varphi_x \, \mathrm{d}x, \tag{2b}$$

for all piecewise linear test functions ϕ, φ defined on an decomposition of the interval (x_-, x_+). No essential boundary conditions are imposed on solutions or test functions. Note that all appearances of h and $x_\pm$ are treated explicitly. In order to arrive at (2) we introduced a new variable $\pi = -h_{xx}$ and split (1a) in two second order equations. Furthermore we used (1c) the zero contact angle $h_x = 0$ and a no-flux condition $|h|^n h_{xxx} = 0$ at $x_\pm$ as natural boundary conditions. Only in (2b) defining π we replaced h by the more implicit expression $h + \tau\dot{h}$ where $\tau = t^{k+1} - t^k$ to obtain a stable method similar to a (semi)-implicit Euler method. For any given h defined on (x_-, x_+) this gives us the time-derivative $\dot{h}$ in the Eulerian reference frame.

However, we need another method to compute $x_\pm$ and h at time t^{k+1} from the corresponding data at time t^k. Here we use the fact that in a reference frame moving

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with velocity $\dot{\psi}$ time derivatives of $H(t, y) = h(t, \psi(t, y))$ simply transform according to

$$\dot{H} = \dot{h} + \dot{\psi} h_x, \tag{3}$$

where $y \in (x_-(t^k), x_+(t^k))$. If we choose $\psi(t, x_\pm(t^k)) = x_\pm(t)$ then $H(t, x_\pm(t^k)) \equiv 0$ which implies $\dot{h} = -\dot{\psi} h_x$ at $x_\pm$. In one spatial dimension we can simply choose

$$\psi(t, y) = x_-(t) + y\big(x_+(t) - x_-(t)\big), \tag{4}$$

with $y = (x - x_-(t^k))/(x_+(t^k) - x_-(t^k))$ as such a mapping. Now we can explicitly and uniquely determine $\dot{H}, \dot{\psi}$ from $\dot{h}$ using the known h_x and (3). For small time steps $\tau \ll 1$ we can assume $h_x \approx h_y$.

Note that for a finite contact angle this procedure makes sense in the discrete and continuous setting. However, one might wonder if evaluating (3) for $\dot{\psi}$ at a zero contact angle is well-defined at the boundary. At least for linear elements the weak derivative h_x is piecewise constant, so that provided h is positive inside (x_-, x_+) at t^k, then h_x has a proper nonzero sign.

Algorithm summarized

Thereby the strategy to solve the free boundary problem(1) is as follows.

For given solution $h, x_\pm$ at time t^k

(i) Solve the semi-implicit in time finite element variational formulation (2) for $\dot{h}, \pi$.
(ii) Use the prior information of h_x at t^k to compute $\dot{H}$ and $\dot{\psi}$ from the previously computed $\dot{h}$ as explained above.
(iii) Evolve h and the domain (x_-, x_+) by updating all vertices of the finite element decomposition and all nodal values according to

$$x^{k+1} = x^k + \tau \dot{\psi}(x^k),$$
$$h^{k+1} = h^k + \tau \dot{H},$$

as it is natural in a comoving coordinate system. Writing this slightly more detailed, what we mean is

$$h_i^{k+1} \equiv h^{k+1}(x_i^{k+1}) = h^k(x_i^k) + \tau \dot{H}_i \equiv h_i^k + \tau \dot{H}_i,$$
$$x_i^{k+1} = x_i^k + \tau \dot{\psi}(x_i^k),$$

for all nodes i of the domain decomposition. Note that the definition of ψ ensures x^{k+1} is again an admissible decomposition provided that $x_- < x_+$.

This concludes a single time-step of the algorithm. Note that this algorithm can be naturally extended to higher dimensions as we discuss later. Note that if we include boundary terms in the definition of π in (2b), then we can also include nonzero contact angles $|h_x| = \tan\theta$ in the problem. Using a variational approach to solve (1) is thereby superior to other numerical methods, e.g. finite differences, in the sense that it allows a simple implementation of all boundary conditions as natural boundary conditions. Furthermore note that (1) has a gradient structure with an energy E that decreases according to

$$\frac{d}{dt} E(h) = -\int |h|^n (\pi_x)^2 \mathrm{d}x < 0,$$

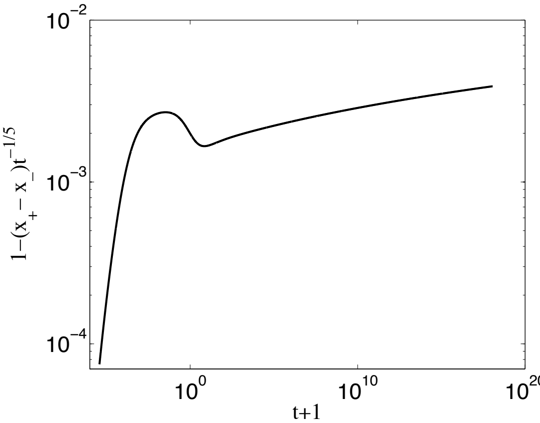

Fig. 2. Relative error of support width of numerical solution compared to exact solution at various times.

and $\pi = \delta E / \delta h$. For the problem here we have

$$E(h) = \int_{-\infty}^{\infty} \frac{1}{2} |h_x|^2 \, \mathrm{d}x.$$

2. NUMERICS FOR SOURCE-TYPE SOLUTIONS

The following section is intended as a validation for the numerical method proposed before. Therefor let us continue with a discussion of source-type solutions. These are solutions of (1) with initial data $h_0(x) = c\,\delta(x)$ of the form

$$h(t, x) = t^{-\alpha} f(\eta), \qquad \eta = x t^{-\alpha}$$

where $\alpha = \frac{1}{n+4}$. It was proven by Bernis et al. (1992) that there exist no source-type solutions for $n \geq 3$, whereas for $0 < n < 3$ there exists precisely one even nonnegative source-type solution. Only for $n = 1$ an explicit expression for a source-type solution is known

$$\hat{f}(\eta) = \begin{cases} \dfrac{1}{120}(a^2 - \eta^2)^2 & \text{for } -a < \eta < a \\ 0 & \text{otherwise,} \end{cases}$$

and it was found by Smyth and Hill (1988). We use this particularly smooth solution as a first test. The general behavior of the singularity for $\eta \to a$ depends on the exponent n. Bernis et al. (1992) furthermore prove the asymptotics of the solution is

$$f(\eta) \sim B_1 (a - \eta)^2 \qquad 0 < n < 3/2,$$
$$f(\eta) \sim B_2 (a - \eta)^2 (-\log(a - \eta))^{2/3} \qquad n = 3/2,$$
$$f(\eta) \sim B_3 (a - \eta)^{3/n} \qquad 3/2 < n < 3$$

as $\eta \nearrow a$. The case $3/2 < n < 3$ has been further sharpened by Giacomelli et al. (2013), who proved that higher order corrections of f can be written as an analytic function in two variables. In particular the next order of the expansion of f is of the form

$$f(\eta) \sim B_4 (a - \eta)^\nu \big(1 - b(a - \eta)^\beta + \mathcal{O}(a - \eta)^{\min\{1, 2\beta\}}\big)$$

where $\nu = 3/n$ and $\beta = \frac{\sqrt{-3\nu^2 + 12\nu - 8} - 3\nu + 4}{2}$. Such singularities are no particularity of source-type solutions but probably present in any moving contact line for $3/2 < n < 3$. In the case $n = 3$ contact lines do not move due to the well known contact line singularity. First we compare with the exact solution for $n = 1$. Using $h_0(x) = \hat{f}(x)$ with $a = 1/2$ gives the numerical and exact solution shown in fig. 3. In the finite element method we have used standard