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PENALTY-PROJECTION SCHEMES FOR THE CAHN-HILLIARD NAVIER-STOKES DIFFUSE INTERFACE MODEL OF TWO PHASE FLOW, AND THEIR CONNECTION TO DIVERGENCE-FREE COUPLED SCHEMES

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Dedicated to Professor William J. Layton on the occasion of his 60^{th} birthday

Abstract. We study and compare fully discrete numerical approximations for the Cahn-Hilliard-Navier-Stokes (CHNS) system of equations that enforce the divergence constraint in different ways, one method via penalization in a projection-type splitting scheme, and the other via strongly divergence-free elements in a fully coupled scheme. We prove a connection between these two approaches, and test the methods against standard ones with several numerical experiments. The tests reveal that CHNS system solutions can be efficiently and accurately computed with penalty-projection methods.

Key words. Cahn-Hilliard-Navier-Stokes system, penalty-projection method and strong divergence-free elements.

1. Introduction

The Cahn-Hilliard-Navier-Stokes (CHNS) system of equations is a diffuse interface model for the evolution of two-phase, immiscible, incompressible flows with uniform mass densities. In contrast to those of sharp interface type, the CHNS model describes a small-thickness transition region (diffuse interface) between the two immiscible fluids. This allows for convenient simulation of topological transitions such as pinch-off and reconnection of drops [25], without the need to explicitly track interfaces. In a domain $\Omega \subset \mathbb{R}^d$, d=2 or 3, with u representing velocity, p pressure, μ the chemical potential, and ϕ the phase field variable (taking a value of 1 in the bulk of one fluid and -1 in the bulk of the other), the CHNS system is given in non-dimensional form by [25]

$$\phi_t + \nabla\cdot(\phi u) = \nabla\cdot(M(\phi)\nabla\mu), \tag{1}$$

$$\mu = f_0'(\phi) - \epsilon^2\Delta\phi, \tag{2}$$

$$u_t + u\cdot\nabla u + \nabla p - \nu\Delta u = -\frac{\epsilon^{-1}}{\mathrm{We}}\phi\nabla\mu, \tag{3}$$

$$\nabla\cdot u = 0, \tag{4}$$

together with initial conditions u_0 and ϕ_0, and boundary conditions

$$\begin{aligned} u|_{\partial\Omega} &= 0, && \text{(no slip, no penetration)},\\ \nabla\phi\cdot n|_{\partial\Omega} &= 0, && \text{(local equilibrium)},\\ \nabla\mu\cdot n|_{\partial\Omega} &= 0, && \text{(no flux)}. \end{aligned}$$

In the system above, ν is the kinematic viscosity ($\nu^{-1} = Re$, the Reynolds number), $\epsilon > 0$ is the transition layer width, We is a modified Weber number (measuring the

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strength of the kinetic and surface energies [21]), $M(\phi)$ is the mobility function, which for simplicity we will take as $M(\phi) = 1$. The function $f_0(\phi) = \frac{1}{4}(1-\phi^2)^2 = \frac{1}{4}\phi^4 - \frac{1}{2}\phi^2 + \frac{1}{4}$ is the homogeneous free energy density function. We note that the energy balance of the system is easily shown to be

$$\frac{\partial}{\partial t}\left(\frac{1}{2}\|u\|^2 + \frac{\epsilon}{2\mathrm{We}}\|\nabla\phi\|^2 + \frac{\epsilon^{-1}}{\mathrm{We}}\int_\Omega f_0(\phi)\,dx\right) + \left(\nu\|\nabla u\|^2 + \frac{\epsilon^{-1}}{\mathrm{We}}\|\sqrt{M(\phi)}\nabla\mu\|^2\right) = 0.$$

By redefining the pressure, we can reformulate the system

$$\phi_t + \nabla\phi\cdot u = \nabla\cdot(M(\phi)\nabla\mu), \tag{5}$$

$$\mu = f_0'(\phi) - \epsilon^2\Delta\phi, \tag{6}$$

$$u_t + u\cdot\nabla u + \nabla p - \nu\Delta u = \frac{\epsilon^{-1}}{\mathrm{We}}\mu\nabla\phi, \tag{7}$$

$$\nabla\cdot u = 0. \tag{8}$$

Numerically solving the CHNS system is known to be very challenging for several reasons, including the fact that Navier-Stokes and Cahn-Hilliard equations can by themselves be difficult. For solutions to the coupled system, there are large spatial derivatives in the small transition regions causing stiff nonlinear systems. Moreover, the nonlinear algebraic equations resulting from discretization are large and strongly coupled, which makes it difficult to even 'get numbers' in a reasonable amount of time. Significant progress was recently made in [15], where a cleverly devised projection method was developed that decouples the pressure and divergence constraint from the system, but while still providing unconditional stability and (seemingly) second order temporal accuracy. Moreover, further decoupling of the system was done in the nonlinear iterations at each timestep, which further decoupled the system into easily solvable pieces. This scheme was shown to perform very well in terms of both accuracy and efficiency on a series of test problems.

The purpose of this paper is to study finite element schemes for (1)-(4) that more strongly enforce the divergence-constraint than what is usually found in the literature. In particular, we consider a coupled scheme that strongly enforces the divergence constraint, and a penalty-projection scheme that uses grad-div stabilization to better enforce the divergence constraint. Recent work in [10, 18, 22] has shown that the error caused in weak enforcement of the divergence constraint used by typical finite element methods for fluid simulations (e.g., using Taylor-Hood elements) is exacerbated when the momentum equation forcing has a large irrotational component [20]. Considering the CHNS system above, the forcing of the momentum equation (3) is observed to be either $-\frac{\epsilon^{-1}}{\mathrm{We}}\phi\nabla\mu$ or $\frac{\epsilon^{-1}}{\mathrm{We}}\mu\nabla\phi$, depending on the definition of the pressure. Since ϵ is small, we can expect the forcing to be large in general, especially in the diffuse interface region. Moreover, since $|\phi| \approx 1$ except in transition regions, we can expect the forcing the be nearly irrotational in bulk flow regions. Thus, the CHNS system seems to fit into a class of problems where stronger enforcement of the divergence constraint can significantly help solution accuracy.

There are many ways of reducing the effect of poor divergence-constraint enforcement in discretizations, including using point-wise divergence-free velocity-pressure elements (e.g., [20, 32, 2, 26, 13, 14, 8]) and using grad-div stabilization. Point-wise divergence-free elements completely eliminate the problem but come with difficulties such as larger (and discontinuous) pressure spaces, restrictive mesh conditions,