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A Second Order Numerical Scheme of the Cahn-Hilliard-Navier-Stokes System with Flory-Huggins Potential

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Abstract. A second order accurate in time, finite difference numerical scheme is proposed and analyzed for the Cahn-Hilliard-Navier-Stokes system, with logarithmic Flory-Huggins energy potential. In the numerical approximation to the chemical potential, a modified Crank-Nicolson approximation is applied to the singular logarithmic nonlinear term, while the expansive term is updated by an explicit second order Adams-Bashforth extrapolation, and an alternate temporal stencil is used for the surface diffusion term. Moreover, a nonlinear artificial regularization term is included in the chemical potential approximation, which ensures the positivity-preserving property for the logarithmic arguments, i.e., the numerical value of the phase variable is always between -1 and 1 at a point-wise level. Meanwhile, the convective term in the phase field evolutionary equation is updated in a semi-implicit way, with second order accurate temporal approximation. The fluid momentum equation is also computed by a semi-implicit algorithm. The unique solvability and the positivity-preserving property of the second order scheme is proved, accomplished by an iteration process. A modified total energy stability of the second order scheme is also derived. Some numerical results are presented to demonstrate the accuracy and the robust performance of the proposed second order scheme.

AMS subject classifications: 35K35, 35K55, 49J40, 65M06, 65M12

Key words: Cahn-Hilliard-Navier-Stokes system, Flory-Huggins energy potential, second order accurate numerical scheme, Crank-Nicolson approximation, positivity preserving.

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1 Introduction

For simplicity, we assume the domain under consideration is the unit square $\Omega=(0,1)^2$. An extension to a rectangular domain, the 3-dimensional case, is straightforward.

The phase variable ϕ is assumed to have a point-wise bound, $-1<\phi<1$. For any $\phi\in H^1(\Omega)$ with such a bound, the Flory-Huggins free energy is formulated as

$$E(\phi)=\int_\Omega\left((1+\phi)\ln(1+\phi)+(1-\phi)\ln(1-\phi)-\frac{\theta_0}{2}\phi^2+\frac{\epsilon^2}{2}|\nabla\phi|^2\right)d\mathbf{x}, \tag{1.1}$$

in which $\epsilon>0$, $\theta_0>0$ are certain physical parameter constants associated with the diffuse interface width and inverse temperature, respectively; see the related references [2,14,17, 23].

For two phase flow problems, the fluid motion plays an important role in the physical process. A well-known two phase flow model is the following Cahn-Hilliard-Navier-Stokes (CHNS) system [36]

$$\mathbf{u}_t+\mathbf{u}\cdot\nabla\mathbf{u}+\nabla p-\nu\Delta\mathbf{u}=-\gamma\phi\nabla\mu, \tag{1.2}$$

$$\phi_t+\nabla\cdot(\phi\mathbf{u})=\Delta\mu, \tag{1.3}$$

$$\mu:=\delta_\phi E=\ln(1+\phi)-\ln(1-\phi)-\theta_0\phi-\epsilon^2\Delta\phi, \tag{1.4}$$

$$\nabla\cdot\mathbf{u}=0, \tag{1.5}$$

in which $\mathbf{u}$ is the advective velocity, p is the pressure variable, and $\nu>0$ is the kinematic viscosity. The constant $\gamma>0$ is associated with surface tension, and term $-\gamma\phi\nabla\mu$ is a diffuse interface approximation of the singular surface force.

For such a coupled system, the following energy dissipation law can be derived:

$$E'_{total}(t)=-\int_\Omega|\nabla\mu|^2d\mathbf{x}-\frac{\nu}{\gamma}\int_\Omega|\nabla\mathbf{u}|^2d\mathbf{x}\le 0,\quad E_{total}=E(\phi)+\frac{1}{2\gamma}\|\mathbf{u}\|^2. \tag{1.6}$$

Many numerical works have been reported for various phase-field-fluid coupled system [3, 6, 7, 26, 27, 34, 35, 41, 42, 47, 48, 53], etc. In particular, the issue of second order accurate numerical schemes have attracted great attentions [15, 32, 54], due to its long time simulation advantages. On the other hand, most existing works of second order schemes have been based on the polynomial approximation in the energy potential. With a singular energy potential (1.1), the analysis will become much more challenging, because of the highly nonlinear, singular and coupled nature of the physical system.

In this article, we propose and analyze a second order accurate numerical scheme for the CHNS system (1.2)-(1.5), with three properties theoretically justified: positivity-preserving (for the logarithmic arguments), unique solvability, and a modified energy stability. In fact, even for the pure gradient model with singular energy potential, the works of second order accurate in time, energy stable numerical schemes are still very