Control and Stabilization of the Cahn-Hilliard Equation. A Numerical Approach

Roland GLOWINSKI[1] Angel Manuel RAMOS[2]

Abstract

Phase separation in a binary mixture is described by the nonlinear evolutionary Cahn-Hilliard equation. In this paper we numerically discuss the Neumann Control of this equation in order to avoid the unstable phase separation phenomenon known as spinodal decomposition.

Introduction

Binary mixtures such as Fe-Al alloys undergo, under certain circumstances (cooling below a critical temperature, for example), a *phase separation* phenomenon known as *spinodal decomposition.* Starting form the pioneering work of J.W. Cahn and J.E. Hilliard (see refs. [2] and [1]), this phenomenon has motivated a large number of investigations and it is generally agreed that spinodal decompositions of binary mixtures are modeled by the *Cahn-Hilliard equation* (which is a *fourth-order parabolic non-linear* equation), with appropriate *initial* and *boundary conditions.* Namely,

$$\begin{cases} \dfrac{\partial \varphi}{\partial t} - \Delta(\varphi^3 - \varphi) + \varepsilon^2 \Delta^2 \varphi = 0 & \text{in } Q := \Omega \times (0,T), \\ \varphi(x,0) = \varphi_0(x) & \text{in } \Omega, \\ \dfrac{\partial \varphi}{\partial n} = \dfrac{\partial}{\partial n} \Delta \varphi = 0 & \text{on } \partial\Sigma := \Omega \times (0,T). \end{cases} \tag{1}$$

Here $\Omega \subset I\!R^d$ ($d = 1, 2$, or 3) is the space region in which the spinodal decomposition is taking place, $\Gamma := \partial\Omega$, φ is equal to $c_2 - c_1$, where c_1 and c_2 are the respective concentrations of the two mixtures components of the spinodal decomposition (therefore φ must satisfy $\varphi \in [-1, 1]$), and φ_0 is a given initial value.

The term $-\Delta(\varphi^3 - \varphi)$ can be also written as $-\nabla \cdot (3\varphi^2 - 1)\nabla\varphi$, which shows that in those regions of Ω where $3\varphi^2 - 1 < 0$ (i.e. $|\varphi| < 1/\sqrt{3}$), the term $3\varphi^2 - 1$ behaves like a *negative diffusion* coefficient (this anti-diffusion is precisely what is the basis of the spinodal decomposition, from the mathematical point of view).

In [3] the authors give a numerical method to solve this problem (without control) and show that, if the initial condition φ_0 is a “small” perturbation of the steady-state solution $\varphi = 0.3$ (we point out that $0.3 < 1/\sqrt{3}$), the solution evolves toward a steady-state solution, where the solution jumps from -1 to +1 through a very narrow layer, showing the spinodal decomposition is taking place.

In [4] the authors give, from a theoretical point of view, some results about the controllability of some *higher-order nonlinear parabolic equations* of Cahn-Hilliard type. That paper is, to the best of our knowledge, the first work dealing with the *controllability* of this type of equations and gives sufficient conditions for the non-linearity in order to guarantee the *approximate controllability property.* That paper also gives some counter-examples showing that this property does not hold for some special non-linearities.

We discuss the *Neumann Control* of this problem to avoid the mentioned spinodal decomposition. To be precise, we consider the problem

$$\begin{cases} \dfrac{\partial\varphi}{\partial t} - \Delta(\varphi^3 - \varphi) + \varepsilon^2\Delta^2\varphi = 0 & \text{in } Q, \\ \varphi(x,0) = \varphi_0(x) & \text{in } \Omega, \\ \dfrac{\partial\varphi}{\partial n} = u\chi_\gamma, \quad \dfrac{\partial}{\partial n}\Delta\varphi = 0 & \text{on } \Sigma, \end{cases} \tag{2}$$

where χ_γ is the characteristic function of $\gamma \subset \partial\Omega$ and u is the external control acting on γ. The goal of this paper is to show that, if we start from a "small" perturbation φ_0 of a constant steady-state solution $\varphi_s \in [-1, 1]$, we can control the solution of the equation, in order to avoid its evolution toward a solution of the type described above, so that it will remain near φ_s.

The plan is the following: 1) First, we linearize the system in the neighborhood of the steady-state solution, 2) next we compute a suitable optimal control for the linearized model and 3) finally we apply the above control to the nonlinear system. This approach was used in [6], where the authors study the control and stabilization of a *second-order nonlinear parabolic system*, which blows up when uncontrolled.

Linearization of the problem in the neighborhood of φ_s.

Let us consider a small variation $\delta\varphi_s$ of φ_s. Then the solution φ of (1) can be written as $\varphi = \varphi_s + \delta\varphi$, where, if φ remains near φ_s, the perturbation $\delta\varphi$ of the steady-state solution φ_s satisfies approximately the following linear model:

$$\begin{cases} \dfrac{\partial\delta\varphi}{\partial t} - \nabla\cdot(3\varphi_s^2 - 1)\nabla\delta\varphi + \varepsilon^2\Delta^2\delta\varphi = 0 & \text{in } Q, \\ \delta\varphi(x,0) = \delta\varphi_s(x) & \text{in } \Omega, \\ \dfrac{\partial\delta\varphi}{\partial n} = \dfrac{\partial}{\partial n}\Delta\delta\varphi = 0 & \text{on } \Sigma. \end{cases}$$

It is clear that this approximate system is no longer valid if $\delta\varphi$ becomes too large. The idea is to compute a control action preventing $\delta\varphi$ from becoming large and hope that this computed control will also stabilize the original nonlinear system. Therefore we look for a control u such that the solution $\delta\varphi$ of

$$\begin{cases} \dfrac{\partial\delta\varphi}{\partial t} - \nabla\cdot(3\varphi_s^2 - 1)\nabla\delta\varphi + \varepsilon^2\Delta^2\delta\varphi = 0 & \text{in } Q, \\ \delta\varphi(x,0) = \delta\varphi_s(x) & \text{in } \Omega, \\ \dfrac{\partial\delta\varphi}{\partial n} = u\chi_\gamma, \quad \dfrac{\partial}{\partial n}\Delta\delta\varphi = 0 & \text{on } \Sigma, \end{cases} \tag{3}$$

remains near 0.

Control Problem for the Linearized Model.

We consider, for the time being, a finite-horizon $T < \infty$. Using the notation $y = \delta\varphi$, we (shall try to) stabilize system (3) via the following control formulation:

$$(\mathcal{CP}) \qquad \begin{cases} u \in \mathcal{U}, \\ J(u) \le J(v), \ \forall v \in \mathcal{U}, \end{cases}$$

where $\mathcal{U} = L^2(\gamma \times (0,T))$,

$$J(v) = \frac{1}{2}\int_{\gamma\times(0,T)} |v|^2 d\Gamma dt + \frac{k_1}{2}\int_Q y^2 dxdt + \frac{k_2}{2}\int_\Omega |y(T)|^2 dx,$$

with $dx = dx_1 \cdots dx_d$, $k_1 \ge 0$, $k_2 \ge 0$, $k_1 + k_2 > 0$, and y obtained from v via the solution of the following *fourth-order linear parabolic problem*:

$$\begin{cases} \dfrac{\partial y}{\partial t} - \nabla \cdot a\nabla y + \varepsilon^2\Delta^2 y = 0 & \text{in } Q, \\ y(x,0) = y_0(x) & \text{in } \Omega, \\ \dfrac{\partial y}{\partial n} = v\chi_\gamma, \quad \dfrac{\partial}{\partial n}\Delta y = 0 & \text{on } \Sigma. \end{cases} \tag{4}$$

Here a denotes the constant $3\varphi_s^2 - 1 \in [-1, 2]$ and $y_0 = \delta\varphi_s$.
Optimality Conditions for problem $(\mathcal{CP})$.
The (unique) solution u of problem $(\mathcal{CP})$ is characterized by $\nabla J(u) = 0$. Let us consider $v \in \mathcal{U}$ and a small perturbation δv of v. Then we have

$$\delta J(v) = \int_{\gamma\times(0,T)} \nabla J(v)\delta v d\Gamma dt = \int_{\gamma\times(0,T)} v\delta v d\Gamma dt + k_1\int_Q y\delta y dxdt + k_2\int_\Omega y(T)\delta y(T)dx,$$

where δy is the solution of

$$\begin{cases} \dfrac{\partial \delta y}{\partial t} - \nabla \cdot a\nabla \delta y + \varepsilon^2\Delta^2 \delta y = 0 & \text{in } Q, \\ \delta y(x,0) = 0 & \text{in } \Omega, \\ \dfrac{\partial \delta y}{\partial n} = \delta v\chi_\gamma, \quad \dfrac{\partial}{\partial n}\Delta \delta y = 0 & \text{on } \Sigma. \end{cases} \tag{5}$$

Then, multiplying in (5) by the solution p of

$$\begin{cases} -\dfrac{\partial p}{\partial t} - \nabla \cdot a\nabla p + \varepsilon^2\Delta^2 p = k_1 y & \text{in } Q, \\ p(x,T) = k_2 y(x,T) & \text{in } \Omega, \\ \dfrac{\partial p}{\partial n} = \dfrac{\partial}{\partial n}\Delta p = 0 & \text{on } \Sigma \end{cases}$$

and integrating by parts, we obtain

$$\int_{\gamma\times(0,T)} \nabla J(v)\delta v d\Gamma dt = \int_{\gamma\times(0,T)} (v + ap - \varepsilon^2\Delta p)\delta v d\Gamma dt.$$

Since δv is arbitrary, we have proved that $\nabla J(v) = v + (ap - \varepsilon^2 \Delta p)\chi_\gamma$. Thus, $\nabla J(u) = 0$ is equivalent to the following (optimality) system

$$u = -(ap - \varepsilon^2 \Delta p)\chi_\gamma;$$

$$\begin{cases} \dfrac{\partial y}{\partial t} - \nabla \cdot a \nabla y + \varepsilon^2 \Delta^2 y = 0 & \text{in } Q, \\ y(x,0) = y_0(x) & \text{in } \Omega, \\ \dfrac{\partial y}{\partial n} = u\chi_\gamma, \quad \dfrac{\partial}{\partial n}\Delta y = 0 & \text{on } \Sigma; \end{cases}$$

$$\begin{cases} -\dfrac{\partial p}{\partial t} - \nabla \cdot a \nabla p + \varepsilon^2 \Delta^2 p = k_1 y & \text{in } Q, \\ p(x,T) = k_2 y(x,T) & \text{in } \Omega, \\ \dfrac{\partial p}{\partial n} = \dfrac{\partial}{\partial n}\Delta p = 0 & \text{on } \Sigma. \end{cases}$$

Stabilization of the Nonlinear Model.

Finally, we apply the control u, obtained via linearization, to the nonlinear model to see if it stabilizes the original nonlinear system. Here we point out that, in general, unless the time horizon T is small enough, the solution of the linearized equation and the the solution of the nonlinear equation is quite different and therefore the control obtained for the linearized equation will not be suitable for the nonlinear equation. To avoid that we consider a partition of the time interval $0 = T_0 < T_1 < T_2 < \cdots < T_r = T$ and use the following algorithm:

a) Set $i = 1$.

b) For the subinterval (T_{i-1}, T_i), we compute the control by using $\varphi_{i-1} - \varphi_s$ as initial data for the linear equation and we call $\varphi_i = \varphi(T_i)$, where φ is the solution of the nonlinear equation, computed with the above control and initial data φ_{i-1}.

c) We do $i = i + 1$ and go to b).

Time Discretization of the Optimal Control Problem $(\mathcal{CP})$.

We consider the time discretization step Δt, defined by $\Delta t = T/N$, where N is a positive integer. Then, if we define $t^n = n\Delta t$, we have $0 < t^1 < t^2 < \cdots < t^N = T$. We approximate then problem $(\mathcal{CP})$ by the following minimization problem:

$$(\mathcal{CP})^{\Delta t} \begin{cases} u^{\Delta t} \in \mathcal{U}^{\Delta t}, \\ J^{\Delta t}(u) \leq J^{\Delta t}(v), \ \forall v \in \mathcal{U}^{\Delta t}; \end{cases}$$

where $\mathcal{U}^{\Delta t} = L^2(\gamma)^N$ is equipped with the scalar product $(\cdot,\cdot)_{\Delta t}$ defined by

$$(v,w)_{\Delta t} = \Delta t \sum_{n=1}^{N} c^n \int_\gamma v^n w^n d\Gamma,$$

where $c^1 = \frac{3}{2}$ and $c^2 = \cdots c^N = 1$, and

$$J^{\Delta t}(v) = \frac{\Delta t}{2}\sum_{n=1}^{N}\int_\gamma c^n|v^n|^2 d\Gamma + \frac{k_1\Delta t}{2}\sum_{n=1}^{N}\int_\Omega |y^n|^2 dx + \frac{k_2}{2}\int_\Omega \frac{|y^{N-1}|^2+|y^N|^2}{2}dx,$$

where $\{y^n\}_{n=1}^N$ is defined from the solution of the following *second order accurate time discretization* scheme of *fourth-order linear parabolic problem* (4):

$$y^0 = y_0,$$

$$\begin{cases} \dfrac{y^1-y^0}{\Delta t} - \nabla\cdot a\nabla y^1 + \varepsilon^2\Delta^2 y^1 = 0 & \text{in } \Omega, \\ \dfrac{\partial y^1}{\partial n} = v^1\chi_\gamma, \quad \dfrac{\partial}{\partial n}\Delta y^1 = 0 & \text{on } \Gamma, \end{cases} \tag{6}$$

and for $n \geq 2$,

$$\begin{cases} \dfrac{\frac{3}{2}y^n - 2y^{n-1} + \frac{1}{2}y^{n-2}}{\Delta t} - \nabla\cdot a\nabla y^n + \varepsilon^2\Delta^2 y^n = 0 & \text{in } \Omega, \\ \dfrac{\partial y^n}{\partial n} = v^n\chi_\gamma, \quad \dfrac{\partial}{\partial n}\Delta y^n = 0 & \text{on } \Gamma. \end{cases} \tag{7}$$

Now, in a way similar to that of the continuous case, it is easy to prove that the solution $u^{\Delta t}$ of $(\mathcal{CP})^{\Delta t}$ is characterized by the following (optimality) system:

$$u = -\{(ap^n - \varepsilon^2\Delta p^n)\chi_\gamma\}_{n=1}^N,$$

$$y^0 = y_0,$$

$$\begin{cases} \dfrac{y^1-y^0}{\Delta t} - \nabla\cdot a\nabla y^1 + \varepsilon^2\Delta^2 y^1 = 0 & \text{in } \Omega \\ \dfrac{\partial y^1}{\partial n} = u^1\chi_\gamma, \quad \dfrac{\partial}{\partial n}\Delta y^1 = 0 & \text{on } \Gamma, \end{cases}$$

and for $n \geq 2$,

$$\begin{cases} \dfrac{\frac{3}{2}y^n - 2y^{n-1} + \frac{1}{2}y^{n-2}}{\Delta t} - \nabla\cdot a\nabla y^n + \varepsilon^2\Delta^2 y^n = 0 & \text{in } \Omega \\ \dfrac{\partial y^n}{\partial n} = u^n\chi_\gamma, \quad \dfrac{\partial}{\partial n}\Delta y^n = 0 & \text{on } \Gamma. \end{cases}$$

$$\begin{aligned} p^{N+2} &= 4p^{N+1} - k_2 y^N, \\ p^{N+1} &= -k_2 y^{N-1}, \end{aligned}$$

and for $n = N, ..., 1$,

$$\begin{cases} \dfrac{\frac{3}{2}p^n - 2p^{n+1} + \frac{1}{2}p^{n+2}}{\Delta t} - c^n\nabla\cdot a\nabla p^n + c^n\varepsilon^2\Delta^2 p^n = k_1 y^n & \text{in } \Omega, \\ \dfrac{\partial p^n}{\partial n} = \dfrac{\partial}{\partial n}\Delta p^n = 0 & \text{on } \Gamma. \end{cases}$$

Time Discretization of the Nonlinear model.

Adapting the scheme developed in [3] for the non-controlled case, we *time discretize* the nonlinear model (2) by the following *second-order accurate time discretization*:

$$\varphi^0 = \varphi_0,$$

$$\begin{cases} \dfrac{\varphi^1 - \varphi^0}{\Delta t} - \nabla \cdot (3\varphi_0^2 - 1)\nabla\varphi^1 + \varepsilon^2\Delta^2\varphi^1 = 0 & \text{in } \Omega, \\ \dfrac{\partial \varphi^1}{\partial n} = u^1\chi_\gamma, \quad \dfrac{\partial}{\partial n}\Delta\varphi^1 = 0 & \text{on } \Gamma, \end{cases}$$

and for $n \geq 2$,

$$\begin{cases} \dfrac{\frac{3}{2}\varphi^n - 2\varphi^{n-1} + \frac{1}{2}\varphi^{n-2}}{\Delta t} - \nabla \cdot \left[3(2\varphi^{n-1} - \varphi^{n-2})^2 - 1\right]\nabla\varphi^n + \varepsilon^2\Delta^2\varphi^n = 0 & \text{in } \Omega, \\ \dfrac{\partial \varphi^n}{\partial n} = u^n\chi_\gamma, \quad \dfrac{\partial}{\partial n}\Delta\varphi^n = 0 & \text{on } \Gamma. \end{cases}$$

As in the continuous case, we divide our interval in subintervals to avoid large differences between the linearized model and the nonlinear model.

Full Discretization.

The full discretization is similar to that of the time discretization and is easy to apply once we know how to fully discretize fourth-order linear elliptic problems of the following form:

$$\begin{cases} \psi - \lambda\nabla \cdot a\nabla\psi + \lambda\varepsilon^2\Delta^2\psi = f & \text{in } \Omega \\ \dfrac{\partial \psi}{\partial n} = u\chi_\gamma, \quad \dfrac{\partial}{\partial n}\Delta\psi = 0 & \text{on } \Gamma. \end{cases}$$

The traditional *finite difference* or *finite element* schemes are not well suited to this type of problems, because of the *fourth-order* term $\lambda\varepsilon^2\Delta^2 y$.

To overcome this difficulty we have adapted to our case the method proposed in [3] for the uncontrolled case. That method consist of an approximate factorization of the fourth-order linear elliptic problem into a system of two second-order linear elliptic problems, making possible its solution by *finite element* techniques together with a Least Square/Conjugate Gradient method. The details can be seen in [7].

Numerical Experiments.

In this section we take $\varepsilon = 10^{-1}$, the domain Ω defined by the interval $\Omega = (0,1)$ and the control domain defined by the points $\gamma = \{0,1\}$. We take $\Delta t = 1/250$ and $h = 1/63$, where h is the space discretization step defined by $h = 1/(N_h - 1)$ and $N_h = 64$ is the number of vertex. We consider the initial condition defined by

$$\varphi_0(x) = 0.3 + \frac{1}{40}\sum_{i=1}^{N_h}\Theta_i w_i(x), \quad \forall\, x \in \Omega,$$

where, Θ_i is a random variable uniformly distributed over $[-1,1]$.

In order to see how the non-controlled solution behaves, we have visualized in Figures 1 and 2 the computed solution for $t \in [0, 0.8]$ and the solution at time $T = 0.8$ respectively. Finally, in Figure 3 we have visualized the computed solution, with control for $t \in [0, 0.8]$, and in Figure 4 we have visualized the computed solution, with control for $t \in [0, 0.8]$ and without control for $t \in (0.8, 2]$.

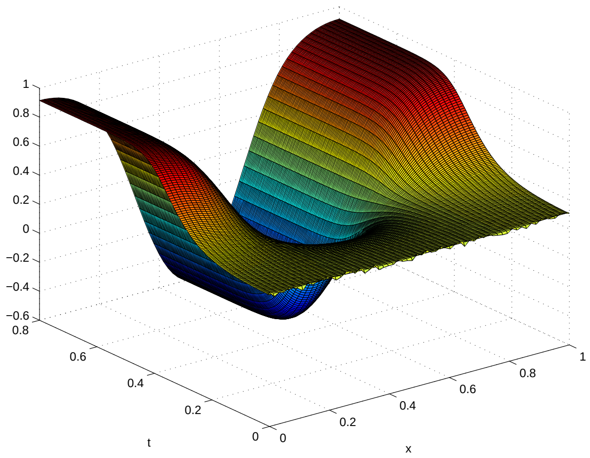

Figure 1: Non-controlled solution during the time-interval $[0, 0.8]$.

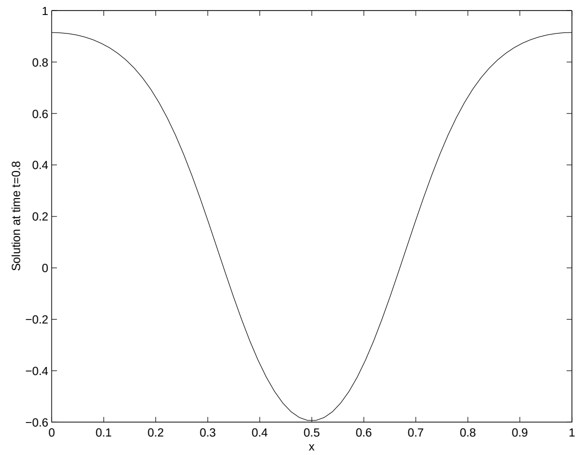

Figure 2: Solution at time $t = 0.8$.

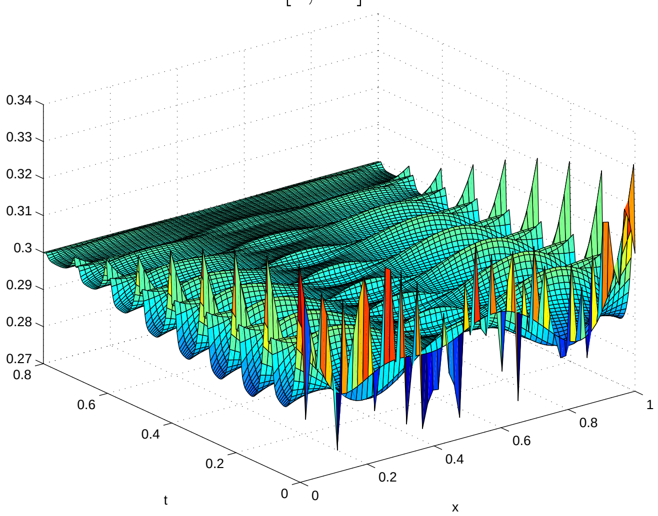

Figure 3: Solution with control during the time interval $[0, 0.8]$.

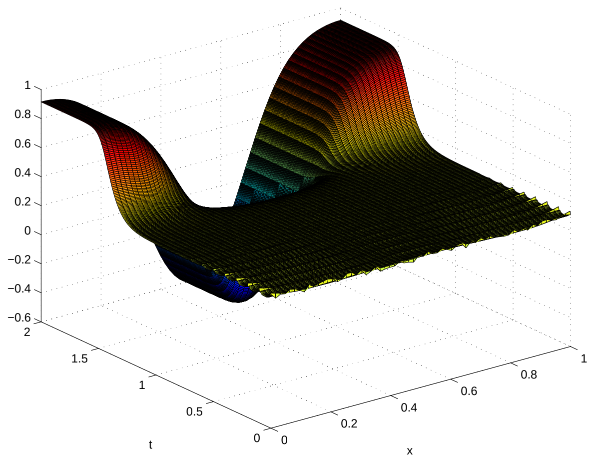

Figure 4: Solution with control for $t \in [0, 0.8]$ and without control for $t \in (0.8, 2]$.

We observe that the system is stabilized for $0 \leq t \leq 0.8$, but if we stop controlling, the small residual perturbations of the steady-state solution $\varphi_s \equiv 0.3$ at $t = 0.8$ are sufficient to destabilize the system, which evolves toward a new steady-state solution, showing that the spinodal decomposition has taken place.

Acknowledgments

The authors are very grateful to E. Dean for helpful comments. The support of a fellowship from the Universidad Complutense de Madrid to the first author to research at the University of Houston, of the Higher Education Texas Coordinating Board and of the DGICYT Spanish Project PB96-0583 is also acknowledged.

References

[1] Cahn, J. W., Phase Separation by Spinodal Decomposition in Isotropic Systems, *J. Chem. Phys.*, 42, 1, pp. 93–99, 1965.

[2] Cahn, J. W. and Hilliard, J. E., Free Energy of a Nonuniform System. I. Interfacial Free Energy, *J. Chem. Phys.*, 28, 2, pp. 258–267, 1958.

[3] Dean, E. J., Glowinski, R., and Trevas, D. A., An approximate Factorization/Least Squares Solution Method for a Mixed Finite Element Approximation of the Cahn-Hilliard Equation, *Anal. Acad. Nac. Cs. Ex. Fís. Nat.*, Buenos Aires, t, 47, pp. 201–215, 1995.

[4] Díaz, A.M. and Ramos, A.M., On the Approximate Controllability for Higher Order Parabolic Nonlinear Equations of Cahn-Hilliard Type. In *Control and Estimation of Distributed Parameter Systems*, International Series of Numerical Mathematics, Birkhäuser Verlag Basel, 1997, pp. 109–127.

[5] Glowinski, R., *Numerical Methods for Nonlinear Variational Problems*, Springer, New York, 1984.

[6] He, J.W. and Glowinski, R., Neumann Control of Unstable Parabolic Systems: Numerical Approach, *Journal of Optimization Theory and Applications*, Vol. 96, No. 1, pp. 1–55, 1998.

[7] Glowinski, R. and Ramos, A.M. A Numerical Approach to the Neumann Control of the Cahn-Hilliard Equation. To appear.

1 Dept. of Mathematics. University of Houston. Houston, Texas 77204-3476.

2 Dept. de Sistemas Informáticos y Programación. Universidad Complutense de Madrid. Avda. Complutense s/n, 28040, Madrid. angel@sunma4.mat.ucm.es.