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Mathematical aspects of the Penrose–Fife phase–field model

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This article gives a survey of the recent mathematical developments in the study of the Penrose-Fife model for phase transitions. It summarizes the analytical aspects of the resulting evolution equations, optimal control problems as well as the numerical treatment of this model.

1. Physical background and derivation of the model

When studying the kinetics of phase transitions one usually ends up analyzing a free boundary problem. In recent years an alternate approach has been pursued by several authors. In this approach a phase-function (or order parameter) ϕ is introduced, which is assumed to describe the state of the system at all times. The free phase boundary is approximately given by level curves of this phase function. Often there is a natural choice for such an order parameter, for example the magnetization per lattice site in a ferromagnet, but the models can be extended to situations where no such choice exists. Several authors have derived state equations for such systems. The most studied case is the system of equations derived by Caginalp (1986), but recently there were other approaches by Alt and Pawłow (1992), Kenmochi and Niezgódka (1992) and many others. Our concern is the approach of Penrose and Fife (1990). In this article we will give a survey of the mathematical developments in the study of the evolution equations. In particular we will outline existence and uniqueness results, results concerning related optimal control problems and a numerical method suitable for problems of this kind. These results have been obtained quite recently and can be found in a number of papers (cf. Horn, Sprekels and Zheng, 1993, Sprekels and Zheng, 1993, Zheng, 1992). We will also include some extensions and generalizations of the known results.

In this first section we will briefly describe the approach of Penrose and Fife, and give the main steps of the derivation of the evolution equations. For a more thorough description of the model we refer the reader to Penrose and Fife (1990).

We will assume that the system occupies a bounded domain $\Omega \subset R^3$. Furthermore, we will assume that the order parameter ϕ is a non-conserved quantity, although the derivation can be carried out for conserved order parameters as well (cf. Penrose and Fife (1990)). The authors of Penrose and Fife (1990) assumed that the free energy density f and the entropy density s depend on ϕ, but still show the same qualitative behaviour with respect to the absolute temperature T and the energy density e as in the absence of an order parameter, i. e. these fuctions are concave with respect to e and T. Furthermore, it is assumed that f and s are connected via the Legendre transform

$$\begin{aligned} f(T,\phi) &= \inf_e [e - Ts(e,\phi)] \\ s(e,\phi) &= \inf_T [\frac{e}{T} - \frac{f(T,\phi)}{T}]. \end{aligned}$$

The total free energy of the system is then given by the functional

$$\begin{aligned} F(T,\phi) &= \int_\Omega \left(f(T,\phi(x)) + \frac{1}{2}\kappa \left|\nabla\phi(x)\right|^2 \right) dx \\ &= \inf_e \left(E(e) - TS(e,\phi)\right). \end{aligned}$$

Using this equation one defines the total energy E and the entropy functional S. The latter is given by

$$S(e,\phi) = \int_\Omega \left(s(e(x),\phi(x)) - \frac{\kappa}{2T} \left|\nabla\phi(x)\right|^2 \right) dx.$$

Observe that the temperature T will generally also depend on the space variable x. To obtain the kinetic behaviour of this system one assumes that the increase of the entropy is maximal along solution paths. It is this entropy approach which distinguishes the model described here from others. The equations for the kinetics of the system are obtained by taking the functional derivatives of S

$$\begin{aligned} \frac{\partial\phi}{\partial t} &= KT\frac{\delta S(e,\phi)}{\delta\phi}, \\ \frac{\partial e}{\partial t} &= -\mathrm{div}\left(M \mathrm{grad}\left(\frac{\delta S(e,\phi)}{\delta e} \right) \right). \end{aligned}$$

The second of these equations is a well-known expression from thermodynamics. We continue by illuminating this derivation of the phase-field equations using a specific example. We use the energy density

$$e(T,\phi) = c_0 T + w(\phi),$$

where

$$w(\phi) = -a\phi^2 + b\phi + c,$$

and the first term describes the kinetic energy of the system. From this we obtain the free energy density

$$\begin{aligned} f(T,\phi) &= T\int_{1/T_0}^{1/T} (c_0\tau + w(\phi))\, d(1/\tau) \\ &= T\int_{1/T_0}^{1/T} c_0\tau\, d(1/\tau) + w(\phi) - Ts_0(\phi). \end{aligned}$$

Using the Legendre transform we get

$$s(e,\phi) = -c_0 \log T + s_0(\phi) + c_1.$$

To continue we have to describe the function $s_0(\phi)$. In this article we will limit ourselves to two specific choices of this function. In the first case we assume that s_0 is a smooth ($C^3(R)$) double well potential with

$$s_0''(\phi) \geq -k, \quad \forall \phi \in R,$$

for a suitable constant $k \geq 0$. In the second case we use

$$s_0(\phi) = -k\phi \log \phi - k(1-\phi)\log(1-\phi),$$

which is the configurational entropy per lattice site in the mean-field theory for Ising ferromagnets, when ϕ is given as the fraction of lattice sites at which the spins are pointing up, i.e. the magnetization per lattice site is proportional to $2\phi - 1$.

Using these specific choices, and following the general outline we arrive at the following system of non-linear parabolic equations

$$\phi_t = K_1\Delta\phi - s_0'(\phi) - \frac{w'(\phi)}{T} \tag{1}$$

$$T_t = -M_1\Delta\left(\frac{1}{T}\right) - w'(\phi)\phi_t + g, \tag{2}$$

where g represents an (optional) heat source. These equations are complemented with initial and boundary conditions. The natural boundary conditions for ϕ are Neumann boundary conditions. In this article we will use the following boundary conditions for T

$$\left.\frac{\partial T}{\partial \nu}\right|_{\partial\Omega} = -\alpha\,(T - T_\Gamma)|_{\partial\Omega}\,. \tag{3}$$

One should note that these boundary conditions are not the natural ones. They were obtained by linearizing the natural boundary conditions about an average temperature T_0. The natural boundary conditions have not been treated so far and are the subject of a forthcoming article.

For the mathematical treatment of these equations it is often more convenient to use the inverse temperature

$$u = \frac{1}{T},$$

which satisfies the following system of equations

$$\begin{aligned} \phi_t &= K_1 \Delta\phi - s_0'(\phi) - w'(\phi)u & (4)\\ \frac{u_t}{u^2} &= M_1 \Delta u + w'(\phi)\phi_t - g, & (5) \end{aligned}$$

with the boundary conditions for u

$$\left.\frac{\partial u}{\partial \nu}\right|_{\partial\Omega} = \left(u - T_\Gamma u^2\right)\big|_{\partial\Omega}. \tag{6}$$

In the following section we will outline the existence and uniqueness results for these equations. These results are found in Zheng (1992) for the one–dimensional case. In three space dimensions the results are given in Sprekels and Zheng (1993) for smooth functions s_0 and in Horn, Sprekels and Zheng (1993) for the logarithmic potential. A non-smooth potential was also treated in Laurençot (1992). We will follow the approach of Sprekels and Zheng (1993), but will allow for some generalizations.

Section 3 will be devoted to an optimal control problem connected with these equations. In this section we will generally follow Sprekels and Zheng (1992). Finally, in section 4 we will describe a suitable numerical method for these equations, which is also described in Horn (1993), Horn and Sprekels (1994).

2. Existence and uniqueness of solutions

In this section we will state the main existence and uniqueness results and outline their proofs. We will assume, that $\Gamma = \partial\Omega$ is sufficiently smooth to apply the results of elliptic and parabolic regularity theory. Furthermore, we make the following assumptions

- The functions g and T_Γ are assumed to be smooth.
- For the function s_0 we assume:
  A $s_0 \in C^3(R)$ and there exists a constant $C > 0$ such that $s_0''(\phi) > -C$ for all $\phi \in R$.
  or
  B $s_0(\phi) = \phi \log\phi + (1-\phi)\log(1-\phi)$.
- $w'(\phi) = a\phi + b$ and $b = 0$. This assumption does not have any effect on the proof of the existence theorem except that it simplifies the notation.
- To further simplify notations we assume that all constants in the equations are equal to one.

We can now state the main existence and uniqueness result.

PROPOSITION 1 *Let $p > 3$ and suppose $\phi_0 \in W_p^s(\Omega)$ and $T_0 \in W_p^s(\Omega)$ satisfy compatibility conditions. Furthermore, suppose that $T_0(x) \geq \beta > 0$ for all $x \in \overline{\Omega}$, and T_Γ is smooth on $\Gamma \times R^+$. Then there exists a unique global smooth solution to the equations (1)–(2) with the boundary conditions (3).*

REMARKS:

- This result is slightly stronger than the results given in Horn, Sprekels and Zheng (1993), Sprekels and Zheng (1993), Zheng (1992). Namely, the statements there require $\phi_0 \in H^4(\Omega)$ and $T_0 \in H^3(\Omega)$ to satisfy stronger compatibility conditions.
- A much stronger local existence result appeared in Theorem 17.3 of Amann (1993). The author allowed for more general non-linearities and potenials. A criterion for global existence is given in the same article. However, at this time we need the specific forms of the potentials in order to prove a global result.

For the proof of Proposition 1 we first observe that we can apply Theorem 17.3 of Amann (1993) to obtain a local existence and uniqueness result. The crucial step of the proof is to obtain uniform a priori estimates from above and below for ϕ and T, i. e. we have to show that the solutions satisfy the criterion for global existence of Amann (1993). To do this it is more convenient to use the equations (4)–(5) for the inverse temperature u. The uniform a priori estimates are obtained in the same way as in Horn, Sprekels and Zheng (1993), Sprekels and Zheng (1993), Zheng (1992). As in these articles one can get some initial estimates for u and ϕ using standard techniques. In particular one gets that $\|\phi(t)\|_{H(\Omega)}$, $\|\phi_t(t)\|_{L^2(\Omega)}$ and $\|u(t)\|_{H^1(\Omega)}$ are all uniformly bounded. In the smooth case one also has a uniform bound for $\|\phi(t)\|_{H^1(\Omega)}$. With these initial properties one can apply the following technical lemma to get a uniform estimate on $\|u(t)\|_{L^\infty(\Omega)}$.

LEMMA 1 *Let w be a positive smooth function which satisfies*

$$\frac{w_t}{w^2} = \Delta w + f, \forall (x,t) \in \Omega \times (0, t^*),$$

with boundary conditions

$$\left.\frac{\partial w}{\partial n}\right|_{\partial\Omega} = \left(w - w^2 T_\Gamma\right)\big|_{\partial\Omega},$$

and $f \in L^\infty(0,t^*; L^2(\Omega))$. Furthermore, let $w(x,0) = w_0(x) \in L^\infty(\Omega)$ and $T_\Gamma \geq \beta > 0$. Then there exists a constant $C > 0$ depending only on t^*, $\|f\|_{L^\infty(0,t^*;L^2(\Omega))}$, $\|w_0\|_{L^\infty(\Omega)}$ and β, such that

$$\max_{0 \leq t \leq t^*} \|w(t)\|_{L^\infty(\Omega)} \leq C.$$

The proof of this Lemma is given in Horn, Sprekels and Zheng (1993) and generally follows a method already found in Alikakos (1979). Multiplying the equation for w by w^{λ_n+1}, where λ_n is a sequence given by

$$\lambda_n = 2\lambda_{n-1} - 2, \quad \lambda_0 = 6,$$

one obtains consecutive estimates on

$$\|w(t)\|_{L^{\lambda_n}(\Omega)}.$$

Taking the limit as $n \to \infty$ one gets the desired result. We remark here that a generalization of this Lemma can be found in Laurencot (1993).

Using almost the same technique as in this Lemma one also obtains a uniform bound on T. In the case of the logarithmic potential one still has to obtain constants $0 < a_{t^*} < b_{t^*} < 1$ such that

$$a_{t^*} \leq \phi(x,t) \leq b_{t^*}, \quad \forall (x,t) \in \Omega \times (0,t^*). \tag{7}$$

This was done in Horn, Sprekels and Zheng (1993) by obtaining consecutive bounds on the L^p-norms of $v_1 = \frac{1}{\phi}$ and $v_2 = \frac{1}{1-\phi}$.

Having obtained these uniform bounds one can apply Theorem of Amann (1993) to finish the proof.

3. A related optimal control problem

The equations (1)–(2) yield an interesting optimal control problem. The object is to control the behaviour of ϕ and T using the source term g and the boundary term T_Γ as controls. The results of this section were obtained in Sprekels and Zheng (1992). The authors treated the specific case when $s_0' = \phi - \phi^3$. However, their arguments can quite easily be extended to the case **A**. Furthermore, one can easily show that the solutions ϕ and T depend continuously on the controls g and T_Γ, as do the constants a_{t^*} and b_{t^*} of (7). Therefore one can conclude that for a compact admissible set of controls, there exist constants $\hat{a}_{t^*}$ and $\hat{b}_{t^*}$ such that $0 < \hat{a}_{t^*} \leq \phi \leq \hat{b}_{t^*} < 1$ for all solutions ϕ corresponding to controls in the admissible set. But $s_0'(\phi)$ is smooth on $[\hat{a}_{t^*}, \hat{b}_{t^*}]$, and therefore the same arguments hold. Since all the arguments are straightforward we will omit the details.

We will generally assume that $(\phi_0, T_0) \in H^4(\Omega) \times H^3(\Omega)$ satisfy the same compatibility conditions as in Sprekels and Zheng (1992,1993). To state the result we introduce the following spaces

$$\begin{aligned}
X_1 &= C([0,t^*]; H^4(\Omega)) \cap C^1([0,t^*]; H^2(\Omega)) \cap C^2([0,t^*]; L^2(\Omega)),\\
X_2 &= C([0,t^*]; H^3(\Omega)) \cap C^1([0,t^*]; H^1(\Omega)) \cap H^{2,4}(\Omega_{t^*}),\\
V &= H^2(0,t^*; L^2(\Omega)) \cap H^1(0,t^*; H^2(\Omega)),\\
W &= H^2(0,t^*; H^{\frac{3}{2}}(\partial\Omega)),\\
K &= V \times \{w \in W : w(x,t) \geq \beta > 0, \text{on}\, \partial\Omega_{t^*}, w(x,0) = T_0(x), \text{on}\, \partial\Omega_{t^*}\}.
\end{aligned}$$

The control problem described in this section is to minimize the cost functional

$$J(\phi,T;g,T_\Gamma) = \frac{\alpha_1}{2}\left\|\phi(t^*)-\hat{\phi}(t^*)\right\|^2_{L^2(\Omega)} + \frac{\alpha_2}{2}\left\|T-\hat{T}\right\|^2_{L^2(\Omega_{t^*})} + \frac{\alpha_3}{2}\|g\|^2_{L^2(\Omega_{t^*})} + \frac{\alpha_4}{2}\int_0^{t^*}\|T_\Gamma(t)\|^2_{L^2(\partial\Omega)}\,dt, \tag{8}$$

where ϕ and T satisfy (1)–(2) and $(g,T_\Gamma)\in U_{ad}$ a closed, convex and bounded subset of K.

Let $B\subset X_1\times X_2$ be defined as follows.

$$B=(C([0,t^*];H^1(\Omega))\cap H^{1,2}(\Omega_{t^*}))\times(C([0,t^*];L^2(\Omega))\cap L^2(0,t^*;H^1(\Omega))).$$

In Sprekels and Zheng (1992) the authors showed for $s_0'(\phi)=\phi-\phi^3$ that the map

$$S: K\to B,$$
$$S:(g,T_\Gamma)\mapsto(\phi,T),$$

is differentiable. It is easy to see that this result also holds for the more general situation considered here.

One can now formulate the adjoint equations and the necessary conditions of optimality. The adjoint state variables p^* and q^* satisfy the following system of linear partial differential equations

$$p_t^*+\Delta p^* = -p^*\left(s_0''(\phi^*)+\frac{1}{T^*}\right)+\phi^* q_t^*, \tag{9}$$

$$q_t^*+\frac{1}{T^{*2}}\Delta q^* = \frac{\phi^*}{T^{*2}}p^*+\alpha_2\left(T^*-\hat{T}\right), \tag{10}$$

together with the boundary and final conditions

$$\frac{\partial p^*}{\partial n} = 0,\quad \frac{\partial q^*}{\partial n}+q^*\left(\frac{2T_\Gamma^*}{T^*}-1\right) = 0,\quad \text{on } \partial\Omega_{t^*}, \tag{11}$$

$$p^*(x,t^*) = -\alpha_1\left(\phi^*(x,t^*)-\hat{\phi}(x)\right),\quad q^*(x,t^*) = 0,\quad \text{on } \overline{\Omega}. \tag{12}$$

These equations admit a unique solution (p^*,q^*) such that

$$p^*,q^*\in C([0,t^*];H^1(\Omega))\cap L^2(0,t^*;H^2(\Omega))\cap H^1(0,t^*;L^2(\Omega)). \tag{13}$$

We conclude this section by stating the main result of Sprekels and Zheng (1992).

PROPOSITION 2 *Under the conditions described above the control problem (8) has at least one solution. Moreover, for any optimal* $(\phi^*,T^*;g^*,T_\Gamma^*)$ *there exists an adjoint state* (p^*,q^*) *satisfying (9)–(13) and the variational inequality*

$$\int_0^{t^*}\int_\Omega(\alpha_3 g^*-q^*)\,h\,dxdt+\int_0^{t^*}\int_{\partial\Omega}\left(\alpha_4 T_\Gamma^*-\frac{q^*}{T^{*2}}\right)k\,dxdt\ge 0,$$

for all (h,k) *in the set*

$$K^+(g^*, T_\Gamma^*) = \{(h,k) \in V \times W : \exists \lambda > 0 \text{ such that } (g^* + \lambda h, T_\Gamma^* + \lambda k) \in U_{ad}\}$$

REMARKS:

- The potential of case **B** gives an implicit state constraint on the order parameter ϕ.
- This is only one of many possible control problems which arise from the phase-field equations studied here. Other interesting problems include state constraints on the temperature T and shape optimization problems.

4. A numerical method

The object of this section is to describe a suitable numerical method for the equations (1)-(2). We will give a time discrete version of these equations and state the major results regarding this scheme. The numerical treatment was initiated for the one-dimensional case in Horn (1993). The mathematical treatment for the one-dimensional case is complete, the higher dimensional analog is currently under preparation (cf. Horn and Sprekels, 1994). We start by giving the time-discrete equations. For a time step h we define

$$f_k(x) = f(x, t_0 + kh),$$

as a time discretization of a function f. Using this notation we introduce the following discrete version of (4)–(5)

$$\frac{\phi_{k+1} - \phi_k}{h} = \Delta\phi_{k+1} - \frac{s_0(\phi_{k+1}) - s_0(\phi_k)}{\phi_{k+1} - \phi_k} + a\phi_{k+1}U_{k+1}, \tag{14}$$

$$\frac{u_{k+1} - u_k}{hu_{k+1}u_k} = \Delta u_{k+1} - a\phi_{k+1}\frac{\phi_{k+1} - \phi_k}{h} - g_{k+1}. \tag{15}$$

The boundary conditions for u_{k+1} become

$$\left.\frac{\partial u_{k+1}}{\partial \nu}\right|_{\partial\Omega} = \left.\left(\frac{u_{k+1} + u_k}{2} - T_{\Gamma,k+1}u_{k+1}^2\right)\right|_{\partial\Omega}. \tag{16}$$

REMARKS:

- This scheme is somewhat different from the one introduced in Horn (1993). Namely, we use the difference quotient of s_0 instead of the analytic derivative s_0'. In Horn (1993) a very specific case $s_0'(\phi) = \phi - \phi^3$ was treated. For more general potentials the difference quotient yields more stability.
- The system (14)-(16) constitutes a highly non-linear system of elliptic PDE. Existence and uniqueness of solutions to that system cannot be taken for granted, and has to be shown separately. However, this can be done by applying a standard contraction argument.

For this scheme one proves the following stability and convergence result.

PROPOSITION 3 *With the hypothesis as in Proposition 1 there exists an* $h_0 > 0$ *such that the system (14)–(16) has a unique solution*

$$(\phi_{k+1}, u_{k+1}) \in H^2(\Omega) \times H^2(\Omega),$$

for all $0 < h \leq h_0$ *and all integers* $0 \leq k \leq [\frac{T}{h}]$. *Moreover, the sequence* (ϕ_{k+1}, u_{k+1}) *is uniformly bounded in* $H^2(\Omega) \times H^2(\Omega)$ *and the sequence of discrete derivatives* $\left(\frac{\phi_{k+1}-\phi_k}{h}, \frac{u_{k+1}-u_k}{h}\right)$ *is uniformly bounded in* $H^1(\Omega) \times L^2(\Omega)$.

REMARKS:

- The uniform boundedness of the derivatives immediately yields an error estimate for the scheme. One can actually show that
$$\|\phi_k - \phi(t)\|^2_{H^1(\Omega)} + \|u_k - u(t)\|^2_{H^1(\Omega)} \leq Ch$$
for all $t \in [kh, (k+1)h)$. Here $(\phi(t), u(t))$ denotes a solution to the system (1)–(3).
- To prove this proposition one basically carries out the same apriori estimates for the discrete scheme as in the continuous system. This is rather technical and has been done for one space dimension in Horn (1993) and for two dimensions in Horn and Sprekels (1994). The result should also hold in three space dimensions, but has not been proven so far.

In order to implement this scheme one solves the non-linear elliptic system by iterating a linearized system in each time step. To solve the resulting linear elliptic equations, one uses a standard solver for elliptic equations. We conclude this section by giving the results of some preliminary computations. More accurate numerical simulations have yet to be done. In Figs. 1–4 we show the results of a two-dimensional experiment. The constant K_1 of (1) was chosen to be equal to 0.1. The function

$$f(\phi, u) = s_0'(\phi) + w(\phi)u = -\log\frac{\phi}{(1-\phi)} + 2\phi - 3 + (50 + 60\phi)\,u, \qquad (17)$$

was used in this experiment. A simple calculation reveals that for $u = \frac{1}{40}$ one has

$$f(\phi, \frac{1}{40}) = -f(1-\phi, \frac{1}{40}),$$

so both phases behave the "same way" at this temperature, i. e. one could call $T = 40$ the "melting point" in this simulation. We used a square domain Ω. As initial value for the temperature we used $u_0 = 0.015$, i. e. $T_0 = 66\frac{2}{3}$. The experiment is therefore a "melting experiment". Figure 1 shows the graph of the function $f(\phi, u_0)$. Figure 2 gives a contour plot of the initial phase distribution. To the left of the contours in Figure 2, we have $\phi_0 = 0.9$, to the right we have $\phi_0 = 0.1$. The function ϕ_0 is changing smoothly in the regions indicated by the contours, which constitutes the so called "mushy region" near the phase boundary.

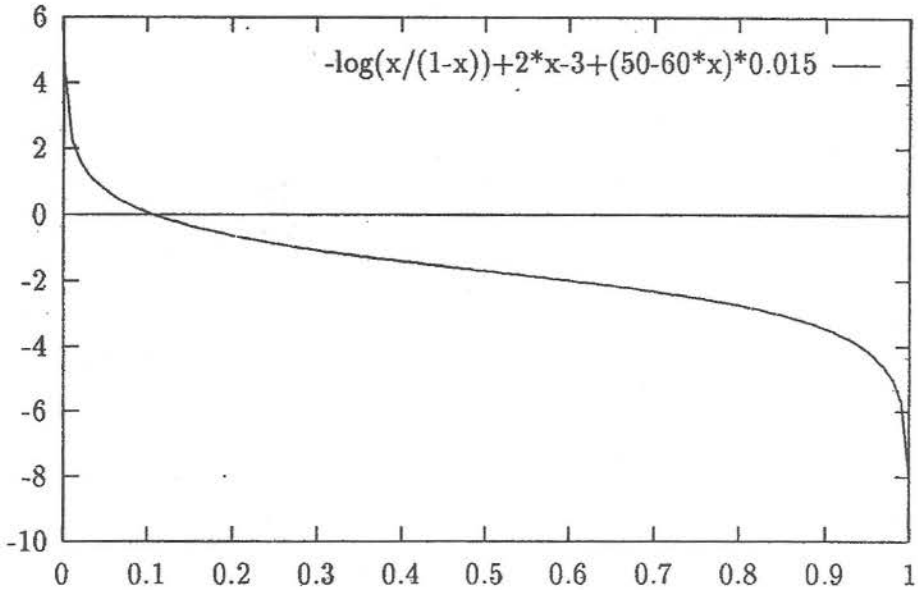

Figure 1. Graph of the function $f(\phi, u_0)$

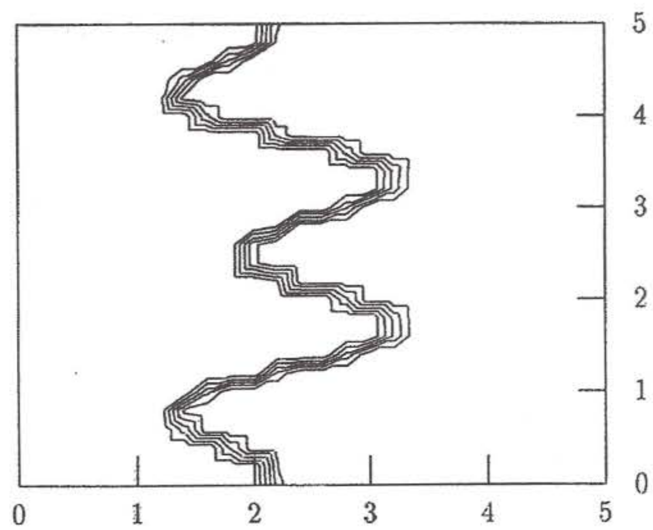

Figure 2. Contour plot of the phase distribution at $t = 0$

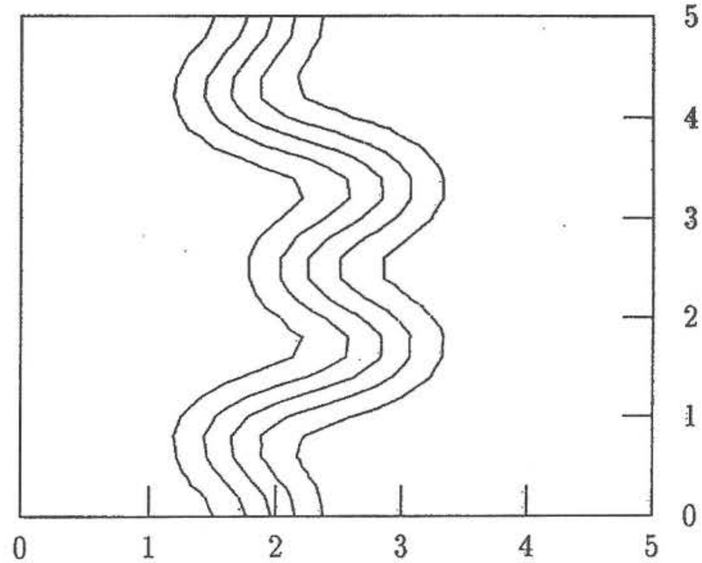

Figure 3. Contour plot of the phase distribution at $t = 200$

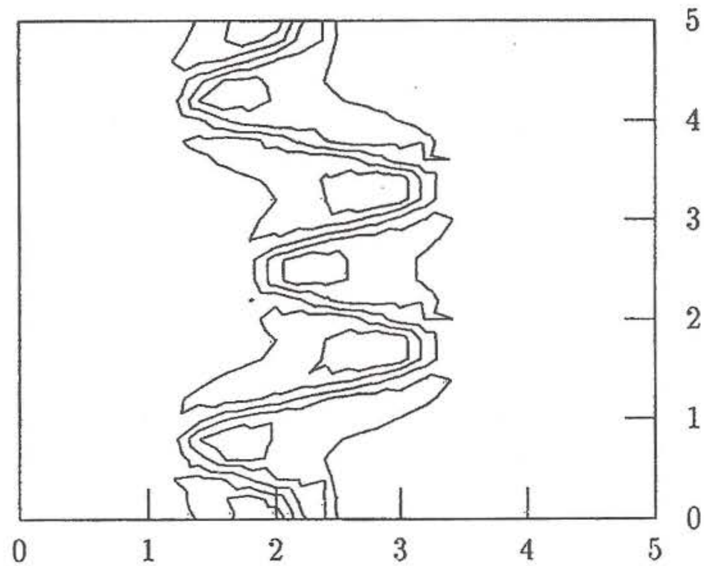

Figure 4. Contour plot of the temperature distribution at $t = 200$

The elliptic equations (14)–(15) were solved using finite differences on a uniform 201×201 grid with a mesh width of 0.01. The time step was 0.000001. The contour plot of the phase distribution ϕ is shown in Figure 3. One sees that the mushy region got wider and that the curvature of the contoures decreased. The contour plot of the temperature shown in Figure 4 gives some more information. One can see distinctive peaks resp. wells in areas where ϕ has maximal resp. minimal curvature. This behaviour is expected from a model, which in the limit as $K_1 \to \infty$ is supposed to model the motion of a phase boundary by mean curvature.

5. Concluding remarks

We conclude this article by mentioning some more recent developments and some interesting problems connected with the model presented in this paper.

- Even though the analysis of the evolution equations seems to be relatively advanced, most existence and uniqueness results cover only the simplest cases of the evolution equations. Aside from the remark on the natural boundary conditions (see section 1) we would like to point out a recent preprint by Ph. Laurençot which treats weak solutions for a some what more complicated set up, Laurençot (1993).
- The analysis of the evolution equations for a conserved order parameter was not covered in this paper. In this case, the equation for the order parameter is a fourth order parabolic equation, similar to the Cahn-Hilliard equation.
- Several interesting optimal control problems are open. These include state constraint optimal control as well as optimal shape design problems.
- The numerical methods for the evolution equations are not very well studied so far. The major problem is, that there is no good discrete equivalent of the powerful theorems of Amann (1993).

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