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ONE DIMENSIONAL PARABOLIC FREE BOUNDARY PROBLEMS

by

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ABSTRACT

The method of lines is used to approximate explicit and implicit free boundary problems for a linear one dimensional diffusion equation with a sequence of free boundary problems for ordinary differential equations. It is shown that these equations have solutions which can be readily obtained with the method of invariant imbedding. It also is established for a model problem that the approximate solutions converge to a unique weak and (almost) classical solution as the discretization parameter goes to zero.

One Dimensional Parabolic Free Boundary Problems

1. Introduction. Among the class of free boundary problems for have been examined in some detail. Perhaps the best understood problem of this kind is the formulation for the melting of a slab of ice in contact with a viscous fluid. If one assumes that the ice is held at 0°C throughout, and that heat transfer in the fluid occurs by conduction only, then the temperature distribution is described by the usual heat equation

$$u_{xx} - cu_t = \mathbf{0}$$

subject to the initial and boundary conditions

$$u(\mathbf{0}, t) = \alpha(\mathbf{0}, t), u(s(t), t) = \mathbf{0}, u_x(s(t), t) = -\lambda \frac{ds}{dt}, s(\mathbf{0}) = \mathbf{0} \quad .$$

Here u denotes the temperature in the fluid between a wall at $x - 0$ held at temperature $\alpha(t)$ and the unknown and moving boundary $s(t)$ between the fluid and ice. The flux condition $u_x(s(t), t) = -\lambda \frac{ds}{dt}$ is obtained from an energy balance and indicates that the heat flowing toward the ice is used to melt it rather than raise its temperature. The condition $s(0) = 0$ means that initially no fluid is present. The constants c and λ are determined from the conductivity, heat capacity, and latent heat of water.

This problem and some natural generalizations to two phase systems (where also the solid has a variable temperature) were studied around 1890 by J. Stefan and today are commonly called Stefan problems. Over the years more and more technical applications were seen to lead to problems of Stefan type and as a result a substantial body of literature has accumulated on the analytical and numerical solution of such free boundary problems. A discussion of the formulation of one dimensional free boundary problems for change of phase, filtration, viscoplastic flow and impact processes as well as a detailed mathematical treatment of certain model problems may be found in the monograph of Rubinstein [14] and in the proceedings of a recent conference on Stefan problems [10].

A common technique for the solution of boundary value problems for the diffusion equation in one space dimension is the so-called method of straight lines in which the partial differential equation is replaced by a sequence of ordinary differential equations at discrete time levels. For fixed boundary problems this method is long established as an analytical and numerical tool {see, e.g. [6], [12] and [2]). Moreover, although not mentioned in [14] the theory has been adapted frequently to free boundary and interface problems (see, e.g. [1], [7], [16], [17] [18], [19] and the references given there). These latter papers differ substantially in detail because a variety of problems are considered, but all follow the same general outline and use the same basic mathematical techniques. It is the purpose of this paper to give an exposition of the method of lines for free boundary problems which illustrates this general outline. Five distinct steps may be identified in the solution process. 1) The formulation of the by-lines approximation; 2) The solution of the by-line equations; 3) The derivation of a-priori bounds on the by-lines solution; 4) The definition of a solution of the given free boundary problem, and 5) The convergence of the method lines solution.

Steps 1 and 2 are algorithmic and will be formulated for quite general problems. In contrast, the a priori bounds and the convergence depend crucially on the given data and hence will be treated for a model problem. Finally, it must be mentioned that in two respects the work of this author differs from most of the cited literature. Step 2 is carried out with the method of invariant imbedding which converts the by-lines boundary value problems into initial value problems, and Step 5 uses the concept of weak solutions rather than classical solutions. However, the general outline will always be adhered to.

2. Straight lines approximation and invariant imbedding. The following problem will be considered

$$(\mathbf{2.1}a)\, Lu \equiv \left(\frac{\partial}{\partial x}\left(k(x,t)\frac{\partial}{\partial x}\right) + a(x,t)\frac{\partial}{\partial x} + b(x,t) - c(x,t)\frac{\partial}{\partial t}\right)u = f(x,t);\; t > \mathbf{0},\; \mathbf{0} < x < s(t)$$

(2.1b) $\alpha_1(t)\,u(0,t) + \alpha_2(t)u_x(0,t) = \alpha(t), \alpha_1^2 + \alpha_2^2 \neq 0; \; t > 0$,

(2.1c) $u(x,0) = u_0(x)$; $0<x<s(0)$

subject to

(2.2) $H\left(u(s,t), u_x(s,t), u_t(s,t), s(t), s'(t), t\right) = 0; \quad t > 0$

where $H = (H_1, H_2)$ is a given function with values in R_2 . Throughout this discussion all data functions are assumed to be as smooth as required for subsequent operations on the set $\Omega_\infty = \{(x,t): 0\leq x<\infty, 0\leq t\leq T\}$ where T is some arbitrary but fixed upper time limit.

The formulation (2.1,2) includes a variety of free boundary problems , among them:

i) Stefan problem: $H \equiv \begin{pmatrix} u \\ u_x + \lambda s' \end{pmatrix}$, or more generally $H \equiv \begin{pmatrix} u+\mu_1(s,t) \\ u_x+\lambda s'+\mu_2(s,t) \end{pmatrix}, \lambda>0$

ii) optimal stopping theory [17] and Bingham plastic flow [14]: $H \equiv \begin{pmatrix} u \\ u_x \end{pmatrix}$

(to be analyzed in the next section)

iii) one phase filtration [16], [193: $H \equiv \begin{pmatrix} u - \mu_1(s,t) \\ u_x - \mu_2(s,t) \end{pmatrix}$

iv) Gibbs-Thompson model for the growth of a bubble in a chemical solution [3]:

$$H \equiv \begin{pmatrix} u - \mu_1 e^{\mu_2/s} \\ u_x - (\mu_3 - u)s' \end{pmatrix}$$

v) Radiation and Arrhenius ablation on the free surface

$$H \equiv \begin{pmatrix} u_x - \mu_1\left(u^4 - \mu_2^4\right) \\ s' - \mu_3 e^{\mu_4/(\mu_5 - u)} \end{pmatrix}$$

where all μ_i. may be functions of t and s. In addition, functional relations on the free boundary can be accommodated (see, e.g. the formulation for viscoplastic impact [5] and the heat transfer problem for fluidized-bed coating [8]).

All these problems have in common that the diffusion equation,. whether cartesian, radial or spherical, with or without additional convection terms, and with a problem dependent source term, must be solved subject to the affine relation (2.1b) and the two relations (2.2). If s(t) were given, the problem would be over-determined and in general have no solution. However, s(t) is not known a priori and must be determined such that the given boundary data are consistent. If one of the equations of (2.2) can be solved for s(t) or s'(t), then the problem is known as an explicit free boundary problem, otherwise it is called implicit. The Stefan problem is an explicit, the optimal stopping problem an implicit formulation.
It is possible to introduce the method of straight lines for the formulation (2.1) without further specifying the structure of the equations. For this purpose we shall define a partition $\{0 = t_0 < t_1 < \,..\, < t_N = T\}$ of $[0,T]$, which for ease of notation is assumed to have equal subintervals $\Delta t = t_i - t_{i-1}$, $i = 1, ..., N$. The simplest, and most commonly used, method of lines approximation for (2.1) requires the substitution

$$u_t(x,t) \approx \frac{u(x,t_n) - u(x,t_{n-1})}{\Delta t}$$

$$s'(t_n) \approx \frac{s(t_n) - s(t_{n-1})}{\Delta t}$$

which reduces the partial differential equation (2.1) to a sequence of free boundary problems for a second order differential equation

$$(k(x,t_n)u'_n)' + a(x,t_n)\,u'_n + b(x,t_n)\,\frac{u_n - u_{n-1}}{\Delta t} = f(x,t_n)$$

$$n = 1, \,..,\, N$$

$$(2.3) \quad \alpha(t_n)u_n(0) + \alpha_2(t_n)\,u_n'(0) = \alpha(t_n)$$

$$H\left(u_n(s_n), u_n'(s_n), \frac{u_n(s_n) - u_{n-1}(s_n)}{\Delta t}, s_n, \frac{s_n - s_{n-1}}{\Delta t}, t_n\right) = 0$$

where $u_n = u(x,t_n)$, $u'_n(s_n), = \frac{d}{dx} u_n$ and $s_n = s(t_n)$. For each n these equations must be solved for the function u_n and the free boundary s_n. (if necessary, u_{n-1} is extended differentiably as a linear function over $[s_{n-1}, \infty)$.)

The equations (2.3) constitute a fully implicit approximation of order Δt since all time derivatives are replaced by simple backward difference quotients. Higher order approximations, such as the Crank-Nicolson scheme, would appear equally feasible although care must be taken to insure that the truncation error on the free boundary is likewise improved. However, for theoretical and numerical work, especially on Stefan problems, the above formulation was found to be attractive because of its simplicity and stability, especially when the initial and boundary data are incompatible, i.e. $\alpha_1(0)u_0(0) + \alpha_2(0)u_0'(0) \neq \alpha(0)$.
A by-lines approximation in which time derivatives are approximated by forward difference quotients is meaningful only if the differential equations in x are discretized as well in order to observe a stability constraint on the ratio $\Delta t / \Delta x^2$. For explicit free boundary problems this approach is simple to use; however, for implicit problems the prediction of the free boundary at the new time level may require considerable continuity of the solution of (2.1) because Taylor expansions of $s(t)$ are commonly used [4]. We shall bypass explicit and semi—explicit approximations of (2.1,2) in favor of the fully implicit formulation (2.3) since the solution algorithm chosen here for its solution is only minimally affected by the presence of the free boundary s_n .

It may be noted that the by-lines approximation involves simply the replacement of time derivatives by difference quotients and does not depend on the linear structure of the equations in (2.1). However, for a linear parabolic operator the equations (2.3) can usually be solved in a consistent manner. In some of the earlier work the linearity of the differential equation was exploited by finding fundamental solutions and a particular integral for (2.3) and combining them in such a manner that the boundary conditions are satisfied. For example. if L in (2.1) is the heat operator $\left(\frac{\partial^2}{\partial X^2} - \frac{\partial}{\partial t}\right)$ then the solution of (2.3) has the representation

$$u_n(x) = c_{1n} \sinh x + c_{2n} \cosh x + \int_0^x \sinh(x-r).[f(r,t_n) - \frac{1}{\Delta t} u_{n-1}(r)]\,dr$$

which on substitution into the boundary conditions yields three equations. in the three unknowns $\{c_{1n}, c_{2n}, s_n\}$. This approach in the basis of the numerical results reported in |16 |. However, UB pointed out in | 7 | use of the fundamental solutions may lead to severe numerical instabilities due to the exponential growth of the basis solutions.

The linearity of the differential equation for u_n may be used in another way which is known, at least for Stefan problems [15], to avoid the instability. The technique to be presented is known as the method of invariant imbedding and has been described in detail in [7]. We shall give a short summary. Problem (2.3) can be written as the first order system

$$(2.4)\qquad v'_n = \frac{c(x,t_n)}{\Delta t}u_n - \left(\frac{a(x,t_n}{k(x,t_n)}\right)v_n - b(x,t_n)u_n + f(x,t_n) - \frac{c(x,t_n)}{\Delta t}u_{n-1}(x)$$

$$u'_n = v_n / k(x,t_n)$$

subject to the given boundary conditions. For definiteness let us assume that $\alpha_2(t) \neq 0$ on [0,T] and for convenience let us set $\alpha_2 \equiv 1$. (For the case of $\alpha_1(t) \neq 0$ the roles of u_n and v_n should be reversed. Details may be found in [7], [9].) Then the boundary conditions for (2.4) are

$$v_n(0) = \alpha(t_n) - \alpha_1(t_n)u_n(0)$$

$$(2.5)\qquad H\left(u_n(s_n), v_n(s_n), \frac{u_n(s_n) - u_{n-1}(s_n)}{\Delta t}, s_n, \frac{s_n - s_{n-1}}{\Delta t}, t_n\right) = \mathbf{0}.$$

The solution of (2.4.5), if it exists, is imbedded in the family $\{v_n(x,r), u_n(x,r)\}$ of solutions of (2.4) subject to

$$(2.6)\qquad \begin{aligned} v_n(0) &= \alpha(t_n) - \alpha_1(t_n)r \\ u_n(0) &= r \end{aligned}$$

where r is a free parameter ranging over all real numbers. (Searching for the value of r consistent with (2.5) would be the usual shooting method for boundary value problems). It is well known that u_n and v_n have the variation of constants representation

$$\begin{pmatrix} v_n \\ u_n \end{pmatrix} = \phi_n(t,0)\begin{pmatrix} -\alpha_1(t_n) \\ r \end{pmatrix} + \phi_n(x,0)\begin{pmatrix} \alpha(t_n) \\ 0 \end{pmatrix} + \int_0^x \phi(x,y)\begin{pmatrix} f(y,t_n) - \frac{c(x,t_n)}{\Delta t} u_{n-1}(y) \\ 0 \end{pmatrix} dy$$

where Φ is the fundamental matrix which satisfies

$$\phi' = \begin{pmatrix} -\hat{a}(x,t_n) & \hat{c}(x,t_n) \\ 1 & 0 \end{pmatrix} \phi, \phi(y,y) = I \quad ,$$

and where

$$\hat{a}(x,t_n) = a(x,t_n)/k(x,t_n)$$

$$\hat{c}(x,t_n) = \frac{c(x,t_n)}{\Delta t} - b(x,t_n) \quad .$$

If the second equation of (2.7) is solved for r, and this expression is substituted into the expression for v_n, we obtain the following relation between u_n and v_n for all $r \in (-\infty,\infty)$

(2.8) $$v_n(x,r) = R_n(x)\, u_n(x,r) + z_n(x) \quad .$$

This expression is the well known Riccati transformation for second order ordinary differential equations. Since it has to hold for all r a comparison with (2.6) shows that

$$R_n(0) = -\alpha_1(t_n), \quad z_n(0) = \alpha(t_n) \quad .$$

Moreover, since u_n and v_n satisfy (2.4) and R_n and z_n are simple combinations of the components of Φ and the particular integral in (2.7), the expression (2.8) may he differentiated to give

$$v'_n = R'_n u_n + R_n u'_n + z'_n \equiv R'_n u_n + R_n [R_n u_n + z_n] + z'_n$$

Substitution of the differential equation for v_n and collecting all terms involving u_n leads to

$$[R' + R^2 - \hat{c}(x,t_n) + \hat{a}(x,t_n) R] u_n(x,r) = [-z'_n - R_n z_n - \hat{a}(x,t_n) z_n + f(x,t_n) - \frac{c(x,t_n)}{\Delta t} u_{n-1}(x)]$$

This relation has to hold for all r and since the "bracketed terms are independent of r they must vanish. Thus we finally obtain that the functions R_n and z_n in the Riccati transformation (2.8) are the solutions of the following well defined initial value problems, the so-called invariant imbedding equations,

$$(2.9) \quad R'_n = \hat{c}(x,t_n) - \hat{a}(x,t_n) R_n - R_n^2, \; R_n(0) = -\alpha_1(t_n)$$

$$(2.10) \quad z'_n = -[R_n(x0 + \hat{a}(x,t_n)] z_n + f(x,t_n) - \frac{c(x,t_n)}{\Delta t} u_{n-1}(x), \; z_n(0) = \alpha(t_n)$$

The representation (2.8) has to hold for all x, hence also at the free boundary s_n . Thus, $u_n(s_n)$ and s_n must be determined such that

$$H(u_n(s_n), R_n(s_n) u_n(s_n) + z_n(s_n), \frac{u_n(s_n) - u_{n-1}(s_n)}{\Delta t}, s_n, \frac{s_n - s_{n-1}}{\Delta t}, t_n) = \mathbf{0} .$$

In other words, the free boundary s and the value $u_n(s_n)$ are roots of the following two equations

$$(2.11) \quad H(u, R_n(x) u + z_n(x), \frac{u - u_{n-1}(x)}{\Delta t}, x, \frac{x - s_{n-1}}{\Delta t}, t_n) = \mathbf{0}$$

If such a root $\{u_n(s_n), s_n\}$ can be found then (2.3) is reduced to an ordinary two-point problem subject to $v_n(0) = \alpha(t_n) - \alpha_1(t_n) u_n(0)$ with $u_n(s_n)$ as computed from (2.11). over the fixed interval $[0,s_n]$. Alternatively, one may obtain $u_n(x)$ by integrating the Riccati transformation (2.8)

(2.12) $k(x,t_n)u'_n \equiv v = R_n(x)u_n + z_n(x)$, with $u_n(s_n)$ as determined from (2.11), backward from s_n to 0. The latter approach is commonly taken in numerical work. In addition, it is frequently possible to reduce (2.11) to a scalar equation $\phi(x) = 0$ by eliminating either u or u_x. For example, only the following scalar equations need be solved for the special problems introduced above

i) $\phi_n(x) \equiv R_n(x)u_n(x) + z_n(x) + \lambda\frac{x - s_{n-1}}{\Delta t} + \mu_2(x,t_n)$

$$\equiv R_n(x)(-\mu_1(x,t_n)) + z_n(x) + \lambda\frac{x - s_{n-1}}{\Delta t} + \mu_2(x,t_n) = 0$$

ii) $\phi_n(x) \equiv z_n(x) = 0$

iii) $\phi_n(x) \equiv -R_n(x)\mu_1(x,t_n) + z_n(x) - \mu_2(x,t_n) = 0$

iv) $\phi_n(x) \equiv R_n(x).k_1 e^{k_2/x} + z_n(x) - (k_3 - k_1 e^{k_2/x})\frac{x - s_{n-1}}{\Delta t} = 0$

where $\psi_n(x) = \mu_5 - \mu_4/(\ln\frac{x - s_{n-1}}{\Delta t} - \ln \mu_3)$.

Thus, for all the sample problems introduced above the same approach may be taken. The invariant imbedding equations (2.9,10) are integrated forward in x and the functional ϕ (x) is evaluated. Where it crosses the x-axis the free boundary s_n is placed and $u_n(s\ )$ is determined from (2.11) which allows the computation of u_n over $[0, s_n]$ for example by integrating (2.12). It is apparent that each of these steps can be realized numerically.

From an analytical point of view several questions now arise. Do the above equations always have a solution, and do these solutions converge, in some form, to a solution of the time dependent problem (2.1).

Many problems, particularly those with a nonlinear coupling u, u_x and s(t) on the free surface, have not yet been examined. However, for Stefan and filtration problems the method of lines is known to converge whenever the data satisfy certain sign and growth conditions [1], [9], [19]. We shall obtain comparable results for a different model problem.

3. Convergence of the method of lines. In order to demonstrate how the above solution technique may be used to give an existence proof we shall consider the model problem

$$(3.1) \qquad \begin{aligned} u_{xx} - u_t &= f(x,t) &&; \quad 0 < x < s(t),\ t \in (0,T] \\ u_x(0,t) &= \alpha(t) &&; \quad t \in (0,T] \\ u(s(t),t) &= u_x(s(t),t) = 0 &&; \quad t \in (0,T] \\ u(x,0) &= s(0) = 0 \ . \end{aligned}$$

As stated, this type of problem occurs in the theory of optimal stopping where u is related to the reward function associated with a Brownian motion and s(t) is the optimum stopping boundary for the process (see [17] and the references given there.) The equations are simple but of some mathematical interest since previous method of lines existence proofs for implicit problems specifically rule out the case of vanishing gradients on the free boundary [16], [19]. Thus some of the following results are new; however, they differ only in detail from those of earlier work. We shall prove in succession that under certain hypotheses

i) the method of lines equations for (3.1) have a solution at each time level

ii) that u_n, u_n', $\frac{u_n - u_{n-1}}{\Delta t}$, and $\frac{s_n - s_{n-1}}{\Delta t}$ are uniformly bounded

iii) that approximate solutions for (3.1) defined in terms of (u_n, s_n) converge to a solution of (3.1).

Two basic tools are used time and again, namely the maximum principle for (elliptic) ordinary differential equations (see e.g.[11]) and Ascoli's theorem about the compactness of a uniformly bounded sequence of equicontinuous functions (see e.g. [13]).

The method of lines approximation for the free boundary problem (3.1) is

(3.2) $$u_n'' - \frac{1}{\Delta t}(u_n - u_{n-1}(x)) = f(x, t_n);\ n = 1,.., N,\ \Delta t = \frac{T}{N},$$

or
$$v'_n = \frac{1}{\Delta t} u_n + f(x, t_n) - \frac{1}{\Delta t} u_{n-1}(x) \qquad v_n(0) = \alpha(t_n)$$
$$u'_n = v_n \qquad u_n(s_n) = v_n(s_n) = 0.$$
$$u_0 = 0$$

The corresponding invariant imbedding equations are

(3.3a) $$v_n(x) = R(x)u_n(x) + z_n(x)$$

(3.3b) $$R' = \frac{1}{\Delta t} - R^2 \qquad , R(0) = 0$$

(3.3c) $$z'_n = - R(x)z_n + f(x, t_n) - \frac{1}{\Delta t} u_{n-1}(x) \ , \ z_n(0) = \alpha(t_n),$$

and the free boundary is determined as a root s_n of the equation

(3.3d) $$\Phi_n(x) = z_n(x) = 0 \ .$$

Let us now establish the existence of a solution $\{u_n, s_n\}$ at each time level and its convergence. Two sets of hypotheses will be required

H1: $\alpha(t) \le 0,\ t \in (0,T];\quad f(x,t) \ge c > 0,\quad (x,t) \in (0,\infty) \times (0,T].$

H2:1) There exist Lipschitz constants $L_i \ge 0,\ i=1,2,3$ such that

$$\alpha(t) - \alpha(r) \le L_1(r-t) \qquad , t,r \in (0,T]$$

$$f(x,t) - f(x,r) \le L_2(r-t) \qquad , t,r \in (0,T] \text{ uniformly in } x$$

$$\left|\frac{\partial f}{\partial x}(x,t) - \frac{\partial f}{\partial x}(x,r)\right| \le L_3 \ |t-r| \ , \quad t,r \in (0,T] \text{ uniformly in } X$$

2) The boundary values are consistent so that $\alpha(0) = 0$.

The existence of $\{u_n, s_n\}$ is easy to obtain.

Lemma 3.1. Under the hypotheses H1 the method of lines solution $\{u_n, s_n\}$ exists for $n = 1, \ldots, N$.

Proof. For given t the Riccati equation has a monotone solution which is bounded above by $\frac{1}{\sqrt{\Delta t}}$. Thus, $z_n(x)$ exists on $[0,\infty)$.

Suppose that s_{n-1} is known, then $u_{n-1} \equiv 0$ for $x \geq s_{n-1}$ and hence $Z'_n(x) \geq c$ on $[s_{n-1}, \infty)$ as long as $z_n(x) \leq 0$; because $z_n(0) \leq 0$ this implies that $z_n(s_n) = 0$ for some $s_n \in [0,\infty)$. Since $\{u_0, s_0\}$ is given the lemma follows by induction.

In order to demonstrate convergence it must be shown that the computed free boundaries $\{s_i\}_{i=0}^{N}$ can be used to define a Lipschitz continuous boundary $s(t)$ as $\Delta t \to 0$. An estimate of the form

$$|s_n - s_{n-1}| \leq K\Delta t$$

is required for this purpose which will be obtained from the Taylor expansion

$$(3.4) \quad u_n(s_{n-1}) = u_n(s_n) + u'_n(s_n)(s_{n-1}) + \frac{1}{2}u''_n(\zeta)(s_{n-1})^2 \; \zeta \in (s_{n-1}, s_n)$$

by bounding $u_n(s_{n-1})$ above and $u''_n(\zeta)$ below. We shall assume that the hypotheses H1 and H2 always apply.

Lemma 3.2. The following monotonicity conditions hold

$$u_n(x) \geq u_{n-1}(x) \quad , \quad s_n \geq s_{n-1}$$

Proof. It follows by inspection from (3.3 c and d) that $s_1 \geq S_0 \equiv 0$ and from (3.2) that u_1 is convex on $[O, S_1]$. Hence $u_1 \geq 0$. Suppose next that $u_{n-1} \geq u_{n-2}$, $s_{n-1} \geq s_{n-2}$. Then

$$(z_n - z_{n-1})' = -R(x)(z_n - z_{n-1}) + f(x, t_n) - f(x, t_{n-1}) - \frac{1}{\Delta t}(u_{n-1}(x) - u_{n-2}(x))$$
$$\leq -R(x)(z_n - z_{n-1}).$$

and $(z_n - z_{n-1})(o)$ imply that $z_n - z_{n-1} \leq 0$ and hence that $s_n \geq s_{n-1}$.

Finally it follows from the maximum principle applied to

$$(u_n - u_{n-1})'' - \frac{1}{\Delta t}(u_n - u_{n-1}) = -\frac{1}{\Delta t}(u_{n-1} - u_{n-2}) + f(x, t_n) - f(x, t_{n-1}) \leq 0,$$

$$u_n(0) - u_{n-1}(0) \leq 0$$

that $u_n - u_{n-1}$ does not have a negative minimum on $[0, s_{n-1}]$. Since by (3.2) $u_n - u_{n-1}$ is convex on $[s_{n-1}, s_n]$ the conclusion $u_n \geq u_{n-1}$ holds for $x \in [0, s_n]$.

In the Stefan and filtration problems the term $u'_n(s_n)$ does not vanish and it suffices to derive a bound like $u_n(s_{n-1}) \leq K\Delta t$ for the Taylor series (3.4) ([9], [19]). For the problem (3.2) a bound like $|u_n(s_{n-1})| \geq K\Delta t(s_n - s_{n-1})$ is necessary which will be obtained by bounding $|u'_n|$ by $K\Delta t$ on $[s_{n-1}, s_n]$.

<u>Lemma 3·3.</u> There exists a constant K such that $|u'_n - u'_{n-1}| \leq K\Delta t$ on $[0, s_n]$.

<u>Proof.</u> Let $K_1 = \max\{L_1, \sqrt{2L_2 c}\}$ and define $K_n = K_{n+1} + L_3\Delta t$. Since u_1 is convex it follows that $0 \geq u'_1(x) \geq \alpha(\Delta t) \geq -L\Delta t$ or $|u'_1 - u'_0| \leq K_1 \Delta t$. Suppose next that $|u'_{n-1} - u'_{n-2}| \leq K_{n-1} \Delta t$ on $[0, s_{n-1}]$. The maximum
principle applied to

$$(u'_n - u'_{n-1})'' - \frac{1}{\Delta t}(u'_n - u'_{n-1}) = -\frac{1}{\Delta t}(u'_{n-1} - u'_{n-2}) + \frac{\partial f}{\partial x}(x, t_n) - \frac{\partial f}{\partial x}(x, t_{n-1})$$

assures that at a relative maximum or minimum on $(0, s_{n-1})$

$$|u'_n - u'_{n-1}| \leq (K_{n-1} + L_3\Delta t)\Delta t = K_n \Delta t.$$

Since $u'_n(0) - u'_{n-1}(0) \leq 0$, $u'_n(s_{n-1}) - u'_{n-1}(s_{n-1}) \equiv u'(s_{n-1}) \leq 0$ we see that

$\max_{x \in [0, s_n]} u'_n(x) - u'_{n-1}(x) \leq K_n\Delta t$. If the minimum occurs at $x = 0$

then $\min [u'_n - n'_{n-1}(x)] \leq L_1\Delta t$; if the minimum occurs at $x = s_{n-1}$

then $u''_n(s_{n-1}) - u''_{n-1}(s_{n-1}) = \frac{1}{\Delta t} u_n(s_{n-1}) + f(x,t_n) - f(x,t_{n-1})$ **0** or

$u_n(s_{n-1}) \le L_2 \Delta t^2$. Since $u''_n \ge c$ on $| s_{n-1}, s_n |$ it follows that

$L_2\Delta t^2 \ge u_n(s_{n-1}) \ge \frac{c}{2}(s_n - s_{n-1})^2$ and $u'_n(s_{n-1}) \ge - c(s_n - s_{n-1})$

$$\ge \sqrt{2L_2 c}\ \Delta t \ge -K_n \Delta t \ .$$

Since the sequence $\{K_n\}$ is uniformly bounded by $K_0 + L_3 T$ it follows that

$$| u'_n - u'_{n-1} | \le K\Delta t \ , \quad x \in [0, s_n] \ .$$

<u>Theorem 3.1.</u> Under the hypotheses H1, H2 there exists a constant K independent of Δt such that

$$s_{n+1} - s_n \le K\Delta t \ .$$

<u>Proof'</u> By convexity $u_n(s_{n-1}) \le u'_n(s_{n-1})(s_{n-1} - s_n)$ and hence by lemma 3.3

$$u_n(s_{n-1}) \le K\Delta t \ (s_n - s_{n-1})$$

Sine $u''_n(x) \ge c$ for $x \in [s_{n-1}, s_n]$ the Taylor series (3.4) leads to

$$c\,(s_n - s_{n-1})^2 \le 2K\Delta t(s_n - s_{n-1})$$

which proves the theorem.

It follows from this theorem that $s_n \le KT$ for some constant K so that henceforth we need to consider problem (3.2) only on the interval $[0, \underline{\overline{X}}]$ for $\underline{\overline{X}} = KT$. Moreover, it follows from lemma 3.3 that $|u_n(x) - u_{n-1}(x)| \le K\Delta t\, |s_n - x|$ so that

$$\left| \frac{u_n(x) - u_{n-1}(x)}{\Delta t} \right| \le K \qquad (3.5)$$

uniformly in x and n for $x \in [0, \underline{\overline{X}}]$.

The method of lines solution $\{u_n, s_n\}$ can now be used to define approximate solutions for the free boundary problem (3.1). We shall set

(3.6) $$S_N(t) = \frac{1}{\Delta t}\{(t - t_{n-1})s_n + (t_n - t)\, s_{n-1}\}$$

$$t \in (t_{n-1}, t_n]$$

$$U_N(t) = \frac{1}{\Delta t}\{(t - t_{n-1})\, u_n(x) + (t_n - t)\, u_{n-1}(x)\}$$

It follows from Theorem 3.1 that $|S_N(t)| \leq \overline{X}$ and $S'_N(t) \leq K$ a.e..

Inequality (3.5) shows that $|U_N(x,t)| \leq K$, $\left|\frac{\partial u_N}{\partial t}(x,t)\right| \leq$ K a.e. while lemma 3.3 assures that $\left|\frac{\partial U_N}{\partial x}\right| \leq K$ uniformly with respect to N. By Ascoli's theorem there exists a subsequence $\{N_\ell\}$ such that $S_{N\ell}$ (t) and $U_{N\ell}$ (x,t) converge uniformly to Lipschitz continuous limit functions s(t) and u(x,t). In what follows we shall consider only this subsequence. $\{N_\ell\}$ and, for ease of notation, suppress the subscript ℓ .

In order to show that s(t) and u(x,t) solve the problem (3.1) we will find it convenient to introduce the concept of a weak solution for the free boundary problem. The appropriate definition is obtained in the usual manner by integrating $(u_{xx} - u_t - f)\cdot\phi$ over Ω $\{(x,t) : 0<x<s(t), t \in (0,T]\}$ subject to the given boundary conditions. Here ϕ is an arbitrary element in a set of test functions D which is chosen so as to annihilate all boundary terms in the integration for which no data are prescribed.

For the model problem (3.1) we choose for D the set of all functions defined on $[0,\underline{X}]x[0,T]$ which are twice continuously differentiable in x and continuously differentiable in t on $[0,\overline{X}]x[0,T]$ and for which $\phi(x,T) = \phi_x(0,t) \equiv 0$.

<u>Definition 3.1.</u> A weak solution of the free boundary problem (3.1) is a bounded measurable function u and a continuous function s(t) with s(0) = 0 which for arbitrary $\phi \in$ D satisfies

(3.7) $$\int_0^T \int_0^{s(t)} [\varphi_{xx} + \varphi_t)\, u - f\varphi\varphi]\, dxd - \int_0^t \varphi(0,t)\alpha(t)dt = 0.$$

As in fixed boundary problems the observation applies that a sufficiently smooth weak solution is necessarily a classical solution of (3.1). Moreover, it is readily shown that there can "be only one weak solution of (3.1).

Lemma 3.4. The weak solution of the free boundary problem (3.1) is unique.

Proof. Assume that $\{u,s\}$ and $\{\hat{u},\hat{s}\}$ are weak solutions. Since s and $\hat{s}$ are continuous we may assume that $s \leq \hat{s}$ on $[0, \hat{t}\,]$ for some $\hat{t} \in [0,T]$. Let Φ be the classical solution of the boundary value problem

$$\phi_{xx} + \phi_t = 0 \ , \qquad (x,t) \in (0, \underline{X}) x(0,T)$$

$$\phi(x, \hat{t}) = 0, \qquad 0 \leq x \leq \underline{X}$$

$$\phi(\underline{X},t) = (\hat{t}-t)^2 \ , \qquad t \in (0, \hat{t})$$

$$\phi_x(0,t) = 0 \ , \qquad t \in (0, \hat{t})$$

After, the change of variable $\tau = \hat{t} - t$ this problem is seen to be a standard boundary value problem of the first kind with smooth boundary data and hence has a smooth solution ϕ which, if extended over $[\hat{t},T]$ as the zero function is seen to belong to D. Substitution of ϕ into (3·6) for $\{\hat{u},\hat{s}\}$ and $\{u,s\}$ and subtraction lead to

$$o = -\int_0^T \int_0^{\hat{s}(t)} f\varphi\varphi dxd + \int_0^T \int_0^{s(t)} f\varphi\varphi dxd = -\int_0^T \int_{s(t)}^{\hat{s}(t)} f\varphi\varphi dxd$$

However, by the strong maximum principle $\phi > 0$ on $(0, \underline{X})\, x(0,T)$. Since $f \geq c > 0$ this implies that $s(t) = \hat{s}(t)$ for $t \in [0, \hat{t}\,]$. Hence we cannot have two distinct free boundaries. To show that $u = \hat{u}$ a.e. we choose as ϕ the solution of $\phi_{xx} + \phi_t = g(x,t)$ $\phi_x(0,t) = \phi(x,0)$ $= \phi(\underline{X},t) = 0$, where g is an arbitrary C^∞ function on $[0, \underline{X}]\, x[0,T]$. Since $s = \hat{s}$ it follows that

$$\int_0^T \int_0^{s(t)} g(x,t)\,(u - \hat{u})\, dxdt = \mathbf{0}$$

This has to hold for arbitrary g, hence $u - \hat{u} = 0$ a.e.

For given K and N let us define the Riemann sum

$$A(K,N) = \sum_{k=1}^{K} \Delta t \int_0^{S_N(t_k)} \phi(x,t_k) \frac{\partial^2 U_N}{\partial x^2}(x,t_k)\,dx$$

where $\phi \in D$, $\Delta t \frac{T}{K}$ and $t_k = k\Delta t$, and where S_N and U_N are given by (3.6).

Integration "by parts shows that

$$A(K,N) = \sum_{k=1}^{K} \Delta t \left\{ \int_0^{S_N(t_k)} \varphi_{xx}(x,t_k) U_N(x,t_k)\,dx - \varphi(0,t_k)\frac{\partial U_N}{\partial x}(0,t_k) \right\}$$

The convergence of A(K,N), uniformly with respect to K as $N \to \infty$, and for all N as $K \to \infty$, allows the conclusion that

$$\lim_{N\to\infty} A(N,N) = \int_0^T \int_0^{s(t)} \varphi_{xx}(x,t)u(x,t)\,dxdt - \int_0^T \varphi(0,t)\alpha(t)\,dt \quad .$$

Similarly, we can conclude that

$$\int_0^T \int_0^{s(t)} \varphi_t(x,t)\,u(x,t)\,dxdt = \lim_{N\to\infty} \int_0^T \int_0^{S_N(t)} \varphi_t(x,t)U_N(x,t)\,dxdt\,.$$

Integration by parts applied to the last term yields

$$\int_0^T \int_0^{S_N(t)} \phi_t U_N dxdt = -\int_0^T \int_0^{S_N(t)} \phi U_N dxdt - \int_0^T \phi(S_N(t),t)\,U_N(S_N(t),t)\,S'_N(t)\,dt\ .$$

It follows from lemma 3.3 and theorem 3.1 that $0 \le U_N\,(S_N\,(t),(t) \le K\Delta t$ so that

$$\lim_{N\to\infty} \int_0^T \phi(S_N(t),t)\,U_N\,(S_N\,(t),t)\,S'_N\,(t)dt = \mathbf{0}\,.$$

In other words,

$$\lim_{N\to\infty} \int_0^T \int_0^{S_N(t)} \phi U_{N_t} dxdt = -\int_0^T \int_0^{s(t)} \phi_t u dxdt\ .$$

We further observe that for $\phi \in D$

$$\int_0^{s_n} \phi(x,t_n)\, U_{N_t}(x,t_n)dx - \int_0^{S_N(t)} \phi(x,t)\, U_{N_t}(x,t)\, dx \le K\Delta t\, , t \in (t_{n-1}, t_n] \ .$$

Hence if we set

$$B(N) = \int_0^T \int_0^{s_n} \phi(x,t_n)\, U_{N_t}(x,t_n)\, dx \equiv \sum_{k=1}^{N} \Delta t \int_0^{s_k} \phi(x,t_k) \frac{u_k(x) - u_{k-1}(x)}{\Delta t}\, dx$$

it follows that

$$\lim_{N \to \infty} B(N) \equiv -\int_0^T \int_0^{s(t)} \phi_t\, u dx dt \ .$$

Finally, if

$$C(N) = \sum_{k=1}^{N} \Delta t \int_0^{s_k} f(x,t_k)\, \phi(x,t_k)\, dx$$

then

$$\lim_{N \to \infty} C(N) = \int_0^T \int_0^{s(t)} f(x,t)\, \phi(x,t)\, dx \ .$$

These relationships will now he used to prove the main result of this paper,,

Theorem 3.2. Under the hypotheses H1, H2 the method of lines solution defined by (3.6) converges uniformly to a classical solution of the free boundary problem (3.1).

Proof. Let us consider first the subsequence $\{U_N , S_N\}$ whose uniform convergence is assured by Ascoli's theorem. It follows from equation (3.2) that

$$A(N,N) - B(N) - C(N) \equiv \sum_{k=1}^{N} \Delta t \int_0^{s_k} \phi(x,t_k)[u_k'' - \frac{1}{\Delta t}(u_k - u_{k-1}) - f(x,t_k)] = \mathbf{0} \ .$$

and consider Instead

$$w_{xx} - w_t = f_\varepsilon (x,t), \quad w_x (0,t) = \alpha_\varepsilon (t)$$

(4.1) $$w(s(t),t) = w_x(s(t),t) = 0, \quad s(0) = 0 \; .$$

It is apparent that for fixed ε the functions f and a satisfy the hypotheses H1 and H2. Hence for $\varepsilon > 0$ the solution w of (4.1) exists and is unique.

Problem (4.1) was solved numerically with the invariant imbedding algorithm of section 2. The Riccati equation (2.9) has the analytical solution

$$R(x) = \frac{1}{\sqrt{\Delta t}} \tanh \frac{x}{\sqrt{\Delta t}} ,$$

while the equations (2.10) and (2.12) were integrated numerically with the trazezoidal rule. The free boundary s_n at the nth time level is a root of $z_n(x) = 0$ and was found by linear interpolation between successive mesh points for which z_n changed its algebraic sign.

Since the case $\varepsilon = 0$ is really of interest, a sequence $\{w^\varepsilon (x,t), s^\varepsilon (t)\}$ was computed where $\varepsilon = \Delta t$ (i.e. the singularity of the data was ignored). Although the computation showed some sensitivity to the space and time step (thought to be largely due to the limited capability of the BASIC compiler) the results converged as $\Delta t, \Delta x \to 0$. Table 1 lists the location of the free boundary s(t) at selected times obtained for (4.1), as well as the corresponding values given in [17].

Table 1 - Location of the Free Boundary s(t) of Problem (4.1)

t	s(t)	s(t) in [17]
.05	.0025	——
.1	.0100	.0099943
.2	.0398	.0398054
.3	.0886	.0885481
.4	.1543	.1542611
.5	.2343	.2341754
.8	.5317	.5307290
1.0	.7565	.7544931
1.4	1.2289	1.223219
1.8	1·7059	1.693958
2.0	1.9420	1.941728

The time and space steps were $\Delta t = 10^{-2}$ and $\Delta x = 2 \times 10^{-3}$ at which, point the computed solution appeared to have settled down since further mesh refinements did not change our results.

It is apprent that the method of lines approach for the formulation in [17] and for (4.1) yield consistent results. However, the method of lines solution technique of this exposition is tied neither to the heat equation nor the specific form of the "boundary data on the fixed and free boundary.

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