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A Multiple Scalar Auxiliary Variables Approach to the Energy Stable Scheme of the Moving Contact Line Problem

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Abstract. In this article, we explore the numerical approximation for a phase-field model to the moving contact line (MCL) problem, governed by the Cahn-Hilliard equation with a dynamic contact angle condition. A difficult and challenging issue comes from the high order, nonlinear and coupled time marching system with a small dimensionless parameter describing the interface thickness. The scalar auxiliary variable (SAV) approach has been recently developed for a large class of gradient flows in principle. Due to the nonlinear gradient terms in both the bulk and boundary energies, we introduce multiple scalar auxiliary variables (MSAV) approach rather than single SAV scheme to deal with phase field contact line model. The MSAV scheme numerically gives a better description of the contact line dynamic in terms of the difference between the modified and original energies. Moreover, the resulting numerical schemes enjoy the advantages of second order accuracy, unconditional energy stability, and only require solving a linear decoupled system with constant coefficients at each time step. Numerical experiments are presented to verify the effectiveness and efficiency of the proposed schemes for a wide range of mobility parameters and phenomenological boundary relaxation parameters.

AMS subject classifications: 35K35, 65M12, 65Z05, 65P40

Key words: Moving contact line, unconditionally energy stable, Cahn-Hilliard equation, multiple scalar auxiliary variables.

1. Introduction

Moving contact line (MCL), is a line where the interface of the two immiscible fluid phases intersects the solid container or the substrate. The equilibrium configuration of

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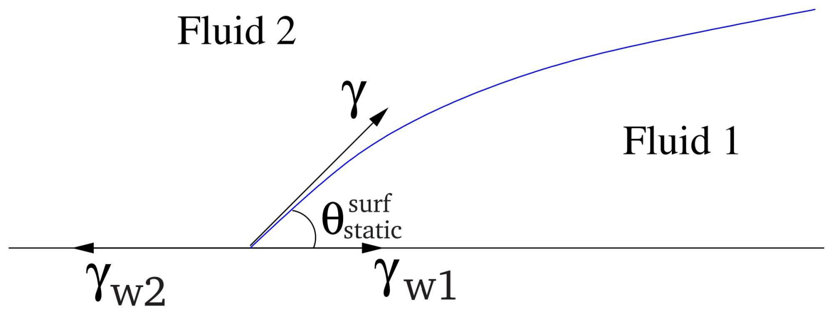

Figure 1: Two immiscible fluid I–fluid II in contact with a solid substrate.

the static contact line is perfectly described by well-known Young's equation (Young, Laplace, and Gauss [65]),

$$\gamma\cos(\theta_{\rm static}^{\rm surf}) = \gamma_{\rm w2} - \gamma_{\rm w1}, \tag{1.1}$$

where $\gamma_{\rm w1}$ and $\gamma_{\rm w2}$ are the coefficients representing the fluid-solid surface tension, γ is the fluid-fluid interfacial tension, and $\theta_{\rm static}^{\rm surf}$ is the contact angle between the fluid interface and the solid surface (see Fig. 1).

Understanding the contact line dynamics is important for many physical and industrial applications such as coating, contact dispensing, inkjet printing, spray cooling, etc. However, the Navier Stokes equation with no-slip boundary condition leads to an unsolved difficult issue for decades due to the non-integrable singularity in the stress and the resulting non-physical divergence in the energy dissipation rate (Huh & Scriven [33] Dussan & Davis in [17,18]). Various models have been proposed for MCL problems such as kinetic models, molecular dynamics (MD) models, hydrodynamic models and diffuse-interface models, which encompass the widely disparate length scales, see [17,18,25,39,40,42,43,52,54,56,66–68] for a review.

Here, we focus on the so-called diffuse-interface or phase-field theory of mesoscopic models, originally proposed by van der Waals [52,66], in which a phase-field variable ϕ is defined to capture the motion of the interface with finite thickness. The dynamics of ϕ is driven by the gradient flow of the total free energy, which can also handle complex morphologies and topological changes. Later, Cahn and Hilliard [10] applied Van der Waals diffuse interface approach to study the binary incompressible fluid system, and describe nucleation and spinodal decomposition. In typical phase field models, there are two main categories of systems based on choices of diffusion rates: the Allen-Cahn equation [9] and Cahn-Hilliard equation. From the numerical point of view, the Allen-Cahn equtaion is a second order system without the volume conservation, while the Cahn-Hilliard equation is a fourth order equation with the volume fixed. Thus, the numerical computation of Cahn-Hilliard equation is relatively harder than that of Allen-Cahn model. The issue of the numerical stiffness for both equations is still far from being solved completely [8,13,21,22,26,27,36,45,55,59,63,69]. Both Allen-Cahn and