PHASE FIELD METHODS FOR FREE BOUNDARY PROBLEMS

by

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ABSTRACT

A phase field model is derived for free boundary problems where the effects of supercooling and surface tension are present. A scheme for obtaining numerical approximations is derived, and sample numerical results are presented.

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1. The H-method for Stefan Problems

The standard description of a solidification process is captured in the classical Stefan problem [1]. In this context $T « T(\underline{x},t)$ denotes a temperature field with T^* denoting the phase transition temperature. In particular, points $\underline{x}$ in the material ft are in the liquid phase when $T > T_A$, and conversely, they are in the solid phase when $T < T^\wedge$. At points ££ft where there is no phase transition, i.e., $TO\underline{c},t) + T^\wedge$, the following diffusion equation is valid:

$$(1.1) \qquad || - \mathrm{div}(D\ \overrightarrow{\mathrm{grad}}\ T) \qquad \underline{x}\ £\ ft,\ t > 0, \quad T(\underline{x},t) + T^*.$$

The transition region is defined by

$$(1.2) \qquad f(t) - \{x\ €R : T(\underline{x},t) - T^*\},$$

and for points in this region

$$(1.3) \qquad Xv + [D^*\overrightarrow{\mathrm{grad}}\ T^*\underline{v}J^*_- - 0, \qquad \underline{x}\ £\ T(t).$$

Here X is the latent heat, v the normal velocity of F(t), $\underline{\backslash}^\wedge$ the normal to F(t), and $[\bullet]^+_-$ denotes the jump across F(t). To complete the specification of the problem v» specify initial conditions, e.g.,

$$(1.4) \qquad T(x,0)\ »\ T_Q(x) \qquad \underline{x}\ €ft,$$

for a given initial temperature field T_Q, and boundary conditions. For simplicity we use Dirichlet type conditions, namely

$$(1\text{-}5) \qquad T(x,t) - T_x(x), \qquad \underline{x}\ £\ 3ft,\ t > 0,$$

where $T^\wedge_-$ is a given temperature field defined on the boundary 3ft of ft.

The H-method [2] is a reformulation of (1.1), (1.3) in terms of a single partial differential equation. To do this we introduce an "enthalpy" as follows:

$$(1.6) \qquad H(u) = \begin{cases} u + X/2, & u > 0 \\ u - A/2, & u < 0_f \end{cases}$$

where

$$(1.7) \qquad o - T - T_{\#}.$$

Then (1.1), (1.3) are formally equivalent to

$$(1.8) \qquad || - \mathrm{div}(D \ \mathrm{grid} \ u).$$

Since H is discontinuous across the free boundary F(t), (1.8) must be interpreted in the weak sense. Perhaps the most easily understood "weak version" of this equation is as a balance law which expresses the conservation of heat. Indeed, let C be any closed curve in ft^{x} [0,°°). Then the balance of heat in C gives

$$(1.9) \qquad /_{C} (Hv_t + Dgr\hat{}du\text{-}\underline{V}_x)dC \ « \ 0,$$

where V » (v.,v) is the outer normal to the space-time curve C.

By shrinking G to a point (x,t) one can formally derive (1.7). Alternately, letting C shrink to a point (x,t), where x. i F(t), one obtains (1 1). If on the other hand x £ T(t), we obtain

$$V[H£+[Dgradu\underline{*}v_x£-0,$$

which is (1.3).

The most common finite element and finite difference approximations to (1.1), (1.3) can be derived directly from (1.9). For example, consider the case where Ω is an interval $[a,b]$, and $[a,b] \times [0,\infty]$ is subdivided into rectangles with nodes at (x_j, t_n). Let Δx denote the spacing in x and Δt denote the space in t with u_j^n denoting the approximation to $u(x_j, t_n)$. Then instead of requiring that (1.8) hold for all closed curves C, we require that it hold only for the rectangular paths shown in Figure 1.1. This along with the use of midpoint quadrature to evaluate the integrals gives the following difference scheme:

$$(1.10)\qquad \frac{H(u_j^{n+1}) - H(u_j^n)}{\Delta t} = D\,\frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{\Delta x^2}$$

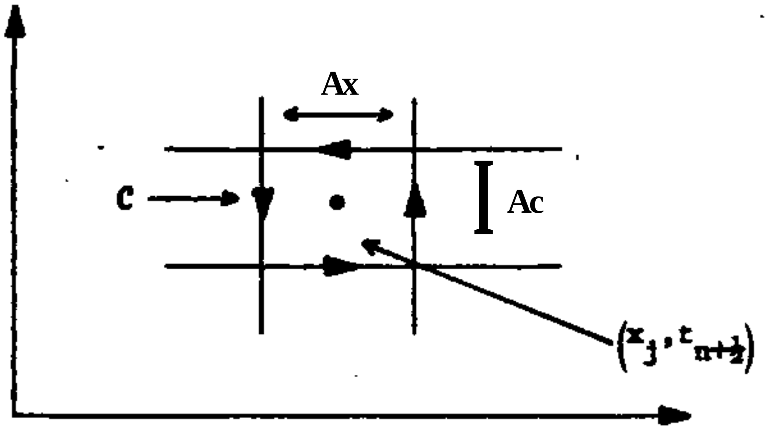

Figure 1.1. Test Curves C.

The scheme (1.10) (plus boundary and initial conditions) represents a set of nonlinear equations for the discrete temperature field $\{u_j^n\}$. Since H is piecewise linear in u this scheme is in fact a "piecewise linear" system in the temperature field u_j^n and as such is easier to solve than a fully nonlinear diffusion problem. This scheme and its multidimensional analogs have proven to be quite effective in practice [3] and [10]. Interestingly, most of the schemes proposed for solving the Stefan problem either directly reduce to (1.9) or to this scheme with minor modifications.

2. A Generalized Stefan Problem - Supercooling and Surface Tension

In many applications — most notably in crystal growth and the fusion and joining of material [4] — there are important effects not captured in the classical Stefan problem. One is the effect of surface tension. As solidification takes place the melting temperature T_* itself will change as the curvature K of the free surface $F(t)$ changes. This can be expressed mathematically by a formula that goes back to Gibbs [5], and which takes the following form:

$$T_K = \bar{T}_*(1-\ell K). \tag{2.1}$$

Here $\bar{T}_*$ is a mean transition temperature, and ℓ is a capillary length.

While (2.1) introduces a full nonlinearity (into the otherwise "piecewise linear" system (1.1) - (1.3)), it is in fact a benign nonlinearity which attempts to stabilize perturbations introduced in the system. For example, if we introduce a perturbation in a planar free surface with a positive curvature $K>0$ as in Figure 2.1, then the transition temperature is lowered, and the perturbation tends to liquidify and disappear.

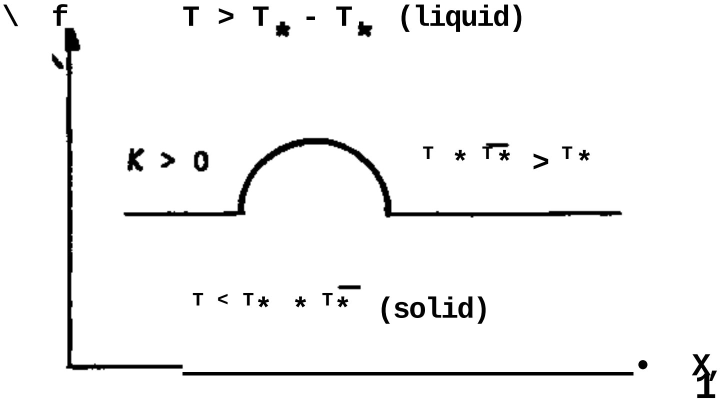

Figure 2.1. Effect of Surface Tension

The second effect of importance is supercooling. It is possible, for example, for a material to be in the liquid phase with its temperature below the transition temperature, or conversely, in the solid phase with its temperature above the transition temperature. This situation can be captured mathematically by permitting the enthalpy $H * H(u)$ to be multivalued (as in Figure 2.2).

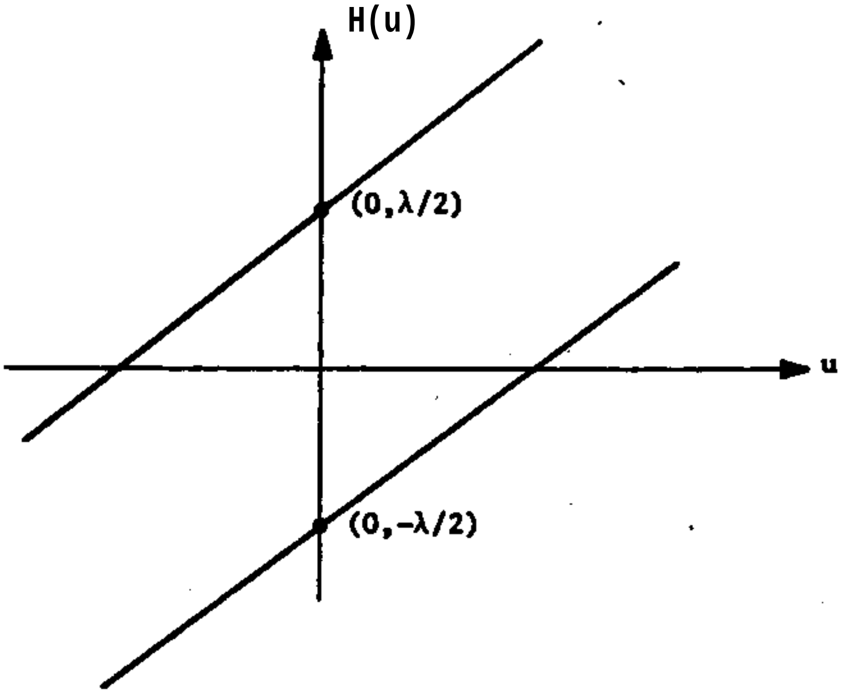

Figure 2.2. The Multivalued Enthalphy

This clearly is an unstable force In solidification. That is, supercooling tends to amplify any perturbation introduced in the system such as shown in Figure 2.1. Without surface tension the influence of supercooling would lead to a totally unstable system. In real physical systems, however, where supercooling is present, local instabilities — often called dendrites — can occur but they are counter balanced by the nonlinear stabilizing effects of surface tension.

One can still use the H-method for problems where surface tension is present (i.e., T^ is given by (2.1)), although it is far more tedious to apply than with standard Stefan problems. The most significant problem is the need to accurately approximate the free surface F(t) so that reasonable approximations to that curvature K of F(t) can be obtained. This unfortunately works against one of the most attractive features of the H-method when applied to standard Stefan problems; i.e., the ability to get reasonable temperature fields without having to sharply resolve the free boundary [6].

The effects of supercooling, on the other hand, cannot directly be introduced into the H-method. Additional information is needed to resolve the ambiguity created by a multivalued enthalpy H(u). Smith [7] has offered one method for doing this by introducing a local criteria for determining which branch of H(u) should be used. In particular, Smith subdivided space-time into cells and used (1.9) to derive a finite difference approximation. He let a spatial cell change phase only when a "majority" of its neighbors were in the opposite phase. Smith's numerical results seem quite realistic, and from the point of view of statistical mechanics, his local criteria seems intuitive. However, a number of important questions can be raised. First, his local criteria is tied to the numerical discretization. How does one interpret his condition as the mesh spacing goes to zero? Secondly, if there is a "limit condition" is it independent of the grids used in the numerical approximation? In short, can one view Smith's scheme as the approximation to an appropriate continuum model?

In the next section we introduce an alternate model which possibly may be of value in answering these questions. In addition, this model itself can also be used for numerical approximation when supercooling and surface tension is present.

3. Phase Field Models

In this model ve introduce a phase variable 4 * $(x,t) which is to be determined by an appropriate field equation. Ideally ve should have • • •÷ in the liquid region and • " •^ in the solid region. Thus the enthalpy is given by

(3.1) $$H - u + \frac{1}{2}\phi .$$

As above a balance of heat gives

(3.2) || - div[D g«id u]f x £ Qf t > 0f

and ve recall that this equation is equivalent to (1.1) and (1.3).

The phase field $, on the other hand, satisfies

(3.3) T ft ≗" ***• + *(*-*3) +Xu ı

for appropriate constants T > 0, A > 0f and £. This equation can be derived by introducing the Helmholtz free energy, which following [8] takes the form

$$F(\phi) = -\int\{\xi^2 \nabla\phi\cdot\nabla\phi + \frac{1}{4}(\phi^2 - \frac{1}{2}\phi^{\textcircled{3}})^{4} + \lambda u\phi\}.$$

One requires that 0 relax in time T > 0 to a critical point of this functional; i.e..

(3.4) $$\tau \frac{\partial\phi}{\partial t} = \frac{\delta F}{\delta\phi} .$$

Here we shall choose a different way of justifying (3.3). In particular, \
we show that in a suitable sense it reduces to the surface tension relation (2.1) which we rewrite as

(3.5) u - -T^IK on T(t).

To do this we view T as a small relaxation time, i.e.,

(3.6)

The diffusion scale £ is also small, but not as small as T:

$$(3.7) \qquad \xi \ll l_f \qquad \tau/\xi \ll 1;$$

i.e., the relaxation to equilibrium takes place at faster rate than the diffusion of the phase.

To study (3.3) under the conditions (3.6) - (3.7) we use the method of matched asymptotic expansions. To take a concrete case consider the situation illustrated in Figure 3.1 where

$$y = \zeta(x,t)$$

describes the free surface

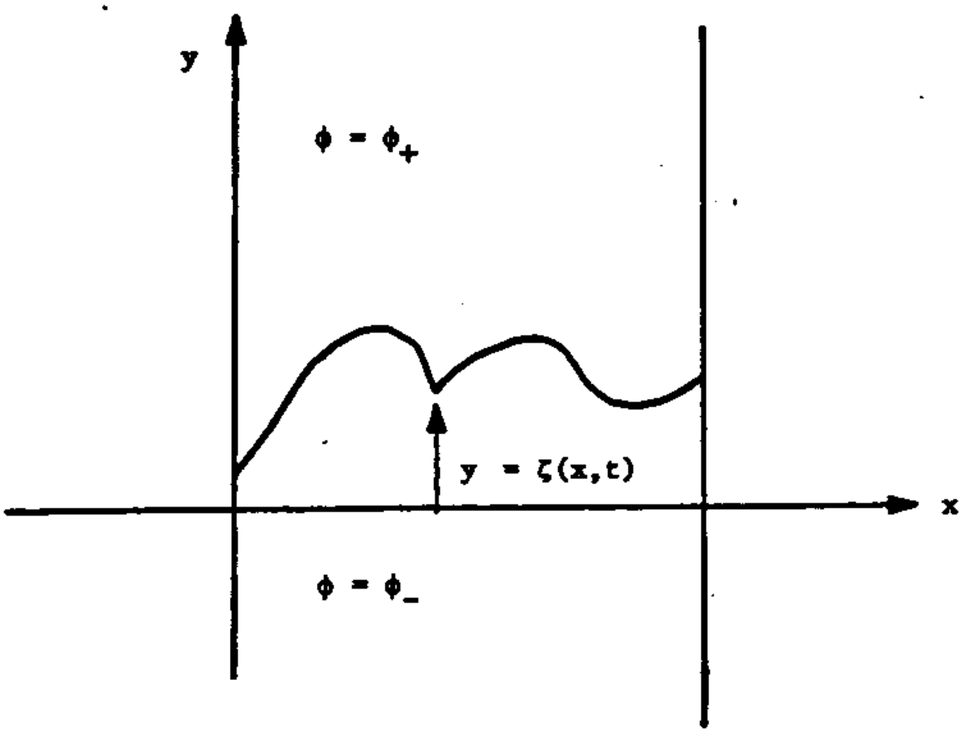

Figure 3.1. The free surface z * £.

The outer solution (to first order) is obtained by setting $\xi = \tau = 0$. This gives

$$\tfrac{1}{2}(\phi - \phi^3) + u = 0. \tag{3.8}$$

For small u this has three real solutions

$$\phi = \phi_+ \approx 1, \qquad \phi \approx 0, \qquad \phi = \phi_- \approx -1. \tag{3.9}$$

It is easy to check that only the first and third are stable orbits of

$$\tau \frac{\partial\phi}{\partial t} = \tfrac{1}{2}(\phi - \phi^3).$$

Thus away from the free surface we have

$$\phi = \phi_+ \quad \text{or} \quad \phi = \phi_-$$

Near the free surface we obtain a boundary layer of order $O(\xi)$. To get the first order contribution we set $\tau = 0$ and obtain the following balance

$$0 = \xi^2 \Delta\phi + \tfrac{1}{2}(\phi - \phi^3) + \lambda u. \tag{3.10}$$

The appropriate boundary layer variables are

$$x^\nabla = x \tag{3.11}$$

$$y^\nabla = [y - \zeta(x,t)]/\xi . \tag{3.12}$$

This gives

$$\xi^2 \frac{\partial^2\phi}{\partial x^{\nabla 2}} - 2\xi \frac{\partial\zeta}{\partial x^\nabla} \frac{\partial^2\phi}{\partial x^\nabla \partial y^\nabla} - \xi \frac{\partial^2\zeta}{\partial x^{\nabla 2}} \frac{\partial\phi}{\partial y^\nabla} + \left(\frac{\partial\zeta}{\partial x^\nabla}\right)^2 \frac{\partial^2\phi}{\partial y^{\nabla 2}} + \tfrac{1}{2}(\phi - \phi^3) + \lambda u = 0. \tag{3.13}$$

Noting that u is small near the free surface $y^{v} - 0$, the 0(1) balance is

$$(3.14) \qquad \left(\frac{\partial\zeta}{\partial x^{\nabla}}\right) \frac{\sigma\ \phi}{\partial y^{\nabla 2}} + \tfrac{1}{2}(\phi - \phi^{3}) = 0.$$

Solution of this equation are approximately

$$\tanh(y^{v}) - \tanh([y - \zeta(x,t)]/\xi).$$

The next balance gives the desired Gibbs-Thompson relation$_9$ namely

(3.15) u · (c/X) (l^/i - |\ ² \3y7\3x‾/ oT r(t).

Noting that the curvature *K* of F(t) is given by

$$K = -\frac{\partial^{2}\zeta}{3x^{2}}\, f$$

we conclude from (3.15) that u is proportional to curvature *K* of the free surface on T(t); i.e., (3.5) holds.

It is interesting to note that this analysis predicts for positve £ > 0 and T > 0 a boundary layer of thickness 0(£) where 4> rapidly changes from $_ to 4>+. Thus it is important when this model is being used to keep £ sufficiently small so that the free surface is not smeared. In addition, the relaxation time x must also be small so that the model is describing phenomena near a thermodynamic equilibrium.

4. Numerical Examples

In this section we present two numerical examples. In the first example supercooling is not present so in effect it is equivalent to a classical Stefan problem. We use this example to illustrate the type of approximations that can be obtained in a setting where one can be reasonably confident about how the solution should behave (although no closed form solution is known). In the second example we display a situation where dendrites appear and then restabilize.

In each example, the diffusion equation (3.2) was integrated by an A.D.I, using a fixed time step AT. The equation (3.3) for the phase <*t*> used the time step

At - T/H.

The number M was chosen so the front velocity was the same order of magnitude as A/At, where A is the smallest mesh length in the grid for $• This is illustrated in Figure 4.1 for one space dimension. In addition, the grid for $ was moved by monitoring values of the second differences in $.

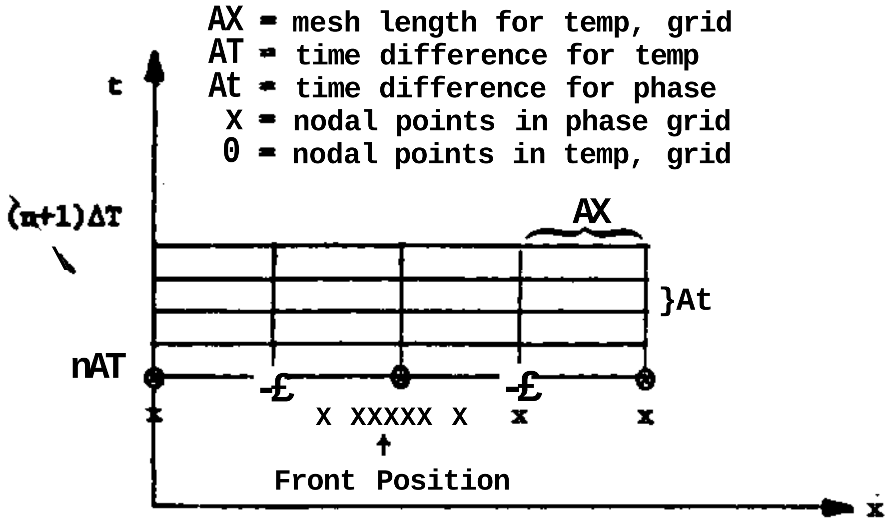

Figure 4.1. Space-time Grid

The calculation started by first marching the phase equation M steps to time ΔT. In this calculation the value of the temperature u was frozen at its previous value, namely at $n\Delta t = 0$. Then one time step of length ΔT was used to compute u at time ΔT. This process was repeated moving from ΔT to $2\Delta T$, etc. In some cases where there were extreme variations in both u and ϕ it became necessary to iterate this process; i.e., recompute the phase based on updated values of u_h.

The first example is shown in Figure 4.2. It is a classical solidification problem where supercooling is not present. The interior of the rectangular domain is initially in the liquid state at the melting temperature $\bar{u}_M = 0$, while the boundary temperature u_Γ is held below $\bar{u}_M$. As time progresses a front moves and the interior starts to solidify. In Figure 4.3 we show sample temperature and phase profiles for $t = 0$ to $t = .5$. The plots represent functions of x for the fixed value $y = .5$. Note that the position of the front is blurred in the temperature plot on the right in Figure 4.3, but is quite sharp in the plot of ϕ on the left.

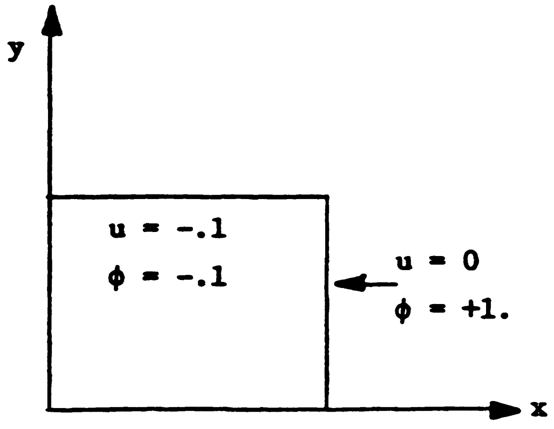

Figure 4.2. Initial Conditions - First Example

In the second example we have a solidification problem that is driven by seed of solid at u « 0 in a background of supercooled liquied at u • -1. (See Figure 4.4). As in the previous example the mean melting temperature $\overline{UL}$, is 0. Two cases were considered. In the first a rather large value for the surface tension was chosen. This tended to act as a strong stabilizing force overriding the tendency of supercooling to promote dendritic growth. The front contours in time are plotted in X-Y geometry in Figure 4.5. The progresssion of the front looks like one that would arise from a standard Stefan problem, except for the bumps in the free surface at the final time when the front neared the boundary. The latter are numerical artifacts.

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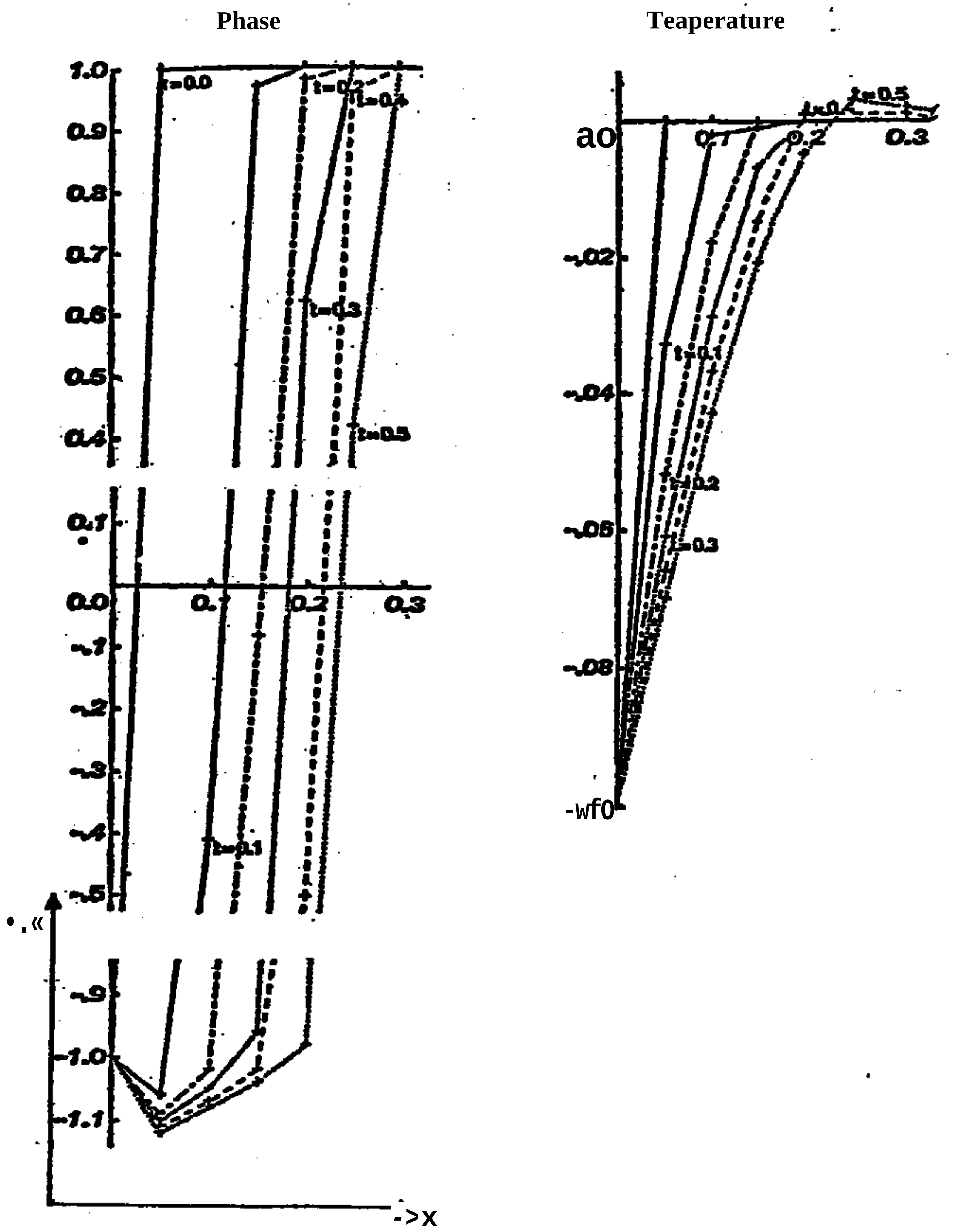

Figure 4.3. Temperature and phase profiles for y - J,

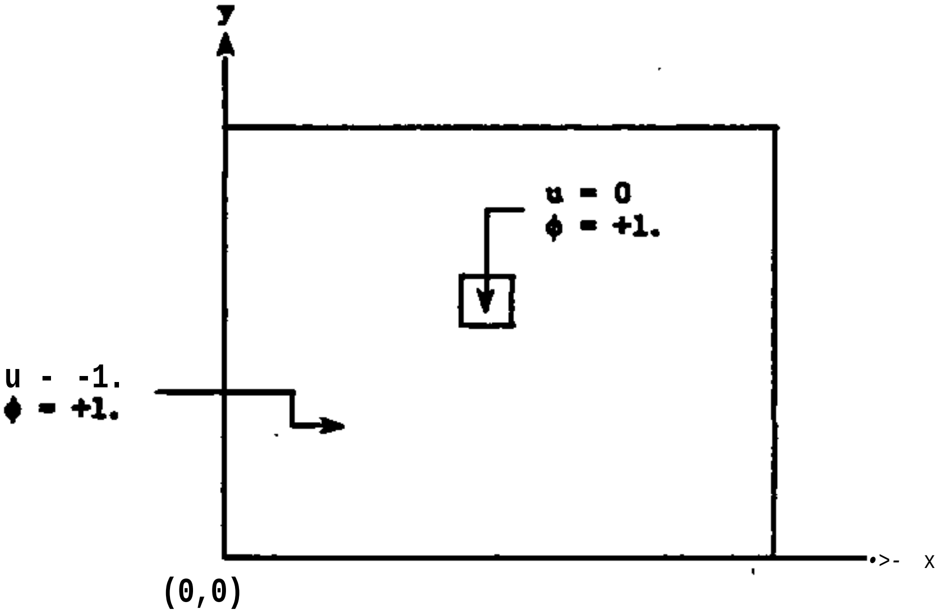

Figure 4.4. Initial conditions - second example.

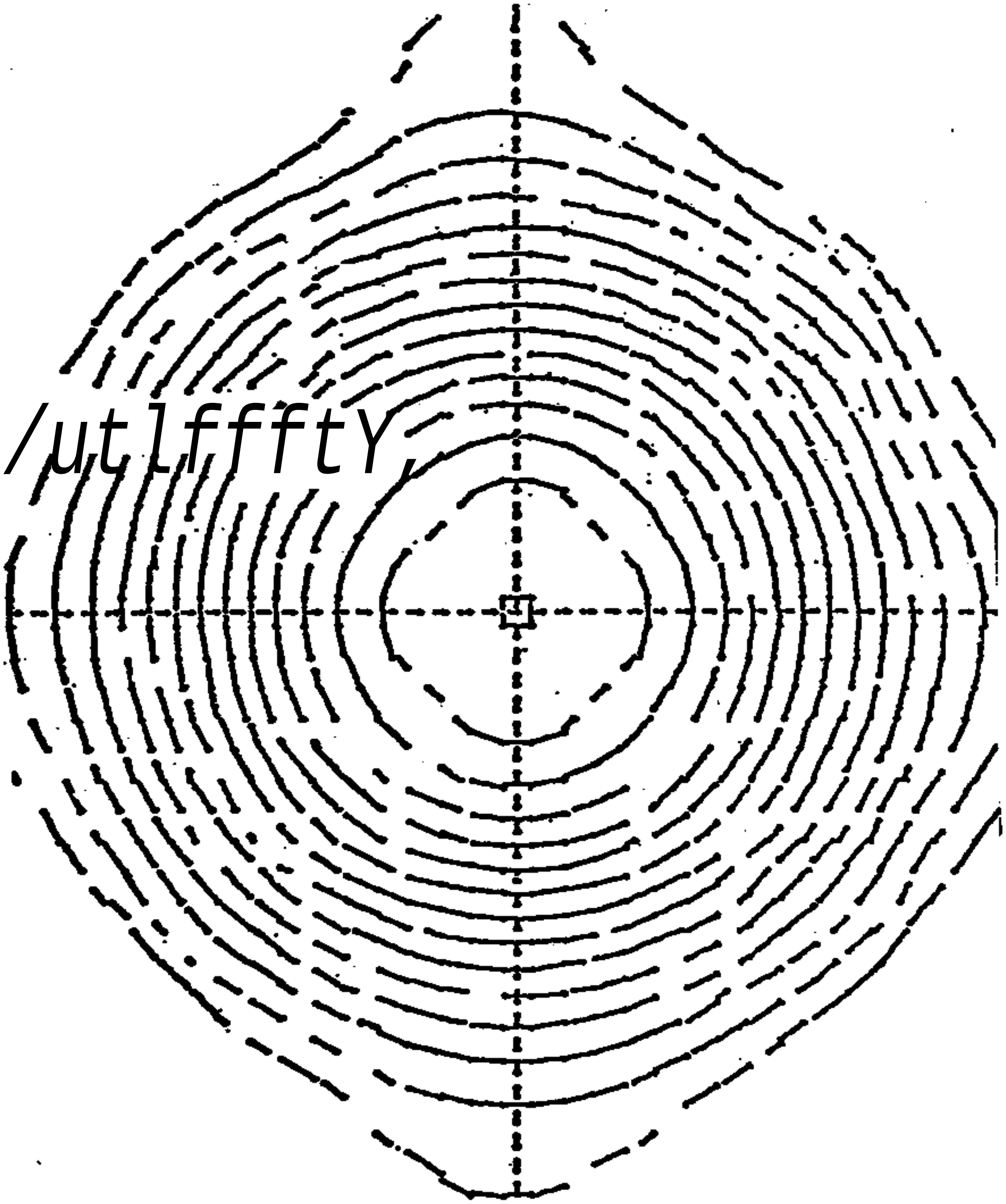

Figure 4.5. First case - large surface tension

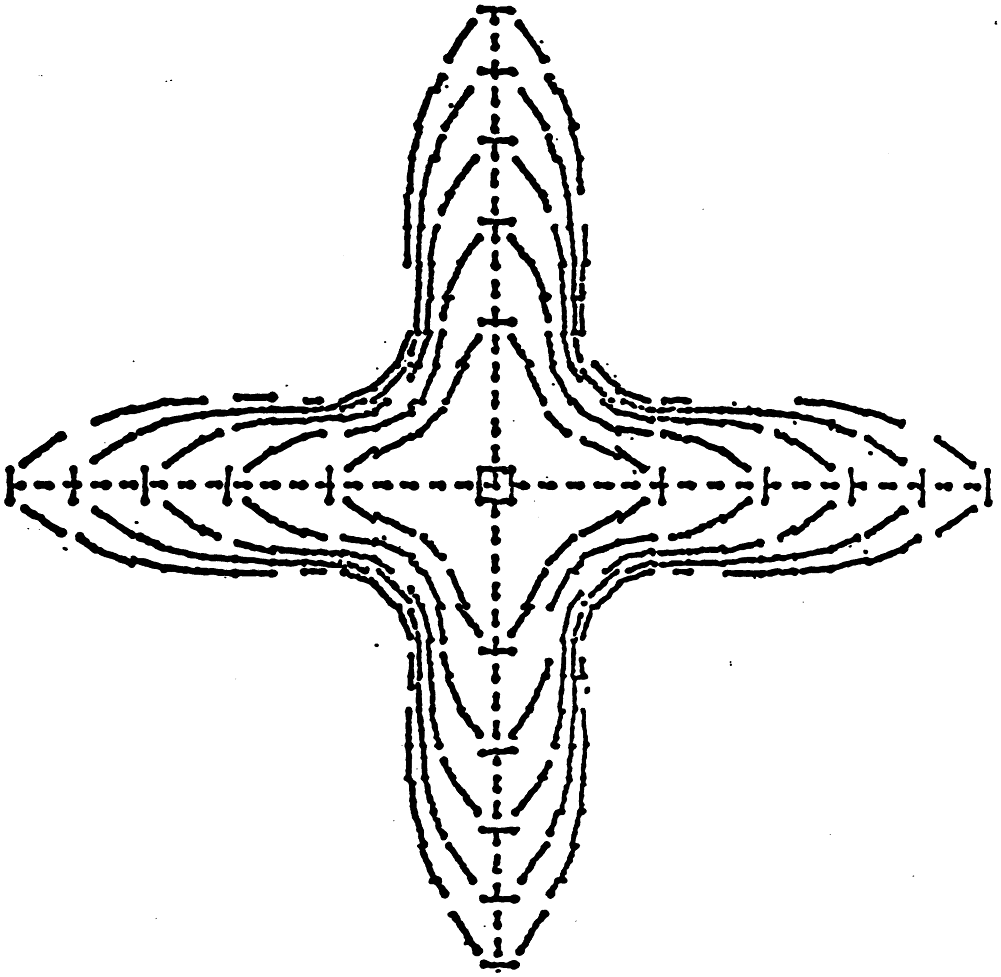

Figure 4.6. Second case - small surface tension.