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# An Adaptive Threshold Dynamics Method for Three-Dimensional Wetting on Rough Surfaces

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**Abstract.** We propose an adaptive threshold dynamics method for wetting problems in three space dimensions. The method is based on solving a linear heat equation and a thresholding step in each iteration. The heat equation is discretized by a cell-centered finite volume method on an adaptively refined mesh. An efficient technique for volume conservation is developed on the nonuniform meshes based on a quick-sorting operation. By this method, we compute some interesting wetting problems on complicated surfaces. Numerical results verify some recent theory for the apparent contact angle on rough and chemically patterned surfaces.

**AMS subject classifications**: 65M08, 65M50, 76T10

**Key words**: Adaptive, threshold dynamics method, wetting.

## 1 Introduction

Wetting describes how liquid stays and spreads on solid surfaces. It appears in many industrial processes, e.g. painting, printing, oil recovery, etc. One important phenomenon in wetting is that the geometric roughness and chemical inhomogeneity of the solid surface can change dramatically the wetting properties. This is the so-called lotus effect. The property is of critical importance in designing self-cleaning materials and hydrophobic surfaces with low contact angle hysteresis.

Theoretical studies for wetting phenomena on rough and inhomogeneous surfaces are enormous(c.f. [3, 12] and the reference therein). The equilibrium wetting problem is

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to minimize the total interface energy in a solid-liquid-vapor system. When the solid surface is rough, there are usually many local minimizers. By the homogenization method, one can show that the local minimizer corresponds to some modified Wenzel and Cassie equations [45, 49]. These equations imply that the macroscopic apparent angle is determined by an average of the chemical and geometric properties along the triple contact line [11, 26, 33]. This is different from the classical Wenzel and Cassies equations [9, 43], which use a surface average instead of the average on the contact line.

Even though there are many theoretical studies, there still exist many controversies and open questions for wetting on rough surfaces [14,16], especially in three dimensional spaces. The three dimensional wetting problem is much more difficult than that in two dimensions. In the latter case, the contact line is reduced to a point and the apparent contact angle has a simple relation to the local Young's angle at the point [4, 48]. In three dimensions, the position of the contact line can be very complicated. In general, the location of the contact line is not known a priori and numerical simulations are needed to predict the wetting properties of a rough surface.

Numerical simulation for wetting on rough surfaces is quite challenging, since it is a free interface problem with complex boundary conditions. For example, a phase-field model for wetting includes a nonlinear boundary condition [10, 32], which is to enforce the Young's equation for the microscopic contact angle [50]. The boundary condition is difficult to implement numerically. In addition, the possible topological change of the liquid-vapor interface in the Wenzel-Cassie transition on rough surfaces may cause difficulties to other standard numerical methods [6, 13, 34, 44, 51].

Recently, a threshold dynamics method is developed for wetting problems in two space dimensions [41,47]. The method alternately diffuses and sharpens the characteristic function of a domain with a free boundary. It is easy to implement and quite efficient. The method is motivated by the work of S. Esedoglu and F. Otto [17] and can originate from the well-known MBO method for motion of interfaces driven by the mean curvature(so-called mean curvature flow) [30]. Theoretical studies show that the MBO method has first order convergence when the surface is smooth [20, 22, 27, 39]. The threshold dynamics method has also been applied to many other problems [15, 19, 31, 37, 40]. It is usually implemented on uniform meshes so that a fast Fourier transform (FFT) method can be used. One exception is the work in [23], where a nonuniform FFT is applied.

In this paper, we propose a new adaptive threshold dynamics method for wetting problems on rough surfaces in three space dimensions. To reduce the computational complexity, the mesh is adaptively refined in the neighborhood of the liquid-vapor interface and the rough solid surface while it is coarsened elsewhere. Different from the previous work [47], we do not use the convolution method to diffuse the characteristic functions. We solve a linear heat equation directly by a cell-centered finite volume method on the locally refined grids. The discrete heat equations on the adaptive but locally uniform grids are solved with a fast composite grid iterative method [7, 8, 29], which further improves efficiency of the algorithm. We also generalize the volume preserving technique in [47] to the case with non-uniform meshes. The technique is based on a quick-sorting operation