Energy Law Preserving $C^0$ Finite Element Schemes for Phase Field Models in Two-phase Flow Computations

Jinsong Hua ∗ Ping Lin † Chun Liu ‡ and Qi Wang §

Revised paper, March 2011

Abstract

We use the idea in [33] to develop the energy law preserving method and compute the diffusive interface (phase-field) models of Allen-Cahn and Cahn-Hilliard type, respectively, governing the motion of two-phase incompressible flows. We discretize these two models using a $C^0$ finite element in space and a modified midpoint scheme in time. To increase the stability in the pressure variable we treat the divergence free condition by a penalty formulation, under which the discrete energy law can still be derived for these diffusive interface models. Through an example we demonstrate that the energy law preserving method is beneficial for computing these multi-phase flow models. We also demonstrate that when applying the energy law preserving method to the model of Cahn-Hilliard type, un-physical interfacial oscillations may occur. We examine the source of such oscillations and a remedy is presented to eliminate the oscillations. A few two-phase incompressible flow examples are computed to show the good performance of our method.

Keywords: two-phase flow, phase-field method, $C^0$ finite elements, energy law preservation.

Mathematics Subject Classification. 65M60, 76A15

∗Department of process and fluid flow technology, Institute for Energy Technology, P.O. Box 40, NO-2027, Kjeller, Norway (e-mail: jinsong.hua@ife.no).
†Department of Mathematics, University of Dundee, Dundee DD1 4HN, Scotland, United Kingdom. (e-mail: plin@maths.dundee.ac.uk).
‡Department of Mathematics, Pennsylvania State University, University Park, PA 18601, USA (e-mail: liu@math.psu.edu).
§Department of Mathematics and NanoCenter at USC, University of South Carolina, Columbia, SC 29208 USA (e-mail: qwang@math.sc.edu).
1 Introduction

Multiphase flows are common and important in a wide range of settings, in which multiple fluids can coexist in their own phases or in mixtures. Gas bubbles trapped in water, water filaments falling in the air, oil-water mixtures, blends of polymers, biological fluids, and cells etc. are easily identifiable examples. Many important biological and industrial processes involve multiphase fluid motions (cf. [26, 6]). Multiphase flow motions have been extensively studied by researchers both theoretically and experimentally, yet still remain an active interdisciplinary research field. In recent years, improved numerical algorithms have resulted in direct numerical simulations of multiphase phenomena leading to a better physical understanding of multiphase flows and their dynamics. The great advantage of numerical simulations is that they can bypass practical difficulties in experiments. At the same time, important data such as the velocity field and the pressure are readily available throughout the computational domain, truly pure fluid phase or component can be assumed in the limited flow domain throughout the simulations, and there are no uncertainties associated with the initial boundary of a distinguished fluid phase. Thus, direct numerical simulations have a great advantage to complement experiments in the pursuit of a better understanding of multiphase flow phenomena.

Many numerical methods for multiphase flows have been developed over the years. These include the volume of fluid method (cf. [19, 7]), Front-tracking method (cf. [23, 45, 22, 21]), level-set method (cf. [39, 40]), immersed boundary method and immersed interface methods (cf. [41, 27]) and boundary integral methods (cf. [5, 20]) etc. In these methods the model for the two-phase flow usually consists of separate hydrodynamic systems of equations for each component and the sharp interface between the phases. The hydrodynamic system describing the two-phase Newtonian fluid flow with a free interface is the usual Navier-Stokes equation in each of the fluid components (possibly with different density and viscosity) together with the kinematic and kinetic boundary conditions at the interface. As an alternative, we may view the interface representing a continuum with rapidly changing properties (such as density, viscosity, etc.) of one fluid but two components. Within this “thin” transition region, the two components or fluids are mixed and have to store certain amount of “mixing energy”. Such an approach coincides with the usual phase field model (cf. [8, 9, 1, 24, 35]) where the mixture may be seen as a special type of non-Newtonian fluids. Its rheological property reflects the competition between the kinetic energy and the “elastic” mixing energy.

The phase field model can be derived from an energetic variational procedure. The resulting coupled system of equations for the two-phase mixture can be expressed in the corresponding variational formulation: the gradient flow for the phase variable, which gives the internal dissipation due to the presence of the phase structures/patterns, and the least action principle for the flow map (See [35]), which provide the reversible part of the linear momentum equation. There is an energy dissipation law naturally associated with the formulation. A few numerical methods have been used to solve the phase field model, for examples, Fourier-spectral method ([35]), adaptive moving mesh method (See e.g. [4, 49])
and finite element method (See e.g. [10, 13, 38, 47]). There are also error analysis of finite element approximation for phase field models without coupling the flow field or coupled with the Stokes flow (See e.g. [3, 11, 12, 15, 16, 48]). Recently [14] provided an error analysis for a mixed finite element approximation of the Navier-Stokes-Cahn-Hilliard diffuse interface model. However, these work did not pay close attention to the preservation of the energy law inherited in the fully discretized system. This feature turns out to be very important to retain in the numerical method in order to produce correct evolution of the solution when a rapid change or a singularity occurs in the solution in such non-Newtonian hydrodynamic systems (cf. [32, 33]). When the underlining energy law is perserved in the fully discretized system, it is also possible to use a relatively coarse mesh in the simulation (See examples in the last section). Consequently such a method can reduce the cost of computation while resolving the prominent features of the flow. In this paper we will introduce a $C^0$ finite element formulation which can accurately preserve the energy law of the system at the discrete level. We emphasize $C^0$ finite elements because they are much simpler than finite elements with higher degree of smoothness and available in most existing finite element software packages. We will develop the numerical methods for both the Allen-Cahn and Cahn-Hilliard phase field model, in which the latter also preserves the volume fraction of each fluid in the two-phase flow. We will also assume that the interface has no contact to the domain boundary. In this case, extra difficulties arise from complicated interface/boundary interacting conditions and should be dealt with separately. Here we just refer to [43] for some available model and discussion in this regard.

The rest of the paper is organized as follows. In §2, we reformulate the phase field model so that the energy law at the discrete level is inherited under a $C^0$ finite element discretization. In §3, we present temporal second order $C^0$ finite element schemes. We then briefly show that a discrete energy law can be derived for this scheme for both models. To our knowledge, such a fully discrete energy law has never been done with $C^0$ elements before in computational methods for multiphase flows. We also show in this section that such a scheme for the Cahn-Hilliard model may be oscillatory near the interface. A low order modification at the initial time step is introduced to damp the oscillation. In §4, we use a fixed point iterative method, which formulates a matrix free time evolution, which is particularly beneficial for a direct linear system solver since the major work of the solver (i.e. the factorization step) is only needed at the initial time but not at later time steps. We show the good performance of our schemes over a method without rigorously preserving the energy law and use our schemes to simulate a few two-phase flow examples in the last section.
2 Phase Field Models and Energy Law Preserving Weak Form

We consider phase field models for mixtures of two isotropic fluids of different densities because of their simplicity in the practical implementation. After applying the classical Boussinesq approximation (assuming the density difference is not large), the governing system of equations is given in the following (cf. [35, 28]).

\[
\rho \left( \frac{u}{t} + (u \cdot \nabla)u \right) - \nabla \cdot \nu \nabla u + \nabla p + \lambda \nabla \cdot (\nabla \phi (\nabla \phi)^T) = s(\phi),
\]

\[
\nabla \cdot u = 0,
\]

\[
\phi_t + (u \cdot \nabla)\phi - \gamma (\Delta \phi - f(\phi)) = 0, \quad \text{(Allen-Cahn)},
\]

or

\[
\phi_t + (u \cdot \nabla)\phi + \gamma \Delta (\Delta \phi - f(\phi)) = 0, \quad \text{(Cahn-Hilliard)},
\]

where vector \( u \) represents the velocity of the fluid mixture, \( p \) is the hydrostatic pressure, and \( \phi \) represents the “phase” of the mixture (\( \phi = 1 \): fluid 1; \( \phi = -1 \): fluid 2), \( \nu \) is the viscosity coefficient, \( f(\phi) \) is the variation of the bulk mixing energy density \( F(\phi) = (|\phi|^2 - 1)^2/4\epsilon^2 \), where \( \epsilon \) is the capillary width (width of the mixing layer), \( s(\phi) = (0, -(1 + \phi)g(\rho_1 - \rho_0) - (1 - \phi)g(\rho_2 - \rho_0))^T \) is the buoyancy force given in 2D with gravity \( g \) (cf [28]), \( \rho_0 \) is the “background” density which may be treated as a constant in the approximation, \( \rho_1 \) and \( \rho_2 \) are the density of fluid 1 and 2, respectively. In addition, \( \lambda \) corresponds to the surface tension coefficient and \( \gamma \) represents the elastic relaxation time of the system. The system is supplied with the initial conditions

\[
\left. u \right|_{t=0} = u_0, \quad \left. \phi \right|_{t=0} = \phi_0,
\]

the Dirichlet boundary condition for \( u \) (\( = b_u \)), and the Neumann boundary condition for \( \phi \): \( \nabla \phi \cdot n = 0 \) for the Allen-Cahn model and \( \nabla \phi \cdot n = 0, \ nabla \Delta \phi \cdot n = 0 \) for the Cahn-Hilliard model, where \( n \) is the unit outward normal vector of the boundary. In this paper we focus on the two dimensional case. But the method can be readily extended to three spatial dimensions. The gradient of the velocity field is defined as:

\[
(\nabla u)_{ij} = u_{i,j} = \frac{\partial u_i}{\partial x_j}.
\]

In the homogeneous case (i.e. the buoyancy force is negligible \( s(\phi) = 0 \) and the boundary value \( b_u = 0 \)), the system obeys an energy dissipation law. Multiplying (2.1) by \( u \) and (2.3) or (2.4) by \( -(\Delta \phi - f(\phi)) \) we have

\[
\frac{dE}{dt} = -\left( \nu \|\nabla u\|_{L^2(\Omega)}^2 + \lambda \gamma \|\Delta \phi - f(\phi)\|_{L^2(\Omega)}^2 \right) \quad \text{(for the Allen-Cahn)}
\]
or
\[
\frac{dE}{dt} = -\left(\nu \|\nabla u\|_{L^2(\Omega)}^2 + \lambda \gamma \|\nabla (\Delta \phi - f(\phi))\|_{L^2(\Omega)}^2\right) \quad \text{(for the Cahn-Hilliard)},
\]

where
\[
E = \frac{1}{2}\rho_0 \|u\|_{L^2(\Omega)}^2 + \frac{\lambda}{2} \|\nabla \phi\|_{L^2(\Omega)}^2 + \lambda \int_\Omega F(\phi)
\]
is the total energy of the mixture system. In addition, for the Cahn-Hilliard model, the total volume of each fluid is conserved, i.e. \(\frac{d}{dt} \int_\Omega \phi \, dx = 0\). The analytical and numerical results in [29, 30, 32, 33] indicate that the energy law is particularly important when orientation dynamics are present in the study of motions of the liquid crystal fluid. The physically interesting solutions we seek are those energetically admissible ones. In this paper about the two-phase flow, the physically interesting dynamics are the solutions undergoing rapid changes at the interface. Hence it is advisable and desirable to use numerical schemes that preserve the energy law at the discrete level. To our best knowledge, whether existing numerical methods for multi-phase flow simulations retains a discrete energy law has not been carefully studied. Such a discrete energy law is also important to serve as a justification in simulating complex systems involving complicated flow equations where normally no benchmark solution is available. We will see Example 5.1 in the last section that if such a law is not rigorously followed spurious solutions may occur.

A direct variational or weak form may be derived straightforwardly by multiplying (2.1) with a test function \(v\) and (2.3) (Allen-Cahn) or (2.4) (Cahn-Hilliard) with a test function \(\psi\), then using integration by parts. In the weak form of the Allen-Cahn model shown below (where \(u, p, \phi\) and test functions \(v, q\) and \(\psi\) are in appropriate spaces),

\[
\int_\Omega (u_t \cdot v + (u \cdot \nabla)u \cdot v + \nu \nabla u : \nabla v - p(\nabla \cdot v) + \lambda \nabla \phi (\nabla \phi)^T : \nabla v) \, dx
= \int_\Omega s(\phi) \cdot v \, dx,
\]

\[
\int_\Omega (\nabla \cdot u) \, q \, dx = 0,
\]

\[
\int_\Omega (\phi_t \psi + (u \cdot \nabla)\phi \psi + \gamma (\nabla \phi \cdot \nabla \psi + f(\phi) \psi)) \, dx = 0,
\]

only first order derivatives of \(u, v, \phi\) and \(\psi\) are present so that the \(C^0\) (conforming) finite element method can be used to solve the problem under this variational form. However, we notice that in deriving the energy law (2.6) the test function \(\psi = - (\Delta \phi - f(\phi))\) is used (implying that the test function space should be in \(H^2\)) a \(C^1\) (or \(H^2\) conforming) finite element method is normally required in order to keep the energy law after the finite element discretization. Actually, in Section 5, we will show an example that a \(C^0\) finite element method would result in a spurious solution under this formulation. While in the so-obtained weak form of the Cahn-Hilliard model, second order derivatives are present and thus a \(C^1\) (conforming) finite element method is normally required to solve the problem.
So to use $C^0$ finite element methods we need to reformulate the flow equations and the phase field equations to obtain a weak form where both trial and test functions are involved with only first order derivatives while at the same time the energy law may be maintained. The benefits of using $C^0$ elements over $C^1$ elements are obvious. The method can be implemented easily and many existing codes may be incorporated to reduce various complications. More importantly, the energy law can be justified rigorously in this weak form with the corresponding $C^0$ finite element method so as to avoid any spurious solutions.

Let $\Omega$ be a bounded domain in $\mathbb{R}^2$. We denote the boundary of $\Omega$ by $\Gamma$ and suppose that $\Gamma$ is sufficiently smooth (for example, Lipschitz-continuous). Denote the following spaces as $W^{1,3}(\Omega) = (W^{1,3}(\Omega))^2$, $W^{1,3}_b = \{ u \in W^{1,3}(\Omega), u = b_u \text{ on } \Gamma \}$, $L^2(\Omega) = (L^2(\Omega))^2$ and $L^2_0(\Omega) = \{ p \in L^2(\Omega), \int_{\Omega} p dx = 0 \}$.

We consider the Allen-Cahn equation first. Usually a mixed formulation may be used to obtain a weak form where a $C^0$ finite element method can be applied (See [36] for such a study of liquid crystal dynamics). However, this introduces extra variables and imposes restrictions on the finite element through the so-called inf-sup condition. For this model, it is not necessary to use the mixed formulation.

We rewrite phase field equation (2.3) as follows

$$
\Delta \phi = \frac{1}{\gamma} (\phi_t + (u \cdot \nabla)\phi + \gamma f(\phi)).
$$

Using the identity

$$
\nabla \cdot (\nabla \phi (\nabla \phi)^T) = \Delta \phi \nabla \phi + \nabla (|\nabla \phi|^2)/2,
$$

it follows that (cf. [35, 32])

$$
\begin{align*}
\nabla \cdot (\nabla \phi (\nabla \phi)^T) &= \Delta \phi \nabla \phi + \nabla (|\nabla \phi|^2)/2 \\
&= \frac{1}{\gamma} (\phi_t + (u \cdot \nabla)\phi) \nabla \phi + \nabla (|\nabla \phi|^2/2 + F(\phi)).
\end{align*}
\tag{2.11}
$$

Substituting the above relation to the momentum transport equation (2.1) and defining a new pressure $p := p + |\nabla \phi|^2/2 + F(\phi)$, we end up with an equation without $\Delta \phi$. By multiplying $v$ and $\psi$ to the equation and (2.3), respectively, we obtain the equations in the following weak form:

Find $u \in W^{1,3}_{b_u}(\Omega), p \in L^2_0(\Omega)$ and $\phi \in W^{1,3}(\Omega)$ such that

$$
\int_{\Omega} \left( \rho_0 u_t \cdot v + \rho_0 (u \cdot \nabla) u \cdot v + \nu \nabla u : \nabla v - p (\nabla \cdot v) + \frac{\lambda}{\gamma} (\phi_t + (u \cdot \nabla)\phi) \cdot (v \cdot \nabla)\phi \right) \, dx
\quad = \int_{\Omega} s(\phi) \cdot v \, dx, \quad \forall v \in W^{1,3}_0(\Omega),
\tag{2.12}
$$

$$
\int_{\Omega} (\nabla \cdot u) \, q \, dx = 0, \quad \forall q \in L^2(\Omega),
\tag{2.13}
$$

$$
\int_{\Omega} (\phi_t \psi + (u \cdot \nabla)\phi \psi + \gamma (\nabla \phi \cdot \nabla \psi + f(\phi)\psi)) \, dx = 0, \quad \forall \psi \in W^{1,3}.
\tag{2.14}
$$
Note that it is possible to use a larger spaces for some variables, e.g. $L^3_0$ for $p$ and $H^1$ for $\psi$. But it will have no essential difference when we apply a $C^0$ finite element approximate space later.

With this weak form, the energy law can be readily obtained in the homogeneous case (i.e. $s(\phi) = 0$ and $b_u = 0$). Taking $v = u$ and $\psi = (\lambda/\gamma)\phi_t$ in (2.12) and (2.14), respectively, summing them up and using integral identities (where (2.13) is used)

$$
\int_{\Omega} (u \cdot \nabla) u \cdot udx = \frac{1}{2} \int_{\Omega} u \cdot \nabla |u|^2 = -\frac{1}{2} \int_{\Omega} |u|^2 \nabla \cdot u = 0,
$$

we have the following energy law:

$$
\frac{d}{dt} \left( \frac{1}{2} \rho_0 \|u\|_{L^2}^2 + \frac{\lambda}{2} \|\nabla \phi\|_{L^2}^2 + \lambda \int_{\Omega} F(\phi) \right) = - \left( \nu \|\nabla u\|_{L^2}^2 + \frac{\lambda}{\gamma} \|\phi_t + (u \cdot \nabla)\phi\|_{L^2}^2 \right).
$$

We next consider the Cahn-Hilliard equation (2.4). In this case, due to the bi-harmonic operator in the equation, we have to introduce an extra variable and use the mixed formulation to arrive at a weak form where a $C^0$ finite element method can be applied. That is, we write (2.4) into the following system (cf [46, 47]).

$$
\phi_t + (u \cdot \nabla)\phi = \frac{\gamma}{\epsilon^2} \Delta (\omega + c\phi)
$$

$$
\omega = -\epsilon^2 \Delta \phi + (\phi^2 - 1 - c)\phi,
$$

where the positive constant $c$ is introduced to enhance the stability of the numerical method (See e.g. [47]). So the weak form for the Cahn-Hilliard model reads: Find $u \in W^{1,3}_{b_u}(\Omega)$, $p \in L_0^2(\Omega)$, $\phi \in W^{1,3}(\Omega)$ and $\omega \in W^{1,3}(\Omega)$ such that

$$
\int_{\Omega} \left( \rho_0 u_t \cdot v + \rho_0 (u \cdot \nabla) u \cdot v + \nu \nabla u : \nabla v - p(\nabla \cdot v) - \frac{\lambda}{\epsilon^2} (\omega + c\phi)^2 \nabla \phi \cdot v \right) d\Omega
$$

$$
= \int_{\Omega} s(\phi) \cdot v d\Omega, \quad \forall v \in W^{1,3}_0(\Omega),
$$

$$
\int_{\Omega} (\nabla \cdot u) q d\Omega = 0, \quad \forall q \in L^2(\Omega),
$$

$$
\int_{\Omega} \left( \phi_t \psi + (u \cdot \nabla)\phi \psi + \frac{\gamma}{\epsilon^2} \nabla (\omega + c\phi) \cdot \nabla \psi \right) d\Omega = 0, \quad \forall \psi \in W^{1,3},
$$

$$
\int_{\Omega} (\omega \chi - \epsilon^2 \nabla \phi \cdot \nabla \chi - (\phi^2 - 1 - c)\phi \chi) d\Omega = 0, \quad \forall \chi \in W^{1,3},
$$

where we have used $\nabla \cdot (\nabla \phi (\nabla \phi)^T) = -\frac{1}{\epsilon^2} (\omega + c\phi)^2 \nabla \phi + \nabla (|\nabla \phi|^2/2 + F(\phi))$ from (2.11) and (2.18) and re-defined the pressure $p := p + \frac{|\nabla \phi|^2}{2} + F(\phi)$ as in the case of the Allen-Cahn model. In the homogeneous case taking $v = u$, $\psi = \frac{\lambda}{\epsilon^2} (\omega + c\phi)$ and $\chi = \lambda \phi_t/\epsilon^2$ in these equations and summing them up, we obtain the following energy law

$$
\frac{d}{dt} \left( \frac{1}{2} \rho_0 \|u\|_{L^2}^2 + \frac{\lambda}{2} \|\nabla \phi\|_{L^2}^2 + \lambda \int_{\Omega} F(\phi) \right) = - \left( \nu \|\nabla u\|_{L^2}^2 + \frac{\lambda \gamma}{\epsilon^2} \|\nabla (\omega + c\phi)\|_{L^2}^2 \right).
$$
From phase field equations (2.3) and (2.18), we can easily see that energy laws (2.16) and (2.23) are consistent to the original ones (2.6) and (2.7), respectively.

A discrete energy law can be similarly obtained with a modified convection in (2.12) (See the next section) and is the same as (2.16) or (2.23) if $C^0$ finite elements are used and if the time remains continuous as long as such finite element solution belongs to the functional spaces required in (2.12)-(2.14) or (2.19)-(2.22). We will present discrete energy laws for fully discretized systems in the next section.

3 Temporal schemes and discrete energy laws

The solution of the weak problem (2.12)-(2.14) or (2.19)-(2.22) is approximated by a finite difference scheme in time and a conformal $C^0$ finite element method in space. It is advisable and desirable for our numerical methods to respect the continuous energy law. In the temporal direction, since phase field models are highly nonlinear, explicit-implicit (or semi-implicit) first order schemes are usually adopted, where a part of the nonlinear term is treated explicitly and the rest is treated implicitly. The fully implicit backward Euler scheme is also used frequently in computational fluid dynamics. Although these two schemes work very well in many practical computations, the discrete energy law may not hold very accurately near the interface of the solution (see more explanation in Remark 3.1). We will use the midpoint scheme proposed for a liquid crystal model in [33] to compute the Allen-Cahn phase field model, where a discrete energy law is obtained and is consistent to the continuous one. However, when we apply the same idea to the Cahn-Hilliard model the resulting scheme may be oscillatory near the interface. This is clearly not physical. We will study the cause of the oscillation and propose a lower order (say, implicit backward Euler) scheme at the initial time as a remedy.

3.1 Numerical Scheme for the Allen-Cahn model

Let

\[ W = W_{b_u}^{1,3}(\Omega) \times L_0^2(\Omega) \times W^{1,3}(\Omega) \]

and $W^h = U^h \times P^h \times H^h \subset W$ be a finite dimensional subspace of $W$ given by a finite element discretization of $\Omega$. $W^h_0$ represents the space $W^h$ satisfying the homogeneous Dirichlet boundary condition. If $\Delta t > 0$ represents a time step size and $(u^n_h, p^n_h, \phi^n_h) \in W^h$ is an approximation of $u(t^n) = u(n\Delta t)$, $p(t^n) = p(n\Delta t)$ and $\phi(t^n) = \phi(n\Delta t)$, the approximation at time $t^{n+1} = (n + 1)\Delta t$ is denoted as $(u^{n+1}_h, p^{n+1}_h, \phi^{n+1}_h) \in W^h$ and computed by
the following finite element scheme

\[
\int_{\Omega} \left( \rho_0 u_t^{n+1} \cdot v + \rho_0 (u_h^{n+\frac{1}{2}} \cdot \nabla) u_h^{n+\frac{1}{2}} \cdot v + \frac{1}{2} \rho_0 (\nabla \cdot u_h^{n+\frac{1}{2}}) u_h^{n+\frac{1}{2}} \cdot v + \nu \nabla u_h^{n+\frac{1}{2}} : \nabla v \right) dx = 0, \tag{3.1}
\]

\[
- p_h^{n+\frac{1}{2}} (\nabla \cdot v) + \frac{\lambda}{2} \left( \phi_t^{n+1} + (u_h^{n+\frac{1}{2}} \cdot \nabla) \phi_h^{n+\frac{1}{2}} \right) (v \cdot \nabla) \phi_h^{n+\frac{1}{2}} \right) dx = 0,
\]

\[
\int_{\Omega} (\nabla \cdot u_h^{n+\frac{1}{2}}) q \ dx = 0, \tag{3.2}
\]

\[
\int_{\Omega} \left( \phi_t^{n+1} \psi + (u_h^{n+\frac{1}{2}} \cdot \nabla) \phi_h^{n+\frac{1}{2}} \psi + \gamma \nabla \phi_h^{n+\frac{1}{2}} \cdot \nabla \psi + \frac{\gamma}{\epsilon^2} g_h(\phi_h^n, \phi_t^{n+1}) \right) dx = 0, \tag{3.3}
\]

for all \((v, q, \psi) \in W_0^h\), where \(u_t^{n+1} = \frac{u_h^{n+1} - u_h^n}{\Delta t}, \ \phi_t^{n+1} = \frac{\phi_h^{n+1} - \phi_h^n}{\Delta t}, \ u_h^{n+\frac{1}{2}} = \frac{1}{2}(u_h^n + u_h^{n+1}), \phi_h^{n+\frac{1}{2}} = \frac{1}{2}(\phi_h^n + \phi_h^{n+1}), \ p_h^{n+\frac{1}{2}} = \frac{1}{2}(p_h^n + p_h^{n+1})\), and

\[
g_h(\phi_h^n, \phi_t^{n+1}) = \frac{1}{2} \left( \left| \phi_h^{n+1} \right|^2 - 1 \right) + \frac{1}{2} \left( \left| \phi_h^n \right|^2 - 1 \right) \left( \phi_h^{n+1} + \phi_h^n \right) \tag{3.4}
\]

is an approximation to the nonlinear function \(g(\phi) = (|\phi|^2 - 1)\phi\) in the phase field equation.

Note that the term \(\frac{1}{2} \nabla \cdot u_h^{n+\frac{1}{2}} \) added in (3.1) corresponds to adding a zero term \(\frac{1}{2} (\nabla \cdot u) u\) to (2.1) following the technique mentioned in [44] in the pseudo-compressibility method. The reason we add this term here is that it aids to attain the discrete energy law (3.6) later. In such a derivation the integral identity in (2.15) which was used in obtaining the continuous energy law is no longer true in the case that the divergence of the velocity is not exactly zero when replacing (3.2) by the penalized system (3.6) later.

If there were no \(g_h\) the scheme given above would be simply the midpoint scheme. The approximation \(g_h\) looks similar to the midpoint scheme but not exactly the same. We call it a modified midpoint scheme. The approximate bulk mixing energy term \(g_h\) is so designed that we are able to derive an accurate discrete energy law for the fully discrete system. The resulting system of the scheme can be solved by a Newton or fixed point iterative method. We will discuss it in the next section.

Now we derive the discrete energy law in the case of zero external force (i.e. \(s(\phi) = 0\)) and homogeneous boundary condition for \(u\). According to the continuous case, we take \(v = u_h^{n+\frac{1}{2}}, q = p_h^{n+\frac{1}{2}}\) and \(\psi = \frac{\lambda}{\gamma} \phi_t^{n+1}\). As shown in [33], we can obtain the discrete energy law:

\[
\left( \frac{1}{2} \rho_0 ||u_h^{n+1}||^2_L^2 + \frac{\lambda}{2} ||\nabla \phi_h^{n+1}||^2_L^2 + \lambda \int_{\Omega} F(\phi_h^{n+1}) \right) = - \left( \nu ||\nabla u_h^{n+\frac{1}{2}}||^2_L^2 + \frac{\lambda}{\gamma} ||\phi_t^{n+1}||^2_L^2 \right) + (u_h^{n+\frac{1}{2}} \cdot \nabla) \phi_h^{n+\frac{1}{2}}||^2_L^2). \tag{3.5}
\]

We can easily see that the energy law (2.16) is accurately preserved by this modified midpoint scheme.
Remark 3.1  The fully implicit backward Euler scheme and explicit-implicit scheme are often used as the time-marching scheme and work well in many practical computations. But the discrete energy law of these schemes are not as accurate as the modified midpoint scheme. For example, the approximation of $g(\phi)$ in the backward Euler scheme is $g_h = (|\phi^{n+1}|^2 - 1)\phi^{n+1}$. To derive the energy law we need to take $\psi = \frac{\lambda}{\gamma} \phi_t^{n+1}$ and the term $\frac{\lambda}{\gamma} g_h \psi$ becomes $\lambda F(\phi_t^{n+1}) + \text{an error term}$:

$$\frac{\lambda \Delta t}{4 \epsilon^2} (2(|\phi^{n+1}|^2 - 1)|\phi_t^{n+1}|^2 + (|\phi^{n+1}|^2 - 1)^2).$$

Obviously, away from the interface $\phi^n$ and $\phi^{n+1}$ are almost equal to 1 or −1 and then this error term is almost zero. But it may not be very small near the interface where $-1 \leq \phi^n, \phi^{n+1} \leq 1$.

We also note that the divergence free equation (3.2) may needs to be treated carefully in incompressible flow computations. The projection method is popular but may be difficult to impose an artificial boundary condition and to derive a discrete energy law. On the other hand, from the viewpoint of differential algebraic equations, the incompressible flow model is of index two because the pressure does not show up in the divergence equation (3.2). The problem is thus not stable and index reduction is needed before applying a differential equation solver (See [31]). The penalty formulation (cf. [44]) is a simple formulation for such a purpose. It does not require any artificial boundary condition either. Furthermore, we are able to derive a discrete energy law based on this formulation. The penalty formulation under the modified midpoint scheme is to replace (3.2) by the following:

$$\int_{\Omega} (\nabla \cdot u_h^{n+\frac{1}{2}} + \delta p_h^{n+\frac{1}{2}}) q \, dx = 0. \quad (3.6)$$

Practically, the divergence free condition may be enforced by choosing a relatively small $\delta$. We will choose $\delta = 10^{-6}$ in our computations. When it is necessary to use a larger $\delta$ in order to improve the stability and accuracy a sequential regularization formulation (See [31, 34, 37]) may be used to replace the penalty formulation. The derivation of the energy law of the penalized system is not much different from the non-penalized formulation. Only the pressure term in (3.1) (i.e. $-p_h^{n+\frac{1}{2}} \nabla \cdot u_h^{n+\frac{1}{2}}$) is relevant to the divergence equation. Now replacing (3.2) by (3.6) the pressure term becomes

$$-\int_{\Omega} p_h^{n+\frac{1}{2}} \nabla \cdot u_h^{n+1} = \delta \int_{\Omega} (p_h^{n+\frac{1}{2}})^2.$$

So under the penalty formulation we can still obtain a discrete energy law:

$$\left( \frac{1}{2} \|u_h^{n+1}\|_{L^2}^2 + \frac{\lambda}{2} \|\nabla \phi_h^{n+1}\|_{L^2}^2 + \lambda \int_{\Omega} F(\phi_h^{n+1}) \right)_{\frac{t}{\Delta t}} = - \left( \nu \|\nabla u_h^{n+1}\|_{L^2}^2 + \delta \|p_h^{n+\frac{1}{2}}\|_{L^2}^2 \right. + \frac{\lambda}{\gamma} \|\phi_t^{n+1} + (u_h^{n+\frac{1}{2}} \cdot \nabla) \phi_h^{n+\frac{1}{2}}\|_{L^2}^2 \right). \quad (3.7)$$
So when $\delta$ is sufficiently small the continuous energy law is approximately maintained under the fully discretized penalty formulation.

### 3.2 Cahn-Hilliard model

We can apply the same idea to the Cahn-Hilliard model (2.19)-(2.22). Let $Q^h = W^h \times H^h$ and $Q^h_0 = W^h_0 \times H^h$. The approximate solution $(u_{h}^{n+1}, p_{h}^{n+1}, \phi_{h}^{n+1}, \omega_{h}^{n+1}) \in Q^h$ can be computed by the following modified midpoint scheme

\[
\begin{align*}
\int_{\Omega} \left( \rho_0 u_{h}^{n+1} \cdot v + \rho_0 (u_{h}^{n+\frac{1}{2}} \cdot \nabla) u_{h}^{n+\frac{1}{2}} \cdot v + \frac{1}{2} \rho_0 (\nabla \cdot u_{h}^{n+\frac{1}{2}}) u_{h}^{n+\frac{1}{2}} \cdot v + \nu \nabla u_{h}^{n+\frac{1}{2}} : \nabla v \\
- p_{h}^{n+\frac{1}{2}} (\nabla \cdot v) - \frac{\lambda}{\epsilon^2} (\omega_{h}^{n+\frac{1}{2}} + c \phi_{h}^{n+\frac{1}{2}}) \nabla \phi_{h}^{n+\frac{1}{2}} \cdot v \right) \, dx &= 0, \\
\int_{\Omega} (\nabla \cdot u_{h}^{n+\frac{1}{2}}) \, q \, dx &= 0, \\
\int_{\Omega} \left( \phi_{h}^{n+1} \psi + (u_{h}^{n+\frac{1}{2}} \cdot \nabla) \phi_{h}^{n+\frac{1}{2}} \psi + \frac{\gamma}{\epsilon^2} \nabla (\omega_{h}^{n+\frac{1}{2}} + c \phi_{h}^{n+\frac{1}{2}}) \cdot \nabla \psi \right) \, dx &= 0, \\
\int_{\Omega} \left( (\omega_{h}^{n+\frac{1}{2}} + c \phi_{h}^{n+\frac{1}{2}}) \chi - \epsilon^2 \nabla \phi_{h}^{n+\frac{1}{2}} \cdot \nabla \chi - g_h(\phi_{h}^{n}, \phi_{h}^{n+1}) \chi \right) \, dx &= 0
\end{align*}
\]

for all $(v, q, \psi, \chi) \in Q^h_0$. In the homogeneous case taking $v = u_{h}^{n+\frac{1}{2}}$, $q = p_{h}^{n+\frac{1}{2}}$, $\psi = \frac{\lambda}{\epsilon^2} (\omega_{h}^{n+\frac{1}{2}} + c \phi_{h}^{n+\frac{1}{2}})$ and $\chi = \lambda \phi_{h}^{n+\frac{1}{2}} / \epsilon^2$ we can obtain a discrete energy law for the Cahn-Hilliard model

\[
\begin{align*}
\left( \frac{1}{2} \rho_0 \| u_{h}^{n+1} \|_{L^2}^2 + \frac{\lambda}{2} \| \nabla \phi_{h}^{n+1} \|_{L^2}^2 + \lambda \int_{\Omega} F(\phi_{h}^{n+1}) \right) &= - \left( \nu \| \nabla u_{h}^{n+1} \|_{L^2}^2 \\
+ \frac{\lambda \gamma}{\epsilon^2} \| \nabla (\omega_{h}^{n+\frac{1}{2}} + c \phi_{h}^{n+\frac{1}{2}}) \|_{L^2}^2 \right).
\end{align*}
\]  

So the energy law (2.23) is accurately preserved by this modified midpoint scheme. Similarly, if we replace (3.9) by the penalty formulation (3.6), we can still obtain the discrete energy law (3.12) with an additional term $-\delta \| p_{h}^{n+1} \|_{L^2}^2$ at its right hand side. However, when we apply this scheme to the Cahn-Hilliard model (decoupled from the momentum transport equation by imposing a zero flow field)
we observe oscillations of the solution at the interface defined by \( \phi = 0 \) no matter how small the time step is. The oscillation is apparently not physical; it results in multi-lines and possible other strange structures of the interface when we draw the interface as a level curve of \( \phi = 0 \) (See Figure 3.1). We also notice small overshoots at the interface due to the lack of the maximum principle for this model. These overshoots may be reduced by refining the grid and the step size (See Figure 5.17 in Section 5). Nevertheless, such overshoots are away from the interface \( \phi = 0 \) and thus are not particularly important in presenting the interface and its motion.

To study the cause of such oscillations near the interface \((\phi = 0)\) we look into the motion of the points near the interface. Figure 3.2 shows the phase variable \( \phi \) vs time in a very short time interval at the interfacial point \((0, 0.25)\) and two neighboring points \((0, 0.25 + 1/128)\) and \((0, 0.25 - 1/128)\).

The phase variable \( \phi \) is supposed to be close to zero near the interface for a short time. But from the figure we see that it oscillates in time and the phase of oscillations at the interfacial point and its neighbors are different, which causes the oscillation in the spatial
direction of $\phi$ as shown in Figure 3.1. So we believe that the oscillation at the interface is due to the time discretization using the midpoint method. Indeed, the Cahn-Hilliard model (2.17)-(2.18) is an index-one partial differential algebraic equation in terms of the temporal variable $t^1$ which is the limit (as $\eta \to 0$) of an extremely stiff but regular (index-zero) differential equation (2.18) when an additional $\eta \omega_t$ term is added to its left hand side. So we can consider (2.18) to be the limit ($\eta \to 0$) equation of an extremely stiff equation. It is well known (See e.g. [2]) that the midpoint scheme, or in general, symmetric schemes cause oscillations for extremely stiff systems. A remedy to this is to solve the system by a stiff decay method, say backward Euler scheme, at a number of beginning time steps (until out of the initial layer (usually of size $O(\eta)$)) and then switch to the midpoint scheme. The equation (2.18) corresponds to the case $\eta \to 0$. So it only requires one time step to get out of the initial layer. We thus suggest the following algorithm: solving (2.17)-(2.18) using the backward Euler temporal scheme at the first time step and then switching to the modified midpoint scheme. Below we re-draw the $\phi$ vs $t$ figure at the interfacial point $(0, 0.25)$ and its two close neighbors over a short time. We see that $\phi$ is close to zero as expected (See Figure 3.3).

Figure 3.3: $\phi(\cdot, \cdot, t)$ vs $t$ at $(x, y) = (0, 0.25), (0, 0.25 + 1/128), (0, 0.25 − 1/128)$ using the combined backward Euler/modified midpoint scheme.

The zero level curve plot of the Cahn-Hilliard solution $\phi$ in the following figure indicates that there is no oscillations anymore at the interface. So the remedy works very well and results in a good algorithm for the Cahn-Hilliard model.

---

1(2.18) may be considered as an algebraic equation in the time variable $t$ since there is no derivatives in terms of $t$ in (2.18)
Figure 3.4: Deformation of the interface through level curves $\phi = 0$ without any flow field.

4 Implementation issues

In this section we discuss how to compute the solution of the scheme (3.1), (3.6) and (3.3). Since the scheme is nonlinearly implicit we need to do a linearization and then solve a linear system at each time step. If we linearize the scheme (3.1)-(3.3) with the Newton method, the resulted linear system depends on time. Consequently, we have to solve a different linear system at any different time step. This indicates that a direct linear system solver would be very costly. On the other hand, iterative methods may not be robust due to the complication of the model and a number of parameters which may be large or small. So the direct method is often preferred in solving the linear system resulted from very complicated PDEs. We thus look for an alternative linearization where the linear system may be symmetric and, more importantly, does not depend on time. Then we only need to do the Cholesky factorization for the symmetric linear system at the initial time step. After the initial time we do not need to factorize the linear system again since the coefficient matrix is independent of time. So we can compute the solution of the implicit scheme as if it is an explicit scheme at any time step other than the initial time.

We are going to use the Cahn-Hilliard model (3.8)-(3.11) to illustrate the procedure. It is straightforward to apply the same procedure to the Allen-Cahn model (See also [33]). To achieve a time independent (or so called matrix free) linear system we propose to use a fixed point iteration as the linearization of all nonlinear terms. We thus have the following iterative scheme (for $s = 1, 2, \ldots$) at every time level $t_n$, i.e. find $\bar{u}_s, \bar{p}_s, \bar{\phi}_s$ and $\bar{\omega}_s$ (as an approximation of $u^{n+1}, p^{n+1}, \phi^{n+1}$ and $\omega^{n+1}$, respectively) to satisfy:

\begin{align*}
\int_{\Omega} \left[ \frac{\bar{u}_s - u^n_h}{\Delta t} \cdot v + \left( \frac{u^n_h + \bar{u}_{s-1}}{2} \cdot \nabla \right) \frac{u^n_h + \bar{u}_{s-1}}{2} \cdot v + \frac{1}{2} \left( \nabla \cdot \frac{u^n_h + \bar{u}_{s-1}}{2} \right) \frac{u^n_h + \bar{u}_{s-1}}{2} \cdot v + \nu \nabla \frac{u^n_h + \bar{u}_{s-1}}{2} : \nabla v \\
- \frac{p^n_h + \bar{p}_s}{2} (\nabla \cdot v) + \frac{\lambda}{\gamma} \left( \frac{\bar{\phi}_s - \phi^n_h}{\Delta t} + \left( \frac{u^n_h + \bar{u}_{s-1}}{2} \cdot \nabla \right) \frac{\phi^n_h + \bar{\phi}_{s-1}}{2} \right) (v \cdot \nabla) \frac{\phi^n_h + \bar{\phi}_{s-1}}{2} \right] dx &= 0, \\
\int_{\Omega} \left( \nabla \cdot \frac{u^n_h + \bar{u}_{s}}{2} + \delta \frac{p^n_h + \bar{p}_s}{2} \right) q dx &= 0, \\
\int_{\Omega} \left[ \frac{\bar{\phi}_s - \phi^n_h}{\Delta t} \psi + \left( \frac{u^n_h + \bar{u}_{s-1}}{2} \cdot \nabla \right) \frac{\phi^n_h + \bar{\phi}_{s-1}}{2} \psi + \gamma \frac{\phi^n_h + \bar{\phi}_{s-1}}{2} \cdot \nabla \left( \frac{\omega^n_h + \bar{\omega}_{s}}{2} + c \frac{\phi^n_h + \bar{\phi}_{s}}{2} \right) \right] dx &= 0, \\
\int_{\Omega} \left[ \left( \frac{\omega^n_h + \bar{\omega}_{s}}{2} + c \frac{\phi^n_h + \bar{\phi}_{s}}{2} \right) \chi - c^2 \nabla \frac{\phi^n_h + \bar{\phi}_{s}}{2} \cdot \nabla \chi - g_b(\phi^n_h, \bar{\phi}_{s-1}) \chi \right] dx &= 0.
\end{align*}
where we choose initial iteration as $\bar{u}_0 = u_n^h$, $\bar{\phi}_0 = \phi_n^h$ and $\bar{\omega}_0 = \omega_n^h$. We can see that the stiffness matrix at each time step is independent of the time step $n$ and the number $s$ of the fixed point iterations, and symmetric if $c = 0$.

According to the discussion in [32] for the liquid crystal model we expect that the step size $\Delta t$ should at least satisfy $\gamma \Delta t < \varepsilon^2$ in order to have the convergence of the fixed point method in the case of the Allen-Cahn model. The restriction is expected to be worse in the case of the Cahn-Hilliard model. We also note that one step of such iteration is actually an implicit-explicit scheme. So the nonlinear iterative implementation procedure may be considered as something like an iterative implicit-explicit scheme.

We would like to emphasize here that we want to use the fixed point iteration whenever possible not only because a symmetric stiffness matrix and a matrix free evolution process can be achieved but also because the system (4.1)-(4.2) for $u$ and $p$ and the system (4.3)-(4.4) for $\phi$ and $\omega$ are automatically separated. We can solve (4.3)-(4.4) first to obtain $\bar{\phi}_s$ and $\bar{\omega}_s$, then solve (4.1)-(4.2) to get $\bar{u}_s$ and $\bar{p}_s$. This further reduces the size of the system and the cost of computation. This dynamic iteration may also be a way to achieve efficient time-domain parallelization (cf. [17]).

5 Numerical examples

In this section we compute a number of examples for interfacial phenomena to demonstrate the proposed energy law preserving $C^0$ finite element method. The computations are carried out with the help of the freefem++ platform ([18]) and MATLAB.

The examples are originally given in [35]. We will let the viscosity $\nu = 0.1$ if not otherwise stated. We apply the fixed point iterative method (cf. (4.1)-(4.4)) with a sufficiently small tolerance. All computations are carried out under the $P_2$ (piecewise polynomial of degree two) finite element space for the velocity $u$ and the phase variables $\phi$ and $\omega$, and the $P_1$ finite element space for the pressure $p$. The initial velocity is set to zero in all examples. In the first two examples, we set the buoyancy force to zero, i.e. $s(\phi) = 0$.

Example 5.1 We study the deformation of an initially rectangular bubble of fluid 1 immersed in fluid 2 using the Allen-Cahn model. The phase variable $\phi = 1$ inside the bubble and $\phi = -1$ outside the bubble. The rectangular bubble quickly deforms into a circular bubble due to the surface tension. We notice that the rectangular bubble deforms into a circular bubble while the size of the bubble shrinks due to the dissipative mechanism in the Allen-Cahn model. In the computation we take $\gamma = 0.1$, $\varepsilon^2 = 0.05^2$, $\Delta t = 0.001$ and use a $32 \times 32$ grid because our numerical tests show that a coarser $16 \times 16$ grid cannot resolve the interface properly (although a $16 \times 16$ grid works well for the velocity field in this case). The level curves of $\phi = 0$ at times $t = 0$, $0.02$, $0.04$ and $0.08$ are depicted in Figure 5.1. Also, the energy law with this energy law preserving scheme is indeed preserved very well under the $32 \times 32$ grid with six fixed point iterations in each time step (See Figure 5.2). Note that the scheme is nonlinear and is solved by a fixed point iterative method. So
Figure 5.1: Deformed interfaces at the first time step, \( t = 0.02, 0.04 \) and 0.08 with an initially zero flow field and the Allen-Cahn model.

Figure 5.2: The error \( \approx O(10^{-8}) \) in the energy law and the total energy vs time with \( \Delta t = 0.001 \).

the energy law is preserved up to the accuracy of the fixed point iteration.

Next we use this example to illustrate that the energy law preserving method performs better than those methods without preserving the energy law. For this purpose we consider the straightforward weak form (2.8)-(2.10) of the Allen-Cahn model (2.1), (2.2), (2.3). We can use our modified midpoint \( C^0 \) finite element scheme to this weak formulation. As described in §2 the scheme does not have a rigorous energy law since we cannot let \( \psi = -(\Delta \phi - f(\phi)) \) for a \( C^0 \) function \( \phi \). We now fix a smaller step size \( \Delta t = 0.0001 \) and compare the performance of the method with that of our energy law preserving method. In the case of \( \nu = 0.1 \), based on our numerical tests, a grid as coarse as \( 16 \times 16 \) can be used to resolve the velocity field using the energy law preserving scheme (See Figure 5.3). However, under the same \( 16 \times 16 \) grid the velocity calculated using the weak form (2.8)-(2.10) goes wrong, for example, at \( t = 0.2 \) (See Figure 5.4). For such a scheme without preserving the energy law a finer grid is required to obtain the correct velocity field (See Figure 5.5 with
Figure 5.3: The energy law preserving scheme: velocity fields at $t = 0.04$ and $0.2$ with $\nu = 0.1$ and a $16 \times 16$ grid.

Figure 5.4: The scheme without theoretically preserving the energy law: velocity fields at $t = 0.04$ and $0.2$ with $\nu = 0.1$ and a $16 \times 16$ grid.
Figure 5.5: The scheme without theoretically preserving the energy law: velocity fields at $t = 0.04$ and 0.2 with $\nu = 0.1$ and a $64 \times 64$ grid.

Figure 5.6: The energy law preserving scheme: velocity fields at $t = 0.04$ and 0.2 with $\nu = 0.001$ and a $64 \times 64$ grid.

a $64 \times 64$ mesh). In the case of $\nu = 0.001$, based on our numerical tests, a $64 \times 64$ grid is needed to resolve the velocity field (See Figure 5.6). Again, using the scheme based on the weak form (2.8)-(2.10) the velocity field under the same $64 \times 64$ grid goes wrong at $t = 0.2$ (See Figure 5.7).

Using the example we may validate the order of the finite element method we use in our computation. The available property of the solution is $\nabla \cdot u = 0$. Using this relation we can calculate the divergence error of the solution in a normalized $L^2$ norm: $\|\nabla \cdot (u(t_n) - u_h)\| = \|\nabla \cdot u_h\| = \left( \frac{1}{|\Omega|} \int_{\Omega} |\nabla \cdot u_h|^2 dx \right)^{\frac{1}{2}}$. We take $t_n = 0.1$ to avoid a possible initial layer associated with the penalty formulation. The results are shown in the following table. The estimated order is calculated by the formula $\log(\|\nabla \cdot (u - u_h)\|/\|\nabla \cdot (u - u_h/2)\|)/\log 2$. 
Figure 5.7: The scheme without theoretically preserving the energy law: velocity fields at $t = 0.04$ and $0.2$ with $\nu = 0.001$ and a $64 \times 64$ grid.

\[
\begin{array}{|c|c|c|c|c|}
\hline
\text{mesh} & 16x16 & 32x32 & 64x64 & 128x128 \\
\hline
\|\nabla \cdot (u - u_h)\| & 0.12782 & 0.0332624 & 0.00482967 & 0.000583337 \\
\text{estimated order} & - & 1.94 & 2.79 & 3.05 \\
\hline
\end{array}
\]

Numerical order has been studied for flow problems, where the velocity and pressure are approximated by the $P_2$-$P_1$ pair as we do. For example, the divergence error $\|\nabla \cdot (u - u_h)\|$ is numerically calculated for a quasi-Stokes problem and found to be two in [25]. Our calculation shows that it tends to be three, probably due to our penalized stabilization formulation for the divergence free equation. In any case this indicates that our computational accuracy is not lower than the expected.

**Example 5.2** We again consider the Allen-Cahn model in this example. We begin with two kissing circular bubbles. As time evolves the two bubbles coalesce into one big bubble. For this kissing bubble example although a $32 \times 32$ grid works but the level curve is not well resolved at earlier times. This might indicate that the Allen-Cahn model is more difficult to handle the topological change of the interface at least in its numerical version than the Cahn-Hilliard model (later we will see that the Cahn-Hilliard model well resolves zero level curves on a $32 \times 32$ grid). We then compute $\phi$ using a finer grid to avoid zig-zag level curves and to obtain good quality interfaces. The deformed interfaces with a $128 \times 128$ grid and $\Delta t = 0.0001$ are shown in Figure 5.8. But for the velocity calculation, a $32 \times 32$ grid is good enough to resolve the result, which is given in Figure 5.9.

**Example 5.3** In this example we consider the Allen-Cahn model for two fluids with different densities $\rho_1 = 1$ and $\rho_2 = 2$ (taking the background density $\rho_0 = \rho_1$), use the Boussinesq approximation for the variable density case and include the buoyancy force $s(\phi)$ as defined in §2. We take $g = 10$ in the computation and see the rise of the bubble. We start with a rectangular bubble at the middle of the domain as shown in Example 5.1. The density of the bubble is lighter than the density of the surrounding fluid. The bubble
Figure 5.8: Deformed interfaces at the first time step, $t = 0.02$, 0.04 and 0.08.

Figure 5.9: Corresponding velocity fields at $t = 0.02$, 0.04 and 0.08.
rises as expected due to the buoyancy force or the gravity differential (See Figures 5.10 and 5.11).

Finally we repeat the computations for some of above examples using the Cahn-Hilliard model. All the computations are done on a $32 \times 32$ grid. We take a smaller time step $\Delta t = 0.0001$ since the Cahn-Hilliard is involved with a fourth order operator which together with a small $\epsilon$ may significantly restrict the time step. All other parameters and initial conditions are taken the same values as given in the previous examples. Figures 5.12 and 5.13 correspond to Example 5.1, Figures 5.14 and 5.15 correspond to Example 5.2. From the computational results we observe the same phenomena as those using the Allen-Cahn model, but the interface deformation speed may be different. After all, these are two different models for binary phase flows at fixed parameters.

Remark 5.1 We observe from the figures that the area of the bubble seems shrinking over the time. This is the hallmark of the Cahn-Hilliard model since the model is dissipative. Although it preserves the volume or area of the bubble in the entire domain (i.e. $\int_\Omega \phi = \text{const}^2$),

\footnote{This is true assuming $u$ is of divergence free. Rigorously speaking, $u$ is not really divergence free due to the penalty treatment (3.6). But in all our computations with the choice of the penalty parameter $\delta = 10^{-6}$ the penalty treatment does not have any explicit effect to the integral of $\phi$ in the entire domain.}
Figure 5.12: Deformed interfaces at the first time step, $t = 0.0002$, $0.002$ and $0.008$ using the Cahn-Hilliard model.

Figure 5.13: Corresponding velocity fields at $t = 0.0002$, $0.002$ and $0.008$.

Figure 5.14: Deformed interfaces at the first time step, $t = 0.002$, $0.004$ and $0.008$ using the Cahn-Hilliard model.
Figure 5.15: Corresponding velocity fields at $t = 0.002, 0.004$ and $0.008$.

Figure 5.16: The integral $\int_{\Omega} \phi$ vs time for the square bubble example using the Cahn-Hilliard model with a $32 \times 32$ grid.

which is $-3.45833$ for the initially rectangular bubble example as depicted in Figure 5.16 and $-3.5$ for the kissing bubble example, in the whole time interval of computation), the high order dissipative mechanism in the diffuse interface model allows a “smeared” interface which makes the immiscible fluid system a weakly mixed one, especially in the neighborhood of the interface. If we want to reduce the effect on the shrinking of the area enclosed by the level curve $\phi = 0$, a smaller $\epsilon$ and finer grid may help. To illustrate this we recalculate the initially rectangular bubble example with $\epsilon^2 = 1e-4$, $\Delta t = 1e-7$ and using a $128 \times 128$ grid. Other parameters are not changed. We obtain that $\int_{\Omega} \phi$ is again equal to $-3.45833$ for the whole time interval of computation. The solution $\phi$ is depicted in Figure 5.17, which is much sharper at the interface region. And then the interface of the bubble does not have much room to “smear” and we observe almost no area shrinking of the bubble in the time frame we computed (See Figure 5.18 in comparison to Figure 5.12).
Figure 5.17: The solution $\phi$ for the square bubble example at the time $t = 0.0002$ using the Cahn-Hilliard model with $\epsilon^2 = 1e-4$ and a $128 \times 128$ grid.

Figure 5.18: The interfaces at times $t = 0.0002, 0.002$ and $0.008$ using the Cahn-Hilliard model with $\epsilon^2 = 1e-4$ and a $128 \times 128$ grid.
Based on our computational results, we conclude that the energy law preserving scheme for the Cahn-Hilliard model performs well with the interface motion and handles the topological change well with only a $32 \times 32$ grid. In general, the energy law preserving scheme renders much better results on coarser grids than other stable convergent schemes which do not obey the energy law at the discrete level.

6 Acknowledgement

Lin is partially supported by the Singapore academic research grant R-146-000-053-112 and R-146-000-099-112 at the early stage of the work. Liu is partially supported by NSF grants DMS-0509094 and DMS-0707595. Wang is partially supported by the NSF through grants DMS-0605029, DMS-0626180, CMMI-0849317, DMS-0819051, and DMS-0908330.

References


