

NUMERICAL ANALYSIS FOR A NONLOCAL PHASE FIELD SYSTEM

SETH ARMSTRONG, SARAH BROWN AND JIANLONG HAN

Abstract. In this paper, we propose a stable, convergent finite difference scheme to solve numerically a nonlocal phase field system which may model a variety of nonisothermal phase separations in pure materials which can assume two different phases, say solid and liquid, with properties varying in space. The scheme inherits the characteristic property of conservation of internal energy. We also prove that the scheme is uniquely solvable and the numerical solution will approach the true solution in the L^∞ - norm.

Key words. Finite difference scheme; Nonisothermal, Long-range interaction.

1. Introduction

In this work, we consider the problem

$$(1.1) \quad u_t = \int_{\Omega} J(x-y)u(y) dy - \int_{\Omega} J(x-y) dy u(x) - f(u) + l\theta,$$

$$(1.2) \quad (\theta + lu)_t = \Delta\theta$$

in $(0, T) \times \Omega$, with initial and Neumann boundary conditions

$$(1.3) \quad u(0, x) = u_0(x), \quad \theta(0, x) = \theta_0(x),$$

$$(1.4) \quad \left. \frac{\partial\theta}{\partial n} \right|_{\partial\Omega} = 0,$$

where $T > 0$ and $\Omega \subset \mathbb{R}^n$ is a bounded domain. Here θ represents temperature, u is an order parameter often used to represent various material phases, l is a latent heat coefficient, the interaction kernel satisfies $J(-x) = J(x)$, and f is bistable.

In order to derive equations (1.1)-(1.2), we begin with the free energy

$$(1.5) \quad E = \frac{1}{4} \int \int J(x-y)[u(x) - u(y)]^2 dx dy + \int \left[F(u(x)) + \frac{1}{2}\theta^2 \right] dx,$$

where F is a double well function.

We consider the gradient flow associated with (1.5) relative to the order parameter u in L^2 and the internal energy e in $H_0^{-1}(\Omega)$, where by H_0^{-1} we mean the dual space of H^1 with mean value zero. This is done because the total internal energy I , with density denoted by $e = \theta + lu$, should be conserved. We have

$$(1.6) \quad u_t = -\frac{\partial E(u, e)}{\partial u},$$

$$(1.7) \quad e_t = -\frac{\partial E(u, e)}{\partial e},$$

where $\frac{\partial E(u, e)}{\partial u}$ is a linear functional on L^2 and $\frac{\partial E(u, e)}{\partial e}$ is a linear functional on H^{-1} .

If we write $F' = f$, the representative of $\frac{\partial E(u,e)}{\partial u}$ in L^2 is

$$(1.8) \quad \frac{\partial E(u,e)}{\partial u} = - \int_{\Omega} J(x-y)u(y) dy + \int_{\Omega} J(x-y)dy u(x) + f(u) - l(e-lu),$$

and the representative of $\frac{\partial E(u,e)}{\partial e}$ in H^{-1} is

$$(1.9) \quad \frac{\partial E(u,e)}{\partial e} = -\Delta(e-lu).$$

The more familiar Ginzburg-Landau free energy

$$\int \left[\frac{d^2}{2} |\nabla u|^2 + F(u) + \frac{l}{2} \theta^2 \right] dx$$

used in [7], [8], and in higher order versions by [6] in deriving phase-field systems, is obtained by approximating the interaction term through a truncated Taylor series. For example, when J is fairly localized, one may hope that

$$\int \int J(x-y)(u(x) - u(y))^2 dx dy$$

is well-approximated by

$$\int \left(\frac{d^2}{2} |\nabla u|^2 \right) dx,$$

where $\frac{d^2}{2} = \int J(y)y_i^2 dy$ is assumed to be independent of coordinate, i . Such an approximation was introduced by Van der Waals in [20] in 1893, and has been adopted ever since for ease of analysis.

If $\int_{\Omega} J(x-y)u(y)dy - \int_{\Omega} J(x-y)dy u(x)$ is replaced by Δu , the system (1.1)-(1.4) becomes

$$(1.10) \quad u_t = \Delta u - f(u) + l\theta,$$

$$(1.11) \quad (\theta + lu)_t = \Delta \theta$$

in $(0, T) \times \Omega$, with initial and Neumann boundary conditions

$$(1.12) \quad u(0, x) = u_0(x), \quad \theta(0, x) = \theta_0(x), \quad \text{and}$$

$$(1.13) \quad \frac{\partial \theta}{\partial n} \Big|_{\partial \Omega} = 0.$$

The system (1.1)-(1.4) and the system (1.10)-(1.13) were proposed as models for nonisothermal phase separation in pure materials which can assume two different phases, say solid and liquid. The function θ represents the temperature field within the material. The function u is an order parameter that describes the phase of the material, where with appropriate scaling $u = 1$ represents the solid phase and $u = -1$ represents the liquid phase; values of u with $-1 < u < 1$ represent a mixture of the two phases. The results about existence, uniqueness, and the structure of solutions for both systems can be found in references [1,3-5,9-13,15-19].

To the best of our knowledge, there are very few results on the numerical solutions to the system (1.1)-(1.4) and the system (1.10)-(1.13).

When temperature is fixed in both systems, (1.1)-(1.4) is the nonlocal Allen-Cahn equation

$$(1.14) \quad u_t = \int_{\Omega} J(x-y)u(y) dy - \int_{\Omega} J(x-y)dy u(x) - f(u)$$