An adaptive variational procedure for a two-phase model with variable density and viscosity

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Abstract. In this paper we present an adaptive variational procedure to solve a two-phase field model with variable density, viscosity. The model is a couple system that consists of incompressible Navier-Stokes equations and Allen-Cahn equation. In the scheme the projection method based on pressure is used to deal with the Navier-Stokes equations and stabilization approach is used for the Allen-Cahn equation. By some subtle explicit-implicit treatments, the proposed scheme is energy stable. In particular the adaptive refinement/coarsening is carried out by evaluating the residual error indicators on the error estimates of the Allen-Cahn equation. Some numerical examples are performed to show the accuracy and efficiency.

1. Introduction
The phase field model is a tool to resolve the motion of free interfaces between two distinct fluid components. Its origin can be traced back to Rayleigh [1] and Waals [2]. It was first formulated to study material mixtures and later adopted as a technique to resolve motion of the interface between different material components in material mixtures [3-5]. The most advantage of the phase-field approach is that the nonlinear partial differential equations satisfy thermodynamics consistent energy dissipation law. So we can carry out mathematical analysis and numerical schemes which can satisfy the corresponding discrete energy dissipation laws.

But most of the analysis of the two-phase model have been restricted to the matched density case. In this paper, we extend the previous study to a two-phase field model with variable density and viscosity in which the Allen-Cahn equation is adopted as the transport equation for the phase variable.

We first investigate the energy stability of the proposed scheme on an unstructured grid over a domain of complex geometry. The proposed procedure aims at reducing the error introduced by the mesh adaptivity while solving the coupled Navier-Stokes and Allen-Cahn equations. The effectiveness of the adaptive algorithm is assessed and several numerical experiments are performed. This article makes a significant contribution to the development of a stable, robust and general nonlinear adaptive variational procedure for solving the coupled Navier-Stokes and Allen-Cahn equations to model two-phase model via phase-field modeling.

The paper is organized as follows. We describe a Navier-Stokes Allen-Cahn coupled model in Section 2. In Section 3 we describe an energy stable scheme and discrete energy law aware derived and fully-discrete variational formulation is given. Finally, some numerical experiments are presented in Section 4 to assess the effectiveness and robustness of the proposed adaptive scheme.
2. A Navier-Stokes Allen-Cahn coupled model
In this paper we consider a two-phase incompressible fluid with variable density and viscosity in a physical domain denoted by $\Omega$ with boundary $\Gamma$. It is showed that this problem can be described by the following coupled system of the Allen-Cahn and Navier-Stokes equations:

Incompressible Navier-Stokes equations for hydrodynamics:

\[
\begin{aligned}
\rho \frac{\partial u}{\partial t} + (u \cdot \nabla) u &= \nabla \cdot \eta D(u) - \nabla p + B\mu \nabla \phi \quad \text{in } \Omega \\
\nabla \cdot u &= 0 \quad \text{in } \Omega \\
u &= 0 \quad \text{on } \Gamma \\
|_{t=0} = u_0 \quad \text{in } \Omega
\end{aligned}
\]  

(1)

Allen-Cahn equation for the dynamics of phase variable:

\[
\begin{aligned}
\frac{\partial \phi}{\partial t} + u \cdot \nabla \phi &= -M\mu \quad \text{in } \Omega \\
\mu &= -\varepsilon \Delta \phi + f(\phi) \quad \text{in } \Omega \\
\partial_n \mu &= 0, \partial_n \phi = 0 \quad \text{on } \Gamma \\
|\phi|_{t=0} = \phi_0 \quad \text{in } \Omega
\end{aligned}
\]  

(2)

To preserve the volume fraction, we add the Lagrangian multiplier $\xi(t)$ corresponding to the constant volume constraint as follows.

$$\mu = -\varepsilon \Delta \phi + f(\phi) + \xi(t), \quad \frac{d}{dt} \int_{\Omega} \phi dx = 0$$

We can easily get that $\xi(t) = \frac{1}{|\Omega|} \int_{\Omega} f(\phi(x,t)) dx$. In the above system, $p$ is the pressure, $\eta D(u) = \eta(\nabla u + \nabla u^T)$ denotes the viscous part of the stress tensor, $\phi$ is the phase-field variable and $\mu$ is the chemical potential. The function $f(\phi) = F'(\phi)$, with $F(\phi)$ being the Ginzburg-Landau bulk potential. More precisely, $F$ is defined as $F(\phi) = \frac{1}{4\varepsilon}(\phi^2 - 1)^2$. And $\nabla$ denotes the gradient operator, $n$ is the outward normal direction on $\Gamma$, scalar operator $\partial_n = n \cdot \nabla$ is the partial derivative along direction $n$, density $\rho = \frac{1+\phi}{2} \rho_1 + \frac{1-\phi}{2} \rho_2$, viscosity $\eta = \frac{1+\phi}{2} \eta_1 + \frac{1-\phi}{2} \eta_2$, where $()_i$ denotes the value of its argument on the phase $i$ of the argument. $B$ denotes the strength of the capillary force comparing the Newtonian fluid stress, $M$ is the phenomenological mobility coefficient, $\varepsilon$ is the ratio between interface thickness and domain size.

3. Numerical energy stable scheme
In this section, we adopt the stabilization method with the adaptive method. The unconditional stability of the stabilization method requires that the second derivative of $F(\phi)$ to be bounded. Thanks to a truncated $F(\phi)$ with quadratic growth at infinity can also guarantee the boundless of $\phi$ in Allen-Cahn equation. More precisely, we replace $F(\phi)$ by $\tilde{F}(\phi)$:
\[
\hat{F}(\phi) = \begin{cases} 
\frac{1}{2\varepsilon}(\phi + 1)^2, & \text{if } \phi < -1, \\
\frac{1}{4\varepsilon}(\phi^2 - 1)^2, & \text{if } -1 \leq \phi \leq 1, \\
\frac{1}{2\varepsilon}(\phi - 1)^2, & \text{if } \phi > 1
\end{cases}
\]  

(3)

Then setting \( \hat{f}(\phi) = \hat{F}(\phi) \), and \( L_i = \max_{\phi \in \mathbb{R}} |\hat{f}'(\phi)| = \frac{2}{\varepsilon} \). Let \( \Delta t > 0 \) be a time discretization step and suppose \( u^n, \phi^n \) and \( p^n \) are given, where the superscript \( n \) on variables denotes approximations of corresponding variables at time \( n \Delta t \). Assuming \( s_1 \) and \( s_2 \) are two positive stabilizing coefficients to be determined. The initial conditions \( \phi^0, p^{-1} = p^0, u^0 \) are given and set \( \rho = \min(\rho_1, \rho_2) \). Now we are ready to present the energy stable scheme:

Step 1: We first solve \( \phi^{n+1} \) and \( \mu^{n+1} \) from

\[
\mu^{n+1} = -\varepsilon \Delta \phi^{n+1} + \hat{f}(\phi^n) + s_1(\phi^{n+1} - \phi^n) + \xi^n(t),
\]

(4)

\[
\frac{\phi^{n+1} - \phi^n}{\Delta t} + u^n_\nu \cdot \nabla \phi^n = -M \mu^{n+1},
\]

(5)

with boundary condition \( \partial_n \mu^{n+1} = 0 \), where \( u^n_\nu = u^n - \varepsilon \cdot \frac{B}{\rho^n} \mu^{n+1} \nabla \phi^n \).

Step 2: Then we solve \( u^{n+1} \) from

\[
\rho^{n+1} = \frac{1 + \phi^{n+1}}{2} \rho_1 + \frac{1 - \phi^{n+1}}{2} \rho_2, \quad \eta^{n+1} = \frac{1 + \phi^{n+1}}{2} \eta_1 + \frac{1 - \phi^{n+1}}{2} \eta_2,
\]

(6)

\[
\frac{1}{\Delta t} \left( \rho^{n+1} + \rho^n \right) u^{n+1} - \rho^n u^n_\nu + \rho^{n+1}(u^n_\nu \cdot \nabla) u^{n+1} + \frac{1}{2} (\nabla \cdot (\rho^{n+1} u^n_\nu) u^{n+1})
\]

\[
= \nabla \cdot (\eta^{n+1} D(u^{n+1})) - \nabla (2 p^n - p^{-1})
\]

(7)

with the boundary condition \( u^{n+1} = 0 \)

Step 3: In the last step, we get \( p^{n+1} \) from

\[
\Delta (p^{n+1} - p^n) = \frac{\rho}{\Delta t} \nabla \cdot u^{n+1}
\]

(8)

With the boundary condition \( \partial_n p^{n+1} = 0 \).

Then we can get the following finite element method and give the weak form. In a standard finite element method the mesh is fitted to the boundary or interpolates the boundary to some suitable order. Let \( T_h \) be a curvilinear triangulation of \( \Omega \), such that \( \Omega \subset T_h \), but \( T_h \subset \Omega \). For all triangles \( K \in T_h \) holds \( K \cap \Omega \neq \emptyset \) and we define the domain covered by \( T_h \) and \( \Omega_r : = \bigcup_{K \in T_h} K \). Let \( h_K \) be the diameter of \( K \) which is less or equal to the grid-parameter \( h \): \( h = \max_{K \in T_h} h_K > 0 \). Associated with \( T_h \) we have the finite element spaces of continuous piece wise polynomial functions
\[ V_h = \{ v_h \in H^1(\Omega_T) : v_h|_K \in P_1(K), \forall K \in T_h \} ; \]
\[ U_h = \{ u_h \in H^1(\Omega_T) : u_h|_K \in P_2(K), \forall K \in T_h \} \]

Where \( P_1(K) \) denotes the space of polynomials of degree less than or equal to \( k \) on the element \( K \).

Then the discrete finite element form can be stated as: first, find \( (\mu_h^{n+1}, \phi_h^{n+1}) \in V_h \times V_h \), such that for \( (\omega_h, \varphi_h) \in V_h \times V_h \)
\[
\frac{\partial (\phi_h^{n+1} + \phi_h^n)}{\partial t} + (M \mu_h^{n+1}, \omega_h) = (\partial_n \cdot \nabla \phi_h^n, \omega_h) \\
(\varepsilon \nabla \phi_h^{n+1}, \nabla \varphi_h) + s_i (\phi_h^{n+1}, \varphi_h) - (\mu_h^{n+1}, \varphi_h) = (s_i \phi_h^n - \tilde{f} (\phi_h^n) - \xi^n (t), \varphi_h) 
\]

Second, from (6) we get \( \rho^{n+1}, \eta^{n+1} \), then we find \( u_h^{n+1} \in U_h \), such that for any \( v_h \in U_h \)
\[
\frac{1}{2} (\rho^{n+1} + \rho^n) u_h^{n+1} + \rho^n (u_h^n \cdot \nabla) u_h^{n+1} + \frac{1}{2} (\nabla \cdot (\rho^{n+1} u_h^n) u_h^{n+1}, v_h) \\
+ (\eta^{n+1} D(u_h^{n+1}), \nabla v_h) = \frac{\partial^n u_h^n}{\partial t} - \nabla (2 p_h^n - p_h^{n-1}), v_h) 
\]

Last, find \( p_h^n \in V_h \), such that for any \( q_h \in V_h \)
\[
(\nabla P_h^{n+1}, \nabla q_h) = (\nabla P_h^n, \nabla q_h) + \frac{\partial}{\partial t} (\nabla \cdot u_h^{n+1}, q_h) 
\]

The above finite element formulation of the Navier-Stokes and the Allen-Cahn equations is simply the differential operator multiplied by the weighting function and integrated by parts as appropriate, which tends to minimize the residual of the equations in a chosen set of weighting functions. When the solution of the underlying differential equation is smooth, as measured relative to the differential equation on the given mesh, the variational error tends to be small at convergence. If the solution exhibits oscillations near sharp gradients due to dominant convection and reaction effects on an underresolved mesh, the residual of the equation has a significantly large value. This residual needs to be minimized to obtain an accurate and close-to-converged solution, defined by the user-defined tolerance limit. Therefore, the mesh has to be refined in those areas to capture the sharp gradients in the solution. This suggests using the residual of the differential equation as an indicator of the error for the adaptive mesh algorithm. For the quantification of the error on which our adaptive algorithm will be based, the residual error estimates are derived for the Galerkin discretization of the Allen-Cahn equation as in [7].

4. A numerical experiment

Let \( \Omega = [0,1] \times [0,1] \) and the periodic boundary conditions are imposed on all the boundaries. The initial condition for this problem is considered as:
\[
\phi(x, y, 0) = 1 + \tanh\left(\frac{R_1 - \sqrt{(x-0.25)^2 + (y-0.25)^2}}{\sqrt{2} \varepsilon}\right) + \tanh\left(\frac{R_2 - \sqrt{(x-0.75)^2 + (y-0.75)^2}}{\sqrt{2} \varepsilon}\right)
\]

Where \( R_1 = 0.1 \) and \( R_2 = 0.15 \) are the radii of the two circles centered at \((0.35, 0.35)\) and \((0.57, 0.57)\), respectively. The interface thickness parameter is chosen as \( \varepsilon = 0.005 \). The results on \( 512 \times 256 \) are taken as the reference solutions and \( \partial t = 0.0005 \), the results regarding the error analysis are showed in Table 1.
Table 1. \( t = 0.06 \), \( L^2 \) error and convergence rate

| h    | \( u_x \)       | Rate | \( u_y \)       | Rate | \( \phi \)      | Rate | \( p \)        | Rate |
|------|-----------------|------|-----------------|------|-----------------|------|----------------|------|
| 0.2022 | 4.6331e-02    | -    | 1.2891e-02    | -    | 2.8933e-01    | -    | 1.2488e-02   | -    |
| 0.1011 | 3.4722e-03    | 2.50 | 2.2548e-03    | 2.92 | 7.7651e-02    | 2.01 | 6.3244e-03   | 1.61 |
| 0.0505 | 4.1561e-04    | 2.71 | 3.6763e-04    | 2.83 | 2.4552e-02    | 2.24 | 2.4419e-03   | 1.82 |

Figure 1. The adaptive mesh at \( t=0, t=400 \)

5. Conclusion
In this paper, a stable, robust and general adaptive variational partitioned procedure has been proposed to solve the coupled Navier-Stokes and Allen-Cahn equations for two-phase fluid flows. The simplicity of the refinement/coarsening avoids complicated tree-type data structures, thus providing the ease of implementation. Several test problems are considered to demonstrate the various aspects of the proposed adaptive variational scheme.

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