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A Physics-Informed Structure-Preserving Numerical Scheme for the Phase-Field Hydrodynamic Model of Ternary Fluid Flows

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Abstract. Phase-field models are widely used in studying multiphase flow dynamics. Given the complexity and strong nonlinearity, designing accurate, efficient, and stable numerical algorithms to solve these models has been an active research field for decades. This paper proposes a novel numerical scheme to solve a highly cited and used phase field hydrodynamic model for simulating ternary phase fluid flows. The main novelty is the introduction of a supplementary variable to reformulate the original problem into a constrained optimization problem. This reformulation leads to several advantages for our proposed numerical algorithms compared with many existing numerical techniques for solving this model. First, the developed schemes allow more straightforward calculations for the hydrodynamic phase-field models by solving a few decoupled Helmholtz or Poisson-type systems with a constant pre-computable coefficient matrix, remarkably reducing the computational cost. Secondly, the numerical schemes can maintain mass conservation and energy dissipation at the discrete level. Additionally, the developed scheme based on the second-order backward difference formula respects the original energy dissipation law that differs from many existing schemes, such as the IEQ, SAV, and Lagrange multiplier approaches for which a modified energy dissipation law is respected. Furthermore, rigorous proof of energy stability and practical implementation strategies are provided. We conduct adequate 2D and 3D numerical tests to demonstrate the proposed schemes' accuracy and effectiveness.

AMS subject classifications: 52B10, 65D18, 68U05, 68U07

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1. Introduction

Multiphase flows exist ubiquitously in nature and arise in many scientific and engineering settings, such as biomedical, chemical, and industrial processes involving three or more liquid components. As one of the most popular approaches for modeling interfacial dynamics, the phase-field method provides a state-of-the-art alternative interface capturing approach for multiphase flow problems (see [4, 13, 16, 18, 21, 27, 28] and references therein). Some reasons include its simplicity of formulation and transparent relations of its model parameters to the physical properties. Additionally, the phase-field models and their hydrodynamic extensions are usually derived by following thermodynamic laws, i.e., thermodynamically consistent, making them physically sound. A typical example extensively studied is the Cahn-Hilliard-Navier-Stokes system for simulating the dynamics of multiphase fluid mixtures. This paper mainly focuses on the ternary-component Cahn-Hilliard-Navier-Stokes (ternary-NSCH) system to better illustrate ideas. Notably, our idea also applies to many other hydrodynamic phase-field models.

The three-component Cahn-Hilliard-Navier-Stokes model is generalized from the two-phase scenario [3] by introducing three independent phase-field variables (ϕ_1, ϕ_2, ϕ_3) while these unknowns are linked through the hyperplane relation $\phi_1 + \phi_2 + \phi_3 = 1$. Please refer to related papers [2, 3, 10, 19, 22] for more details. Traditionally, a Lagrangian multiplier was adopted into the system that introduced the first coupled nonlinear term among the three-phase variables [20,38]. However, such a simple system is not well-posed for the total spreading case, and some nonphysical instabilities at interfaces may occur [2, 3]. To remedy this defect, a sixth-order polynomial-type coupling potential is added to the free energy to ensure the system is well-posed. Developing efficient numerical approximations for solving the three-component Cahn-Hilliard-Navier-Stokes model remains challenging due to the coupling of multi-physical fields with hydrodynamics and their natural nonlinearity.

The phase-field models and their hydrodynamic extensions are usually derived from an energy variational approach, so they naturally admit a free energy dissipation law. This is also known as thermodynamically consistent. When the numerical schemes exploit the variational structure and preserve the dissipation law numerically, they are called energy stable [9]. Suppose such numerical structure-preserving property does not depend on the time step sizes. In that case, the numerical schemes are called ly energy stable. In the past few decades, significant progress in developing structure-preserving algorithms to solve thermodynamical and hydrodynamical phase-field models have been made, for instance, the fully-implicit structure-preserving schemes [3, 33], the convex splitting schemes [5, 8, 41], stabilizer technique [23, 26, 32]. In the past few years, the invariant energy quadratization (IEQ) method and the scalar auxiliary variable (SAV) method, even in combination with stabilization terms, also have fueled the development of energy stable schemes for solving the ternary-component phase-field models [34, 36–38, 42, 43]. However, when some of these methods are applied to solving thermodynamically consistent models, the resulting schemes warrant