Journal of Computational Physics 330 (2017) 510–528

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

An efficient threshold dynamics method for wetting on rough surfaces

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ARTICLE INFO

Article history:
Received 6 February 2016
Received in revised form 26 October 2016
Accepted 6 November 2016
Available online 22 November 2016

Keywords:
Threshold dynamics method
Wetting
Rough surface

ABSTRACT

The threshold dynamics method developed by Merriman, Bence and Osher (MBO) is an efficient method for simulating the motion by mean curvature flow when the interface is away from the solid boundary. Direct generalization of MBO-type methods to the wetting problem with interfaces intersecting the solid boundary is not easy because solving the heat equation in a general domain with a wetting boundary condition is not as efficient as it is with the original MBO method. The dynamics of the contact point also follows a different law compared with the dynamics of the interface away from the boundary. In this paper, we develop an efficient volume preserving threshold dynamics method for simulating wetting on rough surfaces. This method is based on minimization of the weighted surface area functional over an extended domain that includes the solid phase. The method is simple, stable with $O(N \log N)$ complexity per time step and is not sensitive to the inhomogeneity or roughness of the solid boundary.

1. Introduction

Wetting describes how a liquid drop spreads on a solid surface. The most important quantity in wetting is the contact angle between the liquid surface and the solid surface [8]. When the solid surface is homogeneous, the contact angle for a static drop is given by the famous Young's equation:

$$\cos\theta_Y = \frac{\gamma_{SV} - \gamma_{SL}}{\gamma_{LV}}, \tag{1}$$

where γ_{SL}, γ_{SV} and γ_{LV} are the solid–liquid, solid–vapor and liquid–vapor surface energy densities, respectively. θ_Y is the so-called Young's angle [37]. Mathematically, Young's equation (1) can be derived by minimizing the total energy in the solid–liquid–vapor system. If we ignore gravity, the total energy in the system can be written as

$$\mathcal{E} = \gamma_{LV}|\Sigma_{LV}| + \gamma_{SL}|\Sigma_{SL}| + \gamma_{SV}|\Sigma_{SV}|, \tag{2}$$

where Σ_{LV}, Σ_{SL} and Σ_{SV} are respectively the liquid–vapor, solid–liquid and solid–vapor interfaces, and $|\cdot|$ denotes the area of the interfaces. When the solid surface Γ is a homogeneous planar surface, under the condition that the volume of

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http://dx.doi.org/10.1016/j.jcp.2016.11.008

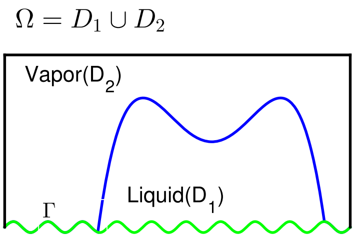

Fig. 1. Wetting on a rough surface.

the drop is fixed, the unique minimizer of the total energy is a domain with a spherical surface in Ω, and the contact angle between the surface and the solid surface Γ is Young's angle θ_Y [33].

The study of wetting and contact angle hysteresis on rough surfaces is of critical importance for many applications and has attracted much interest in the physics and applied mathematics communities [2,11,16,27,36]. Numerical simulation of wetting on rough surfaces is challenging. One must track the interface motion accurately, as well as deal with complicated boundary shapes and boundary conditions. There are many different types of numerical methods for solving interface and contact line problems, including the front-tracking method [22,34], the front-capturing method using the level-set function [38], the phase-field methods [4,10], among others [9].

Merriman, Bence and Osher (MBO) developed an efficient threshold dynamics method to simulate the motion by mean curvature flow [24,25]. This method is based on the observation that the level-set of the solution of a heat equation moves in normal direction at a velocity equal to the mean curvature of the level-set surface. The method alternately diffuses and sharpens characteristic functions of regions and is easy to implement and highly efficient. The method was also extended to problems with volume preservation [19,30] and to some high-order geometric flow problems [14]. Recently, Esedoglu and Otto extended the threshold dynamics method to the multi-phase problems with arbitrary surface tension [13]. There have been many studies on the MBO threshold dynamics method, including some efficient implementations [12,28,29,32] and convergence analysis [3,5,15,18,23]. In particular, Laux and collaborators established the convergence of some computational algorithms including one with volume preservation[20,21].

The generalization of MBO-type methods to the wetting problem where interfaces intersecting the boundary is not straightforward because of a lack of integral representation with a heat kernel for a general domain. In the original MBO scheme, when the interface does not intersect the solid boundary, one can solve the heat equation efficiently on a rectangular domain with a uniform grid using convolution of the heat kernel with the initial condition [28,29]. The convolution can be evaluated using fast Fourier transform (FFT) at $N \log N$ cost per time step where N is the total number of grid points. One way to generalize MBO-type methods to wetting on solid surfaces is to solve the heat equation with a wetting boundary condition before the volume-preserving thresholding step. However, the usual fast algorithms cannot be applied for this case, especially when the boundary is rough.

In this paper, we aim to develop an efficient volume-preserving threshold dynamics method for solving wetting problems on rough surfaces. Our method is based on the approach of Esedoglu–Otto [13]. The key idea is to extend the original domain with a rough boundary to a regular cube and treat the solid part as another phase. In the thresholding step, the solid phase domain remains unchanged. We show that the algorithm has the total interface energy decaying property and our numerical results show that the equilibrium interface satisfies Young's equation near the contact point. The advantage of the method is that it can be implemented efficiently on uniform meshes with a fast algorithm (e.g. FFT) since the computational domain is rectangular and we can simulate wetting on rough boundaries of any shape. We also introduce a fast algorithm for volume preservation based on a quick-sort algorithm and a time refinement scheme to improve the accuracy of the solution at the contact line.

The paper proceeds as follows. In Section 2, we introduce the surface energies of the wetting problem. A direct (but less efficient) MBO-type threshold dynamics method for solving wetting problems is also described. In Section 3, we introduce a new threshold dynamics method which is simple, efficient and easy to implement. Several modifications of the method are also discussed. In Section 4, we discuss the implementation of the algorithm and perform the accuracy check. We also introduce a quick-sort algorithm for volume preservation and a time refinement technique to improve the accuracy of the contact point motion. In Section 5 and Section 6, we present numerical examples of wetting on rough surfaces to demonstrate the efficiency of the new method.

2. The minimization of surface energies

We consider a wetting problem in a domain $\Omega \in \mathbb{R}^n$, $n = 2, 3$ (see Fig. 1). The solid surface Γ is part of the domain boundary $\partial\Omega$. Denote the liquid domain by $D_1 \subset \Omega$. For simplicity, we assume that $\partial D_1 \cap \partial\Omega \subset \Gamma$. The volume of the liquid drop is fixed such that $|D_1| = V_0$. We denote $\Sigma_{LV} = \partial D_1 \cap \Omega$, $\Sigma_{SL} = \partial D_1 \cap \Gamma$ and $\Sigma_{SV} = \Gamma \setminus \partial D_1$ as the liquid–vapor, solid–liquid and solid–vapor interfaces respectively. Then, the equilibrium configuration of the system is obtained by minimizing the total interface energy of the system as follows: