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ERROR ESTIMATION FOR THE CONVECTIVE CAHN – HILLIARD EQUATION

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Abstract. The Cahn–Hilliard phase-field (or diffuse-interface) model has a wide range of applications where the interest is the modelling of phase segregation and evolution of multiphase flow systems. In order to capture the physics of these systems, diffuse-interface models presume a nonzero interface thickness between immiscible constituents, see [1]. The multiscale nature inherent in these models (interface thickness and domain size of interest) urges the use of space-adaptivity in discretization.

In this contribution we consider the a-posteriori error analysis of the convective Cahn–Hilliard [4] model for varying Péclet number and interface-thickness (diffusivity) parameter. The adaptive discretization strategy uses mixed finite elements, a stable time-stepping algorithm and residual-based a-posteriori error estimation [2, 5]. This analysis for the convective model forms a basic step in our research and will be helpful to the coupled Cahn–Hilliard/Navier–Stokes system [3] which is the desired model for future research.

1 INTRODUCTION

1.1 The Model

Let $\Omega \subset \mathbb{R}^d$ be a bounded domain with $d = 1, 2, 3$ and $\partial\Omega$ be the boundary which has an outward unit normal $\mathbf{n}$. The convective Cahn-Hilliard equation can be written as follows:

Find the real valued functions $(c, \mu) : \Omega \times [0, T] \to \mathbb{R}$ for $T > 0$ such that

$$\begin{aligned} \partial_t c - \frac{1}{Pe} \triangle \mu + \nabla \cdot (\mathbf{u} c) = 0 \qquad & \text{in} \quad \Omega_T := \Omega \times (0, T] \\ \mu = \phi'(c) - \epsilon^2 \nabla c \qquad & \text{in} \quad \Omega_T \\ c(\cdot, 0) = c_0 \qquad & \text{in} \quad \Omega \\ \partial_{\mathbf{n}} c = \partial_{\mathbf{n}} \mu = 0 \qquad & \text{on} \quad \partial\Omega_T := \partial\Omega \times (0, T], \end{aligned}$$

where $\partial_t(\cdot) = \partial(\cdot)/\partial t$, $\partial_{\mathbf{n}}(\cdot) = \mathbf{n} \cdot \nabla(\cdot)$ is the normal derivative, ϕ is the real-valued free energy function, $\mathbf{u}$ is a given function such that $\nabla \cdot \mathbf{u} = 0$ in Ω and $\mathbf{u} \cdot \mathbf{n} = 0$ on $\partial\Omega$, Pe is the *Péclet* number and ϵ is the interface thickness.

The nonlinear energy function $\phi(c)$ is of the double well form and we consider the following C^2-continuous function :

$$\phi(c) := \begin{cases} (c+1)^2 & c < -1, \\ \frac{1}{4}\left(c^2 - 1\right)^2 & c \in [-1, 1], \\ (c-1)^2 & c > 1. \end{cases}$$

1.2 Weak Formulation

In order to obtain the weak formulation, we consider the following function space and the corresponding norm as a suitable space for μ:

$$V := L^2(0, T; H^1(\Omega)), \quad \|v\|_V^2 := \int_0^T \|v(t)\|^2_{H^1_{(\Omega)}}\, dt$$

and the space suitable for the phase variable c is

$$W := \{v \in V : v_t \in V'\},$$

where $V' := L^2(0, T; [H^1(\Omega)]')$ is the dual space of V with the norm $\|v_t\|_W^2 := \|v\|_V^2 + \|v_t\|_{V'}^2$, where

$$\|v_t\|_{V'}^2 := \int_0^T \|v_t(t)\|^2_{[H^1(\Omega)]'}\, dt.$$

Then the weak form of the problem becomes:

Find $(c, \mu) \in W_{c_0} \times V$:

$$\begin{aligned} \langle c_t, w \rangle + (u \nabla c, w) + \frac{1}{Pe}(\nabla \mu, \nabla w) = 0 \qquad & \forall w \in H^1(\Omega) \\ (\mu, v) - (\phi(c), v) + \epsilon^2 (\nabla c, \nabla v) = 0 \qquad & \forall v \in H^1(\Omega), \end{aligned}$$

for $t \in [0, T]$, where W_{c_0} is the subspace of W of which the trace at $t = 0$ coincide with c_0.

To derive an a-posteriori error representation, we will employ the mean-value-linearized adjoint problem. The dual problem can be defined in terms of dual variables (p, χ) where the dual variable p is a function in the space

$$W^{\bar{q}} := \{v \in W : v(T) = \bar{q}\}\,.$$

Then the dual problem can be written:
Find $(p, \chi) \in W^{\bar{q}} \times V$:

$$\begin{aligned}
-\partial_t p + u\nabla p + \epsilon^2 \triangle\chi - \phi'(c, \hat{c})\chi = q_1 \qquad & \text{in} \quad \Omega \times [0, T) \\
\chi - \frac{1}{Pe}\triangle p = q_2 \qquad & \text{in} \quad \Omega \times [0, T) \\
p = \bar{q} \qquad & \text{on} \quad \Omega \times \{t = T\} \\
\partial_{\mathbf{n}} p = \partial_{\mathbf{n}}\chi = 0 \qquad & \text{on} \quad \partial\Omega \times [0, T],
\end{aligned}$$

where the nonlinear function $\phi'(c, \hat{c})$ is a mean-value-linearized function

$$\phi'(c, \hat{c}) = \int_0^1 \phi''\left(sc + (1 - s)\hat{c}\right) ds.$$

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