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A NUMERICAL ANALYSIS OF THE COUPLED CAHN-HILLIARD/ALLEN-CAHN SYSTEM WITH DYNAMIC BOUNDARY CONDITIONS

AHMAD MAKKI, ALAIN MIRANVILLE*, AND MADALINA PETCU

Abstract. The numerical analysis of the coupled Cahn-Hilliard/Allen-Cahn system endowed with dynamic boundary conditions is studied in this article. We consider a semi-discretisation in space using a finite element method and we derive error estimates between the exact and the approximate solution. Then, using the backward Euler scheme for the time variable, a fully discrete scheme is obtained and its stability is proved. Some numerical simulations illustrate the behavior of the solution under the influence of dynamical boundary conditions.

Key words. Cahn-Hilliard/Allen-Cahn equations, dynamic boundary conditions, finite element method, error estimates, backward Euler scheme, Lojasiewicz inequality.

1. Introduction

We consider the Cahn-Hilliard/Allen-Cahn system with dynamic boundary conditions

$$(1)\qquad \begin{cases} u_t = \Delta\mu, & x \in \Omega, \\ \mu = -\Delta u + f(u+v) + f(u-v), & x \in \Omega, \\ v_t = \Delta v - f(u+v) + f(u-v) - \alpha v, & x \in \Omega, \\ u_t = \delta\Delta_\Gamma \mu - \partial_n \mu, & x \in \Gamma, \\ \mu = -\sigma\Delta_\Gamma u + g(u+v) + g(u-v) + \partial_n u, & x \in \Gamma, \\ v_t + \partial_n v - \kappa\Delta_\Gamma v + g(u+v) - g(u-v) = 0, & x \in \Gamma, \end{cases}$$

where Ω is a $2d$ or $3d$ slab, i.e.

$$\Omega = \prod_{i=1}^{d-1}(\mathbb{R}/(L_i\mathbb{Z})) \times (0, L_d), \qquad L_i > 0, i = 1, \cdots, d, \quad d = 2 \text{ or } 3,$$

with smooth boundary

$$\Gamma = \partial\Omega = \prod_{i=1}^{d-1}(\mathbb{R}/(L_i\mathbb{Z})) \times \{0, L_d\};$$

in other words, when $d = 2$, Ω is the rectangle $(0, L_1) \times (0, L_2)$, u, μ and v are periodic in x_1-direction and the boundary conditions are valid for $x_2 = 0$ and $x_2 = L_2$; when $d = 3$, Ω is the parallelepiped $(0, L_1) \times (0, L_2) \times (0, L_3)$, u, μ and v are periodic in the x_1 and x_2-directions and the boundary conditions are valid for $x_3 = 0$ and $x_3 = L_3$. The function f is the derivative of some double-well potential (typically, $f(s) = s^3 - s$) and g is the derivative of a surface potential, (typically, $g(s) = a_\Gamma s - b_\Gamma,\ a_\Gamma > 0,\ b_\Gamma \in \mathbb{R}$).

In (1), u and v represent a conserved (typically an average concentration) and a non-conserved order parameter, respectively. See [5] for further relevant references. Furthermore, the parameter α reflects the location of the system within the

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*Corresponding author.

phase diagram and may be either positive or negative. In what follows we consider, without any restriction of generality, α positive (the case α negative can be treated similarly, adapting certain *a priori* estimates). Moreover, δ, σ are nonnegative parameters related to the boundary diffusion and $\kappa > 0$ is a physical coefficient. Also, Δ_Γ is the Laplace-Beltrami operator on Γ and ∂_n is the outward normal derivative. The evolution boundary value problem (1) is completed by initial conditions $u(0) = u_0$ and $v(0) = v_0$. We remark that in the particular case that we consider here, when the domain is a slab, the Laplace-Beltrami operator on Γ reduces to $\partial^2_{x_1x_1}$ for the case $d = 2$ and to $\partial^2_{x_1x_1} + \partial^2_{x_2x_2}$ for the case $d = 3$.

The Cahn-Hilliard/Allen-Cahn system endowed with Neumann boundary conditions was introduced in [4, 5], in order to describe simultaneous order-disorder and phase separation in binary alloys on a BCC lattice in the neighborhood of the triple point. For further references on the physical pertinence of the model, we refer the interested reader to [2]. The authors of [5] explored two phenomenological approaches leading to systems of coupled Allen-Cahn/Cahn-Hilliard (AC/CH) equations. Another important application of the coupled (AC/CH) equations is that under appropriate compositional conditions, ordering can be induced in a previously homogeneous material. If the composition differs slightly from these conditions, the excess composition can emerge as droplets along the boundaries between the ordered regions. This phenomena can be modeled by a coupled (AC/CH) system with degenerate mobilities. In similar applications, surface diffusion coupled with motion by mean curvature appears quite naturally. There are additional effects which are often neglected and which arguably should be included. However, the coupled motion, by itself, is not finally understood and it was thus reasonable to isolate it and study it, even given its limitations (see [9]).

In [4], the authors prove the well-posedness and the existence of maximal attractors and inertial sets (i.e., exponential attractors) for the usual cubic nonlinear term $f(s) = s^3 - \beta s$ in three space dimensions when Neumann boundary conditions are considered. The numerical study using a finite element approximation was treated in [3] for the case of a degenerate Allen-Cahn/Cahn-Hilliard system under Neumann boundary conditions.

A similar system, with a non-constant mobility, was treated in [10] where the existence of weak solutions for a degenerate parabolic system consisting of a fourth-order and a second-order equation with singular lower-order terms in one space dimension with Neumann boundary conditions was proved. In addition, asymptotics for a similar system with a non-constant mobility, proposed as a diffuse interface model for simultaneous order-disorder and phase separation, was studied in [19]. There, A. Novick-Cohen focused on the motion in the plane. This framework yields both sharp interface and diffuse interface models of sintering of small grains and thermal grains boundary grooving in polycrystalline films. This work was extended in [20], where the authors studied the partial wetting case, and their analysis accounts for motion in three space dimensions.

The Cahn-Hilliard/Allen-Cahn system (1) is derived from the following Ginzburg-Landau free energy

$$\begin{aligned} J(u,v) =& \frac{1}{2}(\|\nabla u\|^2_\Omega + \|\nabla v\|^2_\Omega) + \frac{\alpha}{2}\|v\|^2_\Omega \\ &+ \int_\Omega \{F(u+v) + F(u-v)\}\, dx + \frac{\sigma}{2}\|\nabla_\Gamma u\|^2_\Gamma \\ &+ \frac{\kappa}{2}\|\nabla_\Gamma v\|^2_\Gamma + \int_\Gamma \{G(u+v) + G(u-v)\}\, d\Gamma, \end{aligned} \tag{2}$$