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Contact Line Advection using the Level Set Method

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In this work, we consider the geometrical problem of the numerical advection of a hypersurface by a prescribed velocity field in the special case when the hypersurface intersects the domain boundary. This problem emerges from the discretization of continuum models for dynamic wetting. The kinematic evolution equation [1], [2] expresses the fundamental relationship between the rate of change of the contact angle and the structure of the transporting velocity field. We employ a simple version of the Level Set method to numerically solve the hyperbolic transport equation for the interface in two dimensions. The results are validated against an analytic solution of the kinematic evolution equation. Full access to the data and C++-implementations is provided via an open research data repository [3].

1 Introduction

We consider the problem of the advection (i.e. passive transport) of a moving hypersurface $\{\Sigma(t)\}_{t\in I}$ by a prescribed velocity field $v : I \times \overline{\Omega} \to \mathbb{R}^d$ (for $d = 2, 3$ and some interval I). For simplicity, $\Omega \subset \mathbb{R}^d$ is assumed to be a half-space with (planar) boundary $\partial\Omega$. The kinematic boundary condition governing the motion of the hypersurface is

$$V_\Sigma = v \cdot n_\Sigma \quad \text{on} \quad \operatorname{gr} \overline{\Sigma} := \{(t, x) : x \in \overline{\Sigma}(t)\}. \tag{1}$$

Here n_Σ denotes the interfacial normal vector field and V_Σ is the normal velocity of the moving interface, defined as

$$V_\Sigma(t_0, x_0) = \gamma'(t_0) \cdot n_\Sigma(t_0, x_0), \quad (t_0, x_0) \in \operatorname{gr} \overline{\Sigma}, \tag{2}$$

where γ is any $\mathcal{C}^1$-curve in $\operatorname{gr}\overline{\Sigma}$ passing through (t_0, x_0), see e.g. [5]. For the velocity field we assume that it is $\mathcal{C}^1(I \times \overline{\Omega})$ and tangential to the domain boundary, i.e. $v \cdot n_{\partial\Omega} = 0$ at $\partial\Omega$ (see Figure 1 for notation). Within the Level Set method (see, e.g., [5]), the moving hypersurface is described as the zero contour of some function ϕ, i.e. $\Sigma(t) = \{x \in \Omega : \phi(t, x) = 0\}$. The kinematic condition (1) translates to the hyperbolic transport equation

$$\partial_t \phi + v \cdot \nabla\phi = 0 \quad \Leftrightarrow \quad \frac{D\phi}{Dt} = 0 \quad \text{in} \quad \overline{\Omega} \tag{3}$$

for the Level Set function ϕ. One can show by the method of characteristics that (3) is well-posed as an initial value problem under the assumptions on v mentioned above. Notice that $v \cdot n_{\partial\Omega} = 0$ on $\partial\Omega$ prevents the need for boundary conditions for ϕ. We are now interested in the evolution of the *contact line* Γ. This is the curve of intersection of $\partial\Sigma$ with the boundary $\partial\Omega$, and the *contact angle* θ, i.e. the angle at which the interface meets the solid boundary. Mathematically, the contact angle is defined by the relation $n_\Sigma \cdot n_{\partial\Omega} = -\cos\theta$ on $\operatorname{gr}\Gamma$.

2 Contact Line Motion and Contact Angle Evolution

It follows from (1) and $v \cdot n_{\partial\Omega} = 0$ on $\partial\Omega$ that Γ is a material line, i.e. $\operatorname{gr}\Gamma$ is an invariant set for the initial value problem

$$\dot{x}(t) = v(t, x(t)), \quad x(t_0) = x_0 \in \Gamma(t_0). \tag{4}$$

As it has been shown in [1], the evolution of the interface normal vector along such a trajectory satisfies the ordinary differential equation (here $\mathcal{P}_{\Sigma(t)} = \mathbb{1} - n_\Sigma(t) \otimes n_\Sigma(t)$ denotes the orthogonal projector onto the local tangent space of $\Sigma(t)$)

$$\frac{dn_\Sigma}{dt} = -\nabla v(t, x(t))^\mathsf{T} n_\Sigma(t) + [\nabla v(t, x(t)) n_\Sigma(t) \cdot n_\Sigma(t)] n_\Sigma(t) = -\mathcal{P}_{\Sigma(t)}(\nabla v(t, x(t)))^\mathsf{T} n_\Sigma(t). \tag{5}$$

As an example, we consider the class of linear, divergence free velocity fields in two space dimensions, i.e. v satisfies

$$v(x_1, x_2) = (v_0 + c_1 x_1 + c_2 x_2, -c_1 x_2), \quad v_0, c_1, c_2 \in \mathbb{R}. \tag{6}$$

In this case, the ODEs (4) and (5) are explicitly solvable and the solution is (see [4])

$$x_1(t) = x_1^0 e^{c_1 t} + \frac{v_0}{c_1}(e^{c_1 t} - 1), \quad \theta(t) = \frac{\pi}{2} + \arctan\left(-\cot\theta_0\, e^{2c_1 t} \pm c_2 \frac{e^{2c_1 t} - 1}{2c_1}\right), \quad c_1 \neq 0. \tag{7}$$

Here "+" applies for the evolution of the contact angle θ of the right contact point with $n_\Sigma^r = (\sin\theta,\ \cos\theta)$ and "−" applies for the left contact point with $n_\Sigma^l = (-\sin\theta,\ \cos\theta)$.

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3 Numerical Method

To solve (3) numerically, we set up an equidistant Cartesian grid and apply an explicit Euler Finite Volume discretization. Let $\bar{\phi}^k_{i,j}$ denote the cell-averaged value of ϕ in cell (i,j) at time $t_k = k\Delta t$. Then the numerical scheme reads

$$\bar{\phi}^{k+1}_{i,j} = \bar{\phi}^k_{i,j} - \frac{\Delta t}{|V_{ij}|} \int_{\partial V_{ij}} (\phi v \cdot n)(t_k, x)\, d\sigma(x), \tag{8}$$

where n denotes the outer unit normal to ∂V_{ij}. The numerical fluxes over the cell edges are approximated with the first-order upwind method (see [6] p. 72-76 and [3] for the present implementation). For computational purposes, it is convenient to allow for in- and outflow to the computational domain. At inflow boundaries, we impose homogeneous Neumann boundary conditions for ϕ. This can be implemented using a constant extension of $\bar{\phi}$ to a ghost cell layer next to the boundary (see [6], chapter 7). Note that no special care is necessary for cell edges at the solid boundary since we assume a zero normal component of v at solid walls. For the sake of simplicity, we do not reinitialize the level set during the simulation, while this is usually done in order to maintain $|\nabla\phi| \approx 1$ close to the interface.

4 Results and Conclusion

We consider the field (6) with $v_0 = -0.2$, $c_1 = 0.1$, $c_2 = -2$ and an initial spherical cap shape with radius $R = 0.4$. The contact angle is extracted from the Level Set function by a second-order finite differences approximation of the interface normal. A mesh study for the evolution of the contact angle for the left contact point with a fixed Courant number of $\mathrm{CFL} = \|v\|_\infty \Delta t/\Delta x = 0.5$ is reported in Figure 2. A first-order convergence of the numerical solution for $\theta(t)$ to (7) is found, see [3] for details and further examples. The same order of convergence holds for the evolution of the contact point.

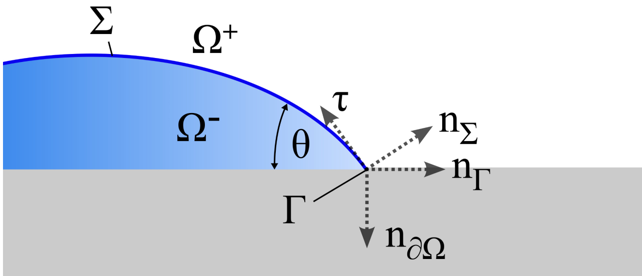

Fig. 1: Notation.

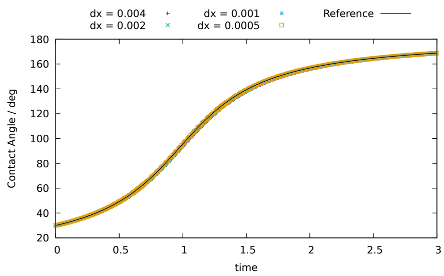

Fig. 2: Mesh study for the contact angle over time.

To summarize, we have demonstrated the validity of the kinematic evolution equation (5) by means of a simple implementation of the Level Set method. The complete source code of this demonstrator along with further data and a short tutorial are provided in [3]. This repository may serve as a database for validation of the numerical transport of the contact angle with other volume tracking methods. An additional publication concerning the contact line advection with the Volume-of-Fluid method is in preparation [4].

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