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A Third Order Accurate Discontinuous Finite Element Method for the One-Dimensional Stefan Problem

R. BONNEROT AND P. JAMET

Commissariat a l'Énergie Atomique, Centre d'Études de Limeil, Service de Mathématiques Appliquées, B.P. 27, 94190 Villeneuve-Saint-Georges, France

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A third order accurate method is proposed for the numerical solution of the one-dimensional Stefan problem. It provides approximations which are continuous with respect to the space-variable x, but which admit discontinuities with respect to the time variable t at each time step. The discretization is based on biquadratic finite elements in the plane (x, t). This method is specially appropriate for the computation of solutions which admit singularities at the initial time or on the boundary. Numerical experiments are described.

1. INTRODUCTION

Many methods have been proposed for the numerical solution of the one-dimensional Stefan problem [1, 4, 5, 6, 9, 10, 11, 12, 13, 14]. Some more general methods for the multi-dimensional Stefan problem can also be applied to the one-dimensional case (see the references contained in [2]). Most of these methods have an accuracy of the first order or less; only two of them (to the authors' knowledge) are of order 2 [1, 6]. In this paper, we describe and experiment a method of *order* 3. The order of the method is not established by a mathematical proof, but is verified by numerical experiments.

This method is based on space-time finite elements like the method that we have proposed in [1]; but, these elements are of a higher degree (biquadratic instead of bilinear). There is also an essential difference between these two methods: the method of [1] yields approximations which are continuous; on the contrary, the present method yields approximations which are continuous with respect to the space variable, but which admit discontinuities with respect to the time variable at each time step. We will call "continuous Q_1 method" the method of [1] and "time-discontinuous Q_2 method" the method of this paper.

In addition to its accuracy, the time-discontinuous Q_2 method has another advantage: it is specially well suited to the *computation* of *solutions with singularities* (discontinuous initial function, discontinuous boundary values, infinite speed of propagation of the free boundary at the initial time); the singularities generate no irregularity of the computed values at later times and the accuracy remains very satisfactory.

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Let us remark that one of the authors has presented a general mathematical theory of time-discontinuous Galerkin-type methods for parabolic equations in a variable domain [8]. However, no numerical experiments had been performed and, moreover, this theory assumes that the moving boundary is given, which excludes the case of free boundary problems like the Stefan problem.

Let us also remark that we describe our method for the one-phase Stefan problem, but it can also be applied to the case of several phases, in particular to the case of phases which can appear or disappear (see the remark of Section 3.2b).

In Section 2 of this paper, we describe the problem that we want to solve. In Section 3, we assume that the free boundary is known and we describe a method for solving the heat equation in a given variable domain. In Section 4, we describe how we compute the free boundary. Section 5 is devoted to numerical experiments. Finally, Appendix 1 gives the explicit expressions of the coefficients of the discrete equations and Appendix 2 contains additional comments related to questions of the referees.

2. Description of the Problem

Let x be the space variable and t the time variable. Let be given three positive numbers a°, T and c, a positive function $u^\circ(x)$ defined in the interval $0 \leqslant x \leqslant a^\circ$ and a positive function $g(t)$ defined in the interval $0 < t \leqslant T$.

Let $\mathscr{R} = \{(x, t);\ 0 < x < a(t),\ 0 < t < T\}$, where $a(t)$ is an unknown function. The problem to be solved is the following: find a positive function $u(x, t)$ defined on $\bar{\mathscr{R}}$(closure of $\mathscr{R}$) and a positive function $a(t)$ defined for $0 \leqslant t \leqslant T$ such that

$$\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} = 0 \qquad \text{in } \mathscr{R}, \tag{2.1}$$

$$u(x, 0) = u^\circ(x) \qquad \text{for } 0 \leqslant x \leqslant a^\circ, \tag{2.2}$$

$$u(0, t) = g(t) \qquad \text{for } 0 < t \leqslant T, \tag{2.3}$$

$$u(a(t), t) = 0 \qquad \text{for } 0 < t \leqslant T, \tag{2.4}$$

$$\frac{da}{dt} = -c \frac{\partial u}{\partial x}(a(t), t) \qquad \text{for } 0 < t < T, \tag{2.5}$$

$$a(0) = a^\circ. \tag{2.6}$$

The partial differential equation (2.1) is the heat equation; the equation (2.2) is the initial condition; the equations (2.3) and (2.4) are the boundary conditions; the equation (2.5) gives the speed of propagation of the free boundary and the equation (2.6) gives its initial position.

These equations represent the melting of a slab of ice. The water lies in the region $0 < x < a(t)$ at the time t and the ice in the region $x > a(t)$; u is the temperature of the water, the temperature of the ice is equal to zero.

Let us replace the partial differential equation (2.1) by an integral relation. Let θ_1 and θ_2 be two arbitrary numbers such that $0 \leqslant \theta_1 < \theta_2 \leqslant T$ and let $G = G(\theta_1, \theta_2)$ be the intersection of the domain $\mathscr{R}$ with the strip $\theta_1 < t < \theta_2$, i.e. $G = \{(x, t);\ 0 < x < a(t),\ \theta_1 < t < \theta_2\}$. Let $\Phi(G)$ be the space of all functions φ which are defined and continuous on $\bar{G}$, which admit bounded first order derivatives in G and which vanish for $x = 0$ and $x = a(t)$ for all t. Let $\Omega(\theta_s) = \{(x, t);\ 0 < x < a(t),\ t = \theta_s\}$, with $s = 1$ or 2 (see Figure 1). Then, if u is a solution of the partial differential equation (2.1), it satisfies

$$A_G(u, \varphi) = 0, \qquad \text{for all} \quad \varphi \in \Phi(G), \tag{2.7}$$

with

$$A_G(u, \varphi) = -\iint_G u \frac{\partial \varphi}{\partial t}\, dx\, dt + \iint_G \frac{\partial u}{\partial x} \frac{\partial \varphi}{\partial x}\, dx\, dt + \int_{\Omega(\theta_2)} u\varphi\, dx - \int_{\Omega(\theta_1)} u\varphi\, dx \tag{2.8}$$

Let us remark that the bilinear form $A_G(u, \varphi)$ does not involve the derivative $\partial u/\partial t$; it is defined even for functions u which admit discontinuities with respect to t. Thus, it will be possible to use the integral relation (2.7) to define approximations which are discontinuous with respect to t.

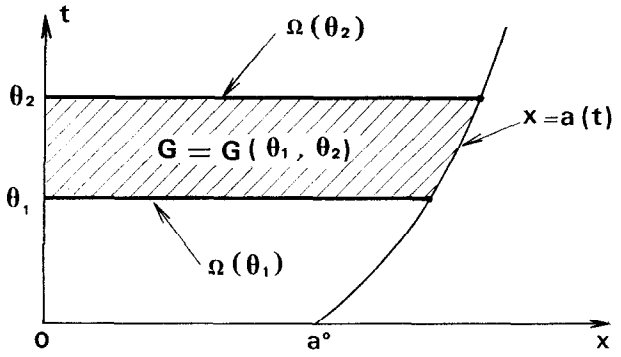

FIG. 1. The subdomain $G = G(\theta_1, \theta_2)$.

3. TIME-DISCONTINUOUS APPROXIMATIONS FOR THE HEAT EQUATION

In this section, we assume that the curve $x = a(t)$ is known and we describe a method for solving the heat equation in a variable domain (problem (2.1)–(2.4)). First, we will give the basic principle of time-discontinuous approximations as described in [8]; then we will specify the particular method that we have chosen.

3.1. *Generalities*

Let $\{t^n;\ 0 \leqslant n \leqslant N\}$ be a finite sequence of real numbers such that $t^\circ = 0$, $t^n < t^{n+1}$, $t^N = T$. Let $G^n = G(t^n, t^{n+1}) = \{(x, t);\ 0 < x < a(t),\ t^n < t < t^{n+1}\}$ and $\bar{G}^n = \{(x, t);\ 0 \leqslant x \leqslant a(t),\ t^n < t \leqslant t^{n+1}\}$, for $0 \leqslant n \leqslant N - 1$. We have $\bar{G}^n = \bar{G}^n - \bar{\Omega}^n$, where $\bar{G}^n$ is the closure of G^n and $\bar{\Omega}^n = \bar{\Omega}(t^n)$ is the portion of the boundary of G^n which lies on the line $t = t^n$.

For each n, let $\Phi_h{}^n$ be a finite dimensional subspace of $\Phi(G^n)$. Let W_h be the space of all functions w_h which are defined on $\bar{\mathscr{R}}$ and which coincide with a function of $\Phi_h{}^n$ on each $\bar{G}^n$; note that the functions w_h are continuous on each $\bar{G}^n$, i.e. for $t^n < t \leqslant t^{n+1}$, but they admit discontinuities with respect to t at each $t = t^n$, $0 \leqslant n \leqslant N - 1$. Let V_h be a set of functions which is affine to the space W_h; each $v_h \in V_h$ is of the form $v_h = v_{0,h} + w_h$, with $w_h \in W_h$, where $v_{0,h}$ is a certain continuous function defined on $\bar{\mathscr{R}}$ which vanishes for $x = a(t)$ and which satisfies the boundary condition (2.3) in a certain approximate way. Then, we approximate the problem (2.1)–(2.4) by the following problem obtained by discretizing the integral relation (2.7).

Discrete problem: *Find a function* $u_h \in V_h$ *such that* $u_h(x, 0) = u^\circ(x)$ *for* $0 \leqslant x \leqslant a^\circ$ *and*

$$A_{G^n}(u_h, \varphi_h) = 0, \tag{3.1}$$

for all $\varphi_h \in \Phi_h{}^n$ *and* $0 \leqslant n \leqslant N - 1$.

For each n, the relation (3.1) involves the known values of u_h at the time t^n (through the fourth integral of (2.8)) and the unknown values of u_h for $t^n < t \leqslant t^{n+1}$ (through the first three integrals of (2.8)). If we write this relation for a set of functions φ_h which is a base of the space $\Phi_h{}^n$ and if we write the function u_h in the strip $t^n < t \leqslant t^{n+1}$ as a linear combination of $v_{0,h}$ and of the functions φ_h, we get a linear system of algebraic equations with a square matrix.

The following result is proved in [8]: the problem (3.1) admits a *unique* solution u_h which is determined by solving a linear system of algebraic equations at each time step; moreover, the method is *unconditionally stable* in L^2 (for any choice of the times t^n and any choice of the discrete spaces $\Phi_h{}^n$).

3.2. *Choice of the Discrete Spaces*

Now, we will make a specific choice for the discrete spaces $\Phi_h{}^n$ and V_h. First, we recall the definition of finite elements "of type Q_2" and introduce some notations (for more details, see [3, 15]).

3.2.a. *Finite Elements of Type* Q_2

Let $\{\xi, \eta\}$ be a system of orthonormal coordinates in a fixed arbitrary plane and let us consider the unit square $\hat{K} = \{(\xi, \eta);\ 0 \leqslant \xi \leqslant 1,\ 0 \leqslant \eta \leqslant 1\}$. Let $\hat{M} = (\xi, \eta)$ denote an arbitrary point of $\hat{K}$ and let $\hat{Q}_2$ denote the space of all functions $\hat{\varphi}(\hat{M}) = \hat{\varphi}(\xi, \eta)$ defined on $\hat{K}$ which are polynomials of degree $\leqslant 2$ with respect to *each* of the variables ξ and η *separately*.

Let $\hat{\Sigma}$ be the set of the nine points $\hat{P} \in \hat{K}$ such that each of their coordinates is equal to 0, $\frac{1}{2}$ or 1. Any function of $\hat{Q}_2$ is uniquely determined by its values on $\hat{\Sigma}$. To each point $\hat{P} \in \hat{\Sigma}$, there corresponds a function $\hat{\varphi}(\hat{M}; \hat{P})$ such that

$$\hat{\varphi}(\hat{M}; \hat{P}) = \begin{cases} 1 & \text{if } \hat{M} = \hat{P}, \\ 0 & \text{if } \hat{M} \in \hat{\Sigma} - \{\hat{P}\}. \end{cases} \tag{3.2}$$

The set $\{\hat{K}, \hat{Q}_2, \hat{\Sigma}\}$ defines a reference finite element and the functions $\hat{\varphi}(\hat{M}; \hat{P})$ are its "shape functions".

Now, let Σ be a set of nine points in the plane (x, t) and let $\mathscr{F}$ be a bijective mapping of $\hat{\Sigma}$ onto Σ. The mapping $\mathscr{F}$ can be extended to the whole square $\hat{K}$ by means of the formula

$$\mathscr{F}(\hat{M}) = \sum_{\hat{P} \in \hat{\Sigma}} \hat{\varphi}(\hat{M}; \hat{P})\, \mathscr{F}(\hat{P}), \qquad \text{for all} \quad \hat{M} \in \hat{K}. \tag{3.3}$$

Let us denote $M = \mathscr{F}(\hat{M})$, $P = \mathscr{F}(\hat{P})$, $K = \mathscr{F}(\hat{K})$ and assume that the extended mapping $\mathscr{F}$ is bijective from $\hat{K}$ onto K. Then, to each function $\hat{\varphi}$ defined on $\hat{K}$, there corresponds a function φ defined on K and conversely, by means of the formula

$$\varphi(M) = \hat{\varphi}(\hat{M}) = \hat{\varphi}(\mathscr{F}^{-1}(M)),$$

where $\mathscr{F}^{-1}$ is the inverse mapping of $\mathscr{F}$.

Let $Q_2 = Q_2(K)$ denote the space of all functions φ such that the corresponding function $\hat{\varphi} \in \hat{Q}_2$. Any function of Q_2 is uniquely determined by its values at the points of Σ. The set $\{K, Q_2, \Sigma\}$ defines a finite element "of type Q_2"; the points of Σ are called the *nodes*.

3.2.b. *The Discrete Spaces V_h and ${\Phi_h}^n$*

We will partition each subdomain $G^n \subset \mathscr{R}$ into elements K which are identical to the element described in 3.2.a. Let us consider an arbitrary subdomain G^n. Let μ and ν be two indices which can take the values 0, $\frac{1}{2}$ and 1; let $t^{n+\nu} = (1 - \nu)\, t^n + \nu t^{n+1}$. For each $t = t^{n+\nu}$, let there be a finite family of points $P_{i+\mu}^{n+\nu} = (x_{i+\mu}^{n+\nu}, t^{n+\nu}) \in \bar{G}^n$, where i is an integer, $0 \leqslant i \leqslant I - 1$, and $x_0^{n+\nu} = 0$, $x_i^{n+\nu} = x_{i+0}^{n+\nu} < x_{i+1}^{n+\nu}$, $x_{i+1/2}^{n+\nu} = (x_i^{n+\nu} + x_{i+1}^{n+\nu})/2$, $x_I^{n+\nu} = a(t^{n+\nu})$. For each index i, one defines a finite element $K = K_i^n$ as follows.

Let $\hat{P}_\mu{}^\nu \in \hat{\Sigma}$ denote the point whose coordinates are $\xi = \mu$, $\eta = \nu$. Let be the correspondance $\hat{P}_\mu{}^\nu \to P_{i+\mu}^{n+\nu}$. There follows a mapping $\mathscr{F}$ defined on $\hat{K}$ and an element $K = \mathscr{F}(\hat{K})$, as in Section 3.2.a. The two sides $\xi = 0$ and $\xi = 1$ of the square $\hat{K}$ are transformed into two arcs of parabolas; the mapping $\mathscr{F}$ is bijective if these two arcs do not intersect. Then, the space $Q_2(K)$ is defined as in paragraph 3.2.a (Fig. 2). The boundaries of two adjacent elements K_i^n and K_{i+1}^n contain a common arc of parabola.

Let $\bar{G}_h{}^n$ be the union of all the elements K_i^n, for $0 \leqslant i \leqslant I - 1$; the set $\bar{G}_h{}^n$ is in general different from the set $\bar{G}^n$ because the portion of the boundary of G^n which coincides with the curve $x = a(t)$ is replaced by an arc of parabola. Let $Y_h{}^n$ be the space of all functions defined and continuous on $\bar{G}_h{}^n$ whose restriction to each

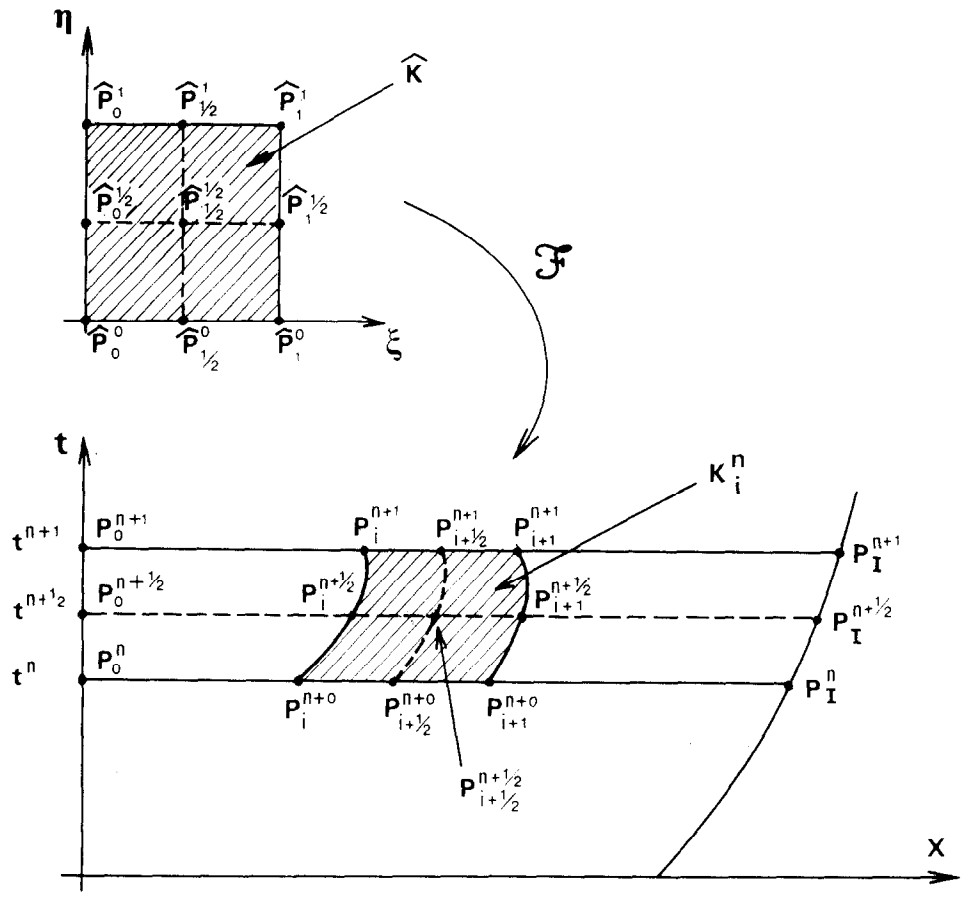

FIG. 2. The correspondence between the reference element $\hat{K}$ and an element $K = K_i^n$.

element K belongs to $Q_2(K)$ and which vanish at the points $P_I^{n+\nu}$ for $\nu = 0, \frac{1}{2}$ and 1 (therefore they vanish on the whole arc of parabola which approximates the curve $x = a(t)$ for $t^n \leqslant t \leqslant t^{n+1}$). Let $\tilde{G}_h^n = \bar{G}_h^n - \bar{\Omega}^n$ and $\bar{\mathscr{R}}_h = \{\bigcup \bar{G}_h^n;\ 0 \leqslant n \leqslant N-1\}$. One defines:

Φ_h^n = set of all functions $\varphi_h \in Y_h^n$ which vanish for $x = 0$. V_h = set of all functions v_h defined on $\bar{\mathscr{R}}_h$, whose restriction to each $\tilde{G}_h^n$ coincides with a function of Y_h^n and which satisfy the boundary condition (2.3) for $t = t^{n+\nu}$, $0 \leqslant n \leqslant N-1$, $\nu = 0, \frac{1}{2}$ or 1.

Remark. The discretization of the domain G^n at each time step can be completely independent of the discretization of the domain G^{n-1}. For example, the nodes P_i^{n+0} of the elements K_i^n can be different from the nodes P_i^n of the elements K_i^{n-1}; the number of elements K_i^n for each n can also depend on n (which can be interesting for the multiphase Stefan problem with appearing and disappearing phases). However, in this paper, we will simply take $P_i^{n+0} = P_i^n$.

3.3. *Structure of the System of Discrete Equations*

Let V_h be the space of functions defined in Section 3.2. For each $v_h \in V_h$, let

$$v_{i+\mu}^n = v_h(P_{i+\mu}^n),$$

$$v_{i+\mu}^{n+0} = \lim\{v_h(M);\ M \in G^n,\ M \to P_{i+\mu}^n\},$$

$$v_{i+\mu}^{n+1/2} = v_h(P_{i+\mu}^{n+1/2}).$$

The restriction to the set $\tilde{G}_h{}^n$ of an arbitrary function $v_h \in V_h$ is uniquely determined by the values of $v_{i+\mu}^{n+\nu}$ for $\frac{1}{2} \leqslant i + \mu \leqslant I - \frac{1}{2}$ and $\nu = 0$, $\frac{1}{2}$ and 1. Hence, for each n, the system of discrete equations (3.1) can be written in terms of the unknowns $u_{i+\mu}^{n+\nu}$ for $\frac{1}{2} \leqslant i + \mu \leqslant I - \frac{1}{2}$ and $\nu = 0$, $\frac{1}{2}$ and 1. Let us numerate these unknowns in the following order: $u_{1/2}^n, \ldots, u_i^n, u_i^{n+1/2}, u_i^{n+1}, u_{i+1/2}^n, u_{i+1/2}^{n+1/2}, u_{i+1/2}^{n+1}, u_{i+1}^n, \ldots, u_{I-1/2}^{n+1}$. Let $\mathscr{S}^n$ denote the set of corresponding nodes $P_{i+\mu}^{n+\nu}$ numerated in the same order. For each $P \in \mathscr{S}^n$, let $\varphi_{h,P}$ be the function in the space $\Phi_h{}^n$ such that

$$\varphi_{h,P}(M) = \begin{cases} 1, & \text{if } M = P, \\ 0, & \text{if } M \in \mathscr{S}^n - \{P\}. \end{cases} \tag{3.4}$$

The set of all the functions $\varphi_{h,P}$ is a base of $\Phi_h{}^n$.

Let us take φ_h in (3.1) successively equal to each of the functions $\varphi_{h,P}$ with $P \in \mathscr{S}^n$. Then, it is easy to check by looking only at the support of the functions $\varphi_{h,P}$, that the matrix B of the resulting system of linear algebraic equations has a block pentadiagonal structure of the form represented on Fig. 3. Each block is a square 3×3 matrix denoted $B_j{}^k$. One has $B_j{}^k \neq 0$, only if

$$k = \begin{cases} j \\ j \pm 1 \\ j \pm 2 \text{ and } j \text{ even} \end{cases}$$

3.4. *Introduction of Numerical quadrature Formulae*

Instead of an exact computation of the integrals involved in the left handside member of (3.1), we will use numerical quadrature formulae. The advantage is to simplify the coefficients of the system of equations (3.1).

The integrals with respect to x are approximated by using the Simpson formula on each of the segments $[P_i^{n+\nu}, P_{i+1}^{n+\nu}]$ i.e.

$$\int_{P_i^{n+\nu}}^{P_{i+1}^{n+\nu}} \psi\, dx \sim J_i^{n+\nu}(\psi) = \tfrac{1}{6}(x_{i+1}^{n+\nu} - x_i^{n+\nu})(\psi_i^{n+\nu} + 4\psi_{i+1/2}^{n+\nu} + \psi_{i+1}^{n+\nu}),$$

where ψ is an arbitrary function.

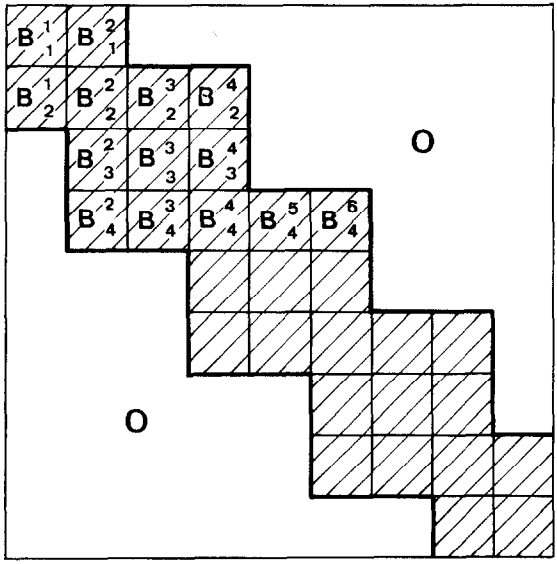

FIG. 3. The structure of the matrix B of the system of discrete equations.

The integrals with respect to x and t are approximated by using the Simpson formula, first with respect to x, then with respect to t, in each of the elements K_i^n, i.e.

$$\iint_{K_i^n} \psi \, dx \, dt \sim \tfrac{1}{6}(t^{n+1} - t^n)(J_i^{n+0}(\psi) + 4J_i^{n+1/2}(\psi) + J_i^{n+1}(\psi))$$

(see Appendix 2).

Using these quadrature formulae does not change the structure of the matrix B of the system (3.1), but the submatrices B_j^k become *diagonal* for $k \neq j$. This property is easy to check by noticing that, for any $P \in \mathscr{S}^n$, the points $P' \in \mathscr{S}^n$ at which the function $\varphi_{h,P}$ vanishes together with its first order derivatives are not involved in the equation corresponding to P.

Explicit formulae for computing the coefficients of the equations (3.1) are given in the appendix at the end of this paper.

3.5. *Approximation of the Flux at the Boundary*

The value of the derivative $\partial u/\partial x$ for $x = a(t)$ represents the heat flux through the moving boundary. Let us denote it by $Du(t)$. It can be approximated by the corresponding derivative of the approximate solution u_h. But, we prefer to use the following method which permits to gain one order of accuracy.

Let n be arbitrary and $\nu = 0, \frac{1}{2}$ or 1. Denote by $\tilde{u}_h^{n+\nu}$ the function of the variable x obtained by cubic interpolation of the values $u_{i+\mu}^{n+\nu}$ at the nodes $P_{i+\mu}^{n+\nu}$ for $i + \mu = I - \frac{3}{2}, I - 1, I - \frac{1}{2}$ and I. Let $(Du)_h^{n+\nu}$ denote the value of the x-derivative of $\tilde{u}_h^{n+\nu}$ at

the end-point $P_l^{n+\nu}$. Then, we approximate $Du(t)$ in the interval $t^n < t \leqslant t^{n+1}$ by the function $(Du)_h(t)$ obtained by quadratic interpolation of the three values of $(Du)_h^{n+\nu}$ for $\nu = 0, \frac{1}{2}$ and 1.

4. Computation of the Free Boundary

In the preceding section, we have assumed that the moving boundary was known. Now, we will consider the complete problem (2.1)–(2.6) and describe a method for computing the free boundary.

We approximate the curve $x = a(t)$ by a continuous curve $x = a_h(t)$ whose restriction to each interval $t^n \leqslant t \leqslant t^{n+1}$ is an arc of parabola $x = q_2^{(n)}(t)$, where $q_2^{(n)}(t)$ denotes a polynomial of degree $\leqslant 2$ with respect to the variable t. Let $a^{n+\nu} = a_h(t^{n+\nu})$. At each time step, the values of $a^{n+1/2}$ and a^{n+1} are computed by means of the following formula which is an analogue of the relation obtained by integrating (2.6) with respect to t:

$$a^{n+\nu} = a^n - c \int_{t^n}^{t^{n+\nu}} (Du)_h(t)\, dt, \tag{4.1}$$

for $\nu = \frac{1}{2}$ and 1, where $(Du)_h(t)$ denotes the approximation of $Du(t)$ obtained by the method of paragraph 3.5.

This formula is implicit since the values of $(Du)_h(t)$ in the interval $t^n < t \leqslant t^{n+1}$ depend on the computed values of u_h in the strip $t^n < t \leqslant t^{n+1}$ which in turn depend on $a^{n+1/2}$ and a^{n+1}. We will use the following iterative procedure.

The equations (3.1) together with the method of paragraph 3.5 for approximating $Du(t)$ define a function

$$(a^{n+1/2}, a^{n+1}) \to u_h(x, t) \to (Du)_h(t) \qquad \text{for} \quad t^n < t \leqslant t^{n+1}.$$

The equation (4.1) defines a function

$$\{Du_h(t);\ t^n < t \leqslant t^{n+1}\} \to (a^{n+1/2}, a^{n+1}).$$

We will perform the iterations:

$$(a^{n+1/2,l}, a^{n+1,l}) \to (u_h(x, t))^l \to ((Du)_h(t))^l, \tag{4.2}$$

$$((Du)_h(t))^l \to (a^{n+1/2,l+1}, a^{n+1,l+1}), \tag{4.3}$$

where l denotes the iteration index.

To start the iterations, we take

$$a^{n+\nu,0} = q_2^{(n-1)}(t^{n+\nu}), \qquad \text{for} \quad \nu = 1/2 \text{ and } 1, \text{ and } n \geqslant 1, \tag{4.4}$$

i.e. we use the quadratic extrapolation of the values a^{n-1}, $a^{n-1/2}$ and a^n.

For $n = 0$, we take $a^{1,0} = a^{1/2,0} = a^0$.

5. Numerical Experiments

First, we compute a smooth solution of problem (2.1)–(2.6) and determine the order of convergence of the method; we consider the same test-problem as in [1]. Also, we compare the results with those obtained in [1] and we check the stability of the method by increasing the time steps and the speed of propagation of the free boundary.

Then, we compute solutions which admit singularities. We consider two cases: in problem 2, the initial function is discontinuous at a point inside the interval $(0, a^\circ)$; in problem 3, the initial function does not vanish at the end-point $x = a^\circ$ and therefore the initial speed of propagation of the free boundary is infinite.

In all this section, we use a constant time step $\Delta t = t^n - t^{n-1}$ and the nodes are equally spaced in each interval $(0, a^{n+\nu})$, i.e.

$$x_i^{n+\nu} = ia^{n+\nu}/I$$

We denote by h the initial space step, i.e.

$$h = a^\circ/I.$$

5.1. *Problem* 1 (Smooth Solution)

We want to solve the problem (2.1)–(2.6) with $c = 1$, $a(0) = 1$,

$$u^\circ(x) = (1 - x)^2, \qquad \text{for} \quad 0 \leqslant x \leqslant 1,$$
$$g(t) = 1, \qquad \text{for} \quad t > 0.$$

5.1.a. *Order of Convergence*

Let us choose the time step $\Delta t = \lambda h$, where λ is a constant. Let $z = z(u)$ be a certain functional of the solution u, for example the value of u at a given point (x, t) or the value of a derivative of u at a given point or the value of $a(t)$ for a given time t. Let z_h be the approximate value of z computed with the initial mesh-size h. We want to determine a positive number p such that

$$z_h - z \simeq Ch^p, \tag{5.1}$$

for h small, where C is a constant.

Let h_1, h_2 and h_3 be three values of h with $h_1 > h_2 > h_3$ and assume that (5.1) holds. Then,

$$\frac{z_{h_1} - z_{h_3}}{z_{h_2} - z_{h_3}} \simeq \frac{(h_1)^p - (h_3)^p}{(h_2)^p - (h_3)^p} = \frac{(r_1)^p - 1}{(r_2)^p - 1} \tag{5.2}$$

with $r_1 = h_1/h_3$ and $r_2 = h_2/h_3$.

Let $f(p) = ((r_1)^p - 1)/((r_2)^p - 1)$. This function increases from 1 to $+\infty$ as p increases from $-\infty$ to $+\infty$ and we have

$$f(0) = \frac{\log r_1}{\log r_2} = \frac{\log h_1 - \log h_3}{\log h_2 - \log h_3} \qquad \text{(see appendix 2).}$$

It follows that, if

$$\frac{z_{h_1} - z_{h_3}}{z_{h_2} - z_{h_3}} > \frac{\log h_1 - \log h_3}{\log h_2 - \log h_3}, \tag{5.3}$$

one can determine a unique positive number $p = p(h_1, h_2, h_3)$ such that

$$(z_{h_1} - z_{h_3})/(z_{h_2} - z_{h_3}) = f(p).$$

The method is of order p^*, for the computation of the functional z, if the condition (5.3) is satisfied for all sufficiently small h_1, h_2 and h_3 and if the corresponding number $p = p(h_1, h_2, h_3)$ converges to p^* as h_1, h_2 and h_3 decrease.

This procedure to determine the order oaccuracy is more general than the procedure used in [1] since h_1, h_2 and h_3 can be chosen arbitrarily whereas the condition $h_1/h_2 = h_2/h_3$ was required in [1]. It permits one to choose a sequence of values of h which decreases more slowly than the sequence used in [1].[1]

We have performed the computations until the time $T = 1$ with $\Delta t = h = 1/I$ for values of I which are multiples of 8. Tables I and II show the convergence of the method for the following functionals $z(u)$.

TABLE I

Problem 1. Convergence for the Value of u at the Point $x = 1$, $t = 1$, with $\Delta t = h = 1/I$.

I	$\tilde{u}_h$	p
8	0.3124 | 4739	
16	0.3124 6 | 431	
24	0.3124 6 | 595	3.05
32	0.3124 6 6 | 35	3.01

[1] The advantage of this procedure has been mentioned to us by Professor R. DeVogelaere, University of California, Berkeley (private communication).

TABLE II

Problem 1. Convergence for the Position of the Free Boundary at the Time $t = 1$

I	a_h	p
8	1. 5 6 0 4 4 4 2 8	
16	1. 5 6 0 4 9 0 4 5	
24	1. 5 6 0 4 9 4 8 2	3. 1 0
32	1. 5 6 0 4 9 5 8 6	3. 0 4
40	1. 5 6 0 4 9 6 2 3	3. 0 3

Table I: value of $u(x, t)$ for $x = 1$ and $t = 1$.

Table II: value of $a(t)$ for $t = 1$.

Moreover, Table III gives the value of the discontinuity $u_h^{n+0} - u_h^n$ at the node $P_{I/2}^{N-1}$ located at the midpoint of the interval $(0, a(t))$ for $t = 1 - \Delta t$.

The first column of these tables gives the values of $I = 1/h$, the second one gives the computed values z_h of the functional $z(u)$ and the third one gives the values of p computed for the last three values of h. Let us remark that, on Table I, the value of u at the point $M = (x, t) = (1, 1)$ is not approximated by $u_h(M)$, but by an improved value $\tilde{u}_h(M)$ obtained by cubic interpolation of u_h with respect to x at the four neighbour nodes (two on each side of M). The introduction of cubic interpolation does not improve the accuracy of the method, but yields a convergent sequence for the computed values of p; otherwise, these values have a randomlike variation which is related to the distance of the point M to the closest mesh-point. The same phenomenon is described in [1].

TABLE III

Problem 1. Values of the Jump $d_h = u_h^{n+0} - u_h^n$ at the Middle Node for $t = 1 - \Delta t$[a]

I	$10^5 \cdot d_h$	p
8	0. 5 9 5 2	
16	0. 0 6 8 4	
24	0. 0 1 9 6	3. 1 3
32	0. 0 0 8 1	3. 0 8
40	0. 0 0 4 1	3. 0 6

[a] The values of d_h have been multiplied by 10^5.

Tables I and II show that *the method is of order* $p = 3$ (for the values of $u(x, t)$ and $a(t)$) and Table III shows that *the discontinuities are also of order* 3.

At each time step we have used the Gauss method to solve the linear system of algebraic equations (3.1) and we have performed the iterations on the position of the free boundary until the relative difference between two successive iterated values becomes inferior to $\epsilon = 10^{-8}$, i.e.

$$| a^{n+\nu,l+1} - a^{n+\nu,l} | / a^{n+\nu,l} < \epsilon, \qquad \text{for} \quad \nu = \tfrac{1}{2} \quad \text{and} \quad 1.$$

For $I = 40$, the average number of iterations at each time step is equal to 3.5 and the total computation time until $t = 1$ is equal to 27 seconds on a computer *CDC* 7600; Tables I and II show that the relative errors on the values of u and on the position of the free boundary are inferior to 10^{-6}.

If we seek only an accuracy of the order of 10^{-4}, it is sufficient to take $I = 8$ and $\epsilon = 10^{-5}$. Then, the relative errors on $u(1, 1)$ and $a(1)$ are respectively equal to 0.6×10^{-4} and 0.3×10^{-4}; the average number of iterations is equal to 3.75 and the computation time is equal to 1.04 second.

Let us remark however, that the program has been written without trying to minimize the computation time.

TABLE IV

Problem 1. Value of u at the Point $x = 1$, $t = 1$: Comparison of Two Methods

I	Method I	Method II
8	0.312 3557 64	0.312 4473 9
16	0.312 4097	0.312 4631
32	0.312 4565	0.312 4663 5
40		0.312 4663 9
64	0.312 4613 2	
128	0.312 4652 7	
256	0.312 4662 9	
512	0.312 4665 5	

[a] Method I: Continuous Q_1 method of [1]. Method II: Time-discontinuous Q_2 method (this paper).

5.1.b. *Comparison with the Continuous Q_1 Method*

Tables IV and V permit to compare the accuracy of the time-discontinuous Q_2 method (method 2) with the continuous Q_1 method (method 1). Table IV gives the computed values of $u(x, t)$ for $x = 1$ and $t = 1$ and Table V gives the computed values of $a(t)$ for $t = 1$.

TABLE V

Problem 1. Position of the Free Boundary: Comparison of Two Methods

I	Method I	Method II
8	1.5 5 9 6 4 8 1 7	1.5 6 0 4 4 4 2 8
16	1.5 6 0 2 0 6 4 0	1.5 6 0 4 9 0 4 5
32	1.5 6 0 4 1 5 0 3	1.5 6 0 4 9 5 8 6
40		1.5 6 0 4 9 6 2 3
64	1.5 6 0 4 7 5 1 4	
128	1.5 6 0 4 9 1 1 1	
256	1.5 6 0 4 9 5 2 2	
512	1.5 6 0 4 9 6 2 6	

These tables show that it is sufficient to take $I = 40$ to obtain relative errors inferior to 10^{-6} if we use method 2, while we need $I = 512$ if we use method 1. For both methods, the total number of elements until the time $t = 1$ is equal to I^2. But, the total number of unknowns is approximately I^2 for method 1 and approximately $6\,I^2$ for method 2 (since for each i and n, we must compute u_i^{n+0}, $u_i^{n+1/2}$, u_i^{n+1}, $u_{i+1/2}^{n+0}$, $u_{i+1/2}^{n+1/2}$, $u_{i+1/2}^{n+1}$), i.e.

$$\mathcal{N}_1 \simeq (512)^2 \qquad \text{for method 1,}$$
$$\mathcal{N}_2 \simeq 6 \times (40)^2 \qquad \text{for method 2.}$$

The ratio of these two numbers is

$$\mathcal{N}_1/\mathcal{N}_2 \simeq 27.$$

5.1.c. *Stability*

In the preceding sequence of computations we have taken $\Delta t = h$. Now, we want to check the stability of the method when we increase the ratio $\lambda = \Delta t/h$.

We have performed computations with $\lambda = 2$, 4 and 8. The computed values remain quite regular; no oscillation appears, neither on the values of u nor on the position of the free boundary. An illustration is given by Fig. 4 and 5 which represent the displacement $a^{n+1} - a^n$ of the free boundary at each time step for $\lambda = 1$ and $\lambda = 8$ respectively and $h = 1/32$.

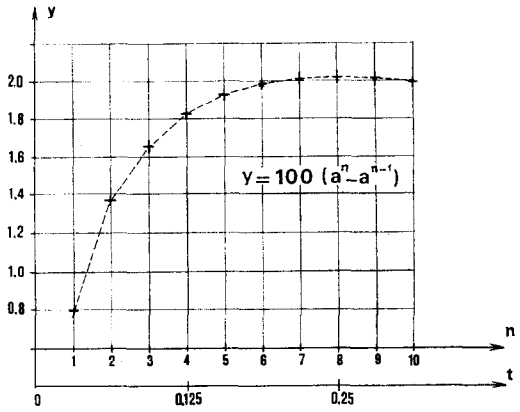

FIG. 4. Problem 1. Displacement of the free boundary at each time step for $\Delta t = h = 1/32$.

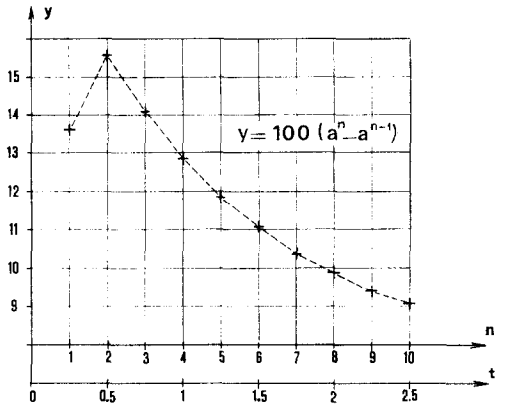

FIG. 5. Problem 1. Same as figure 4 with $\Delta t = 8h$, $h = 1/32$.

Let us remark that the maximum of $a^{n+1} - a^n$ on each of the figures 4 and 5 corresponds to a maximum of the speed of propagation of the free boundary; the speed of propagation is equal to zero at the initial time, increases until the time $t \simeq 0.25$, then decreases.

In order to study if the stability may depend on the speed of propagation of the free boundary, we have increased the coefficient c of equation (2.5). For $c = 4$ and $\lambda = 8$, the results remain very regular.

These various computations permit to conclude that *the method is unconditionally stable.*

5.2. *Problem 2 (Discontinuity at the Initial Time)*

Now, we want to compute a non smooth solution of problem (2.1)–(2.6). We take $c = 1$, $g(t) = 1$ for $t > 0$ and

$$u^\circ(x) = \begin{cases} 1, & \text{for } 0 \leqslant x \leqslant 1/2, \\ 1 - x, & \text{for } 1/2 < x \leqslant 1 = a(0). \end{cases}$$

The solution u is discontinuous at the point $x = 1/2$, $t = 0$.

We have performed computations with $\Delta t = h = 1/64$. Figure 6 represents the function u_h^n computed at the time t^n for $n = 1, 2, 3, 4, 5$.

No oscillation appears. This is an important quality of the method. Let us recall, for example, that the continuous Q_1 method, like the Crank–Nicolson scheme of which it is an extension, admits oscillations of the computed values when the exact solution is discontinuous (unless the time step Δt is taken of the order of h^2).

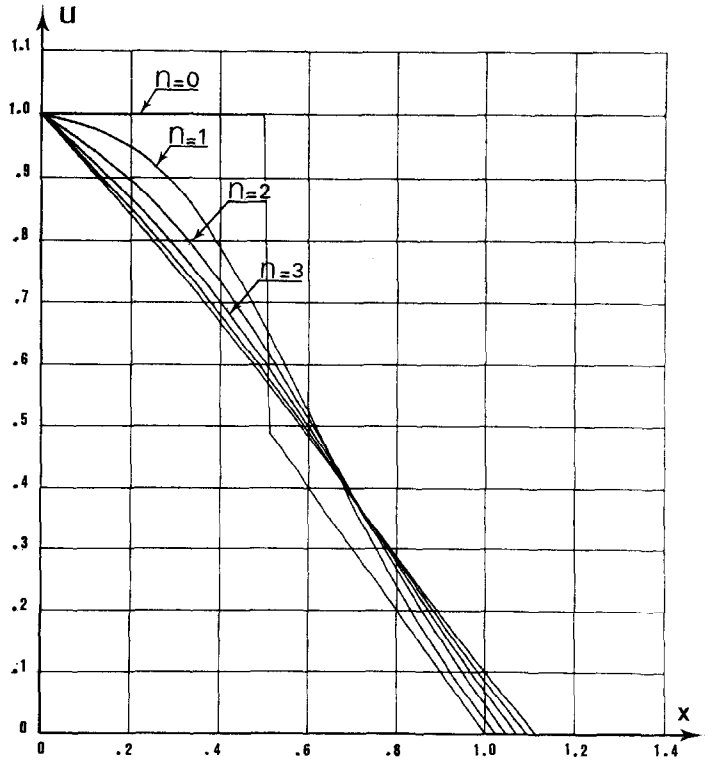

FIG. 6. Problem 2. Functions u_h^n computed at the first five time steps, with $\Delta t = h = 1/64$.

5.3. *Problem* 3 (Discontinuity on the Free Boundary)

Now, we take

$$u^\circ(x) = 1, \qquad \text{for} \quad 0 \leqslant x \leqslant 1 = a(0).$$

The constant c and the function $g(t)$ are the same as in problems 1 and 2.

The solution u is discontinuous on the free boundary at the time $t = 0$, since $u(a(0), 0) = u^\circ(1) = 1$ and $u(a(t), t) = 0$ for $t > 0$. The derivative $\partial u/\partial x$ is infinite in the neighbourhood of the discontinuity and therefore, the speed of propagation of the free boundary is *infinite* at the time $t = 0$.

Despite this singularity, the method can be applied without any trouble: *no oscillation appears* on the computed values and *the accuracy is good.* These results are exhibited on Figs. 7 and 8 and Table VI.

Figure 7 represents the function u_h^n computed at the time $t^n = nh$ for $h = 1/40$ and $n = 1, 2, 3, 4, 5$. Figure 8 represents the corresponding function $a(t)$. Table VI gives a comparison of the values of $a(t)$ computed with $h = 1/32$ and $h = 1/64$ during the first time steps; the first column gives the values of n; the second column

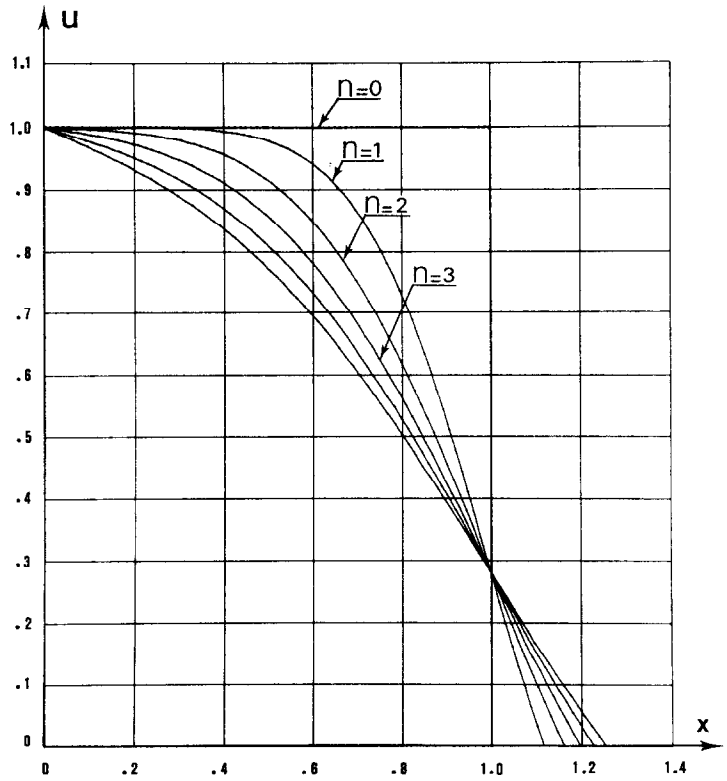

FIG. 7. Problem 3. Functions u_h^n computed at the first five time steps, with $\Delta t = h = 1/40$.

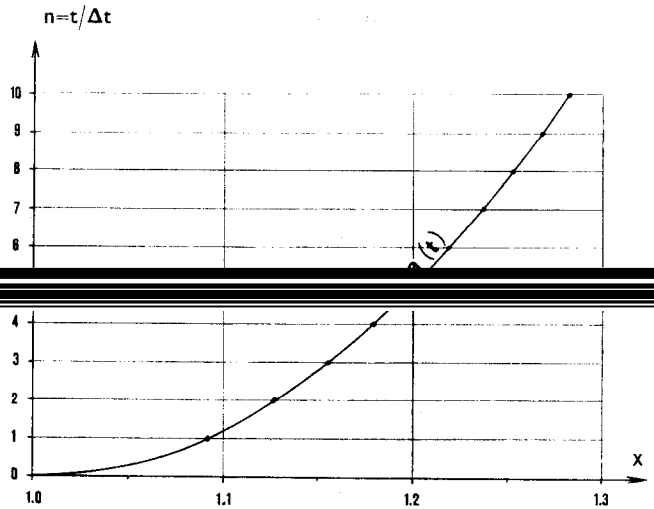

FIG. 8. Problem 3. Movement of the free boundary during the first ten time steps, with $\Delta t = h = 1/64$.

TABLE VI

Problem 3. Position of the Free Boundary: Comparison of the Computed Values at the First Time Steps with $h = 1/32$ and $h = 1/64$.

n	$\Delta t = h = 1/32$ a_h^n	$\Delta t = h = 1/64$ a_h^{2n}	Difference
0	1. 0 0 0 0 0	1. 0 0 0 0 0	
1	1. 1 2 8 8 2	1. 1 2 7 6 4	0. 0 0 1 1 8
2	1. 1 8 0 4 9	1. 1 7 9 7 0	0. 0 0 0 7 9
3	1. 2 2 0 4 1	1. 2 1 9 7 6	0. 0 0 0 6 5
4	1. 2 5 4 1 4	1. 2 5 3 5 7	0. 0 0 0 5 7
5	1. 2 8 3 8 9	1. 2 8 3 3 8	0. 0 0 0 5 1

gives the values of $a(t)$ computed for $t = t^n = nh$ with $h = 1/32$; the third column gives the values of $a(t)$ computed for $t = t^{2n} = 2nh$ with $h = 1/64$; the fourth column gives the difference between the values of column 2 and column 3: we observe that the relative difference between these values is of the order of 10^{-3} for $n = 1$ and decreases as n increases. For a solution with such a singularity this result is very satisfactory.

Remark 1. The three problems presented in this section have been chosen in order to exhibit and isolate the main difficulties which may be encountered in the numerical solution of the one-phase Stefan problem. The hardest case corresponds of course to problem 3 with a discontinuity of the solution on the free boundary which implies

an infinite speed of propagation of the front at the initial time. Various other numerical experiments have been performed although they are not reported in this paper. In particular, we have tested the case of a discontinuity on the fixed boundary ($g(t)$ discontinuous); this case is simpler than the case of problem 3 and presents no difficulty.

Let us also mention that the cases of an appearing phase ($a(0) = 0$), of several phases and of disappearing phases are presently being experimented with.

Remark 2. Another possibility for solving the one-dimensional Stefan problem is to make the change of variable $\xi = x/a(t)$ in order to transform the moving boundary into a fixed boundary. This leads to a system of two ordinary differential equations and a non-linear parabolic equation. Since the submission of this paper, Nitsche [16] has established error estimates for an appropriate Galerkin approximation of this new problem. However, as far as the authors know, no high order accurate approximation of the Stefan problem has yet been computed by this method.

Also, it should be noted that, in the case of problem 3, the transformation $(x, t) \rightarrow (\xi, t)$ is singular at the initial time since $a'(t)$ is infinite. Moreover, this method cannot be applied to problems with appearing and disappearing phases, for example to the case $a(0) = 0$. Finally, in practical problems, heat transfer is often coupled with other phenomenons, so that we have to solve other partial differential equations which are coupled with the heat equation: for these other equations the change of variable $x \rightarrow \xi$ may be inconvenient; so, it seems preferable to solve the whole problem directly without transformation.

APPENDIX 1. Explicit Formula for Computing the Coefficients of the Discrete Equations

Assume that we have performed the computations until the time $t = t^n$. Let

$\mathscr{S}'^n$ = the set of all nodes of $\bar{G}^n$ which are not located on the moving boundary $x = a(t)$,

$\mathscr{S}^n$ = the set of all nodes of $\bar{G}^n$ which are not located on the moving boundary $x = a(t)$ nor on the fixed boundary $x = 0$.

To each point $P = P_{i+\mu}^{n+\nu} \in \mathscr{S}^n$, there corresponds one unknown $u_{i+\mu}^{n+\nu}$ and one equation of the system (3.1); this equation is obtained by taking $\varphi_h = \varphi_{h,P}$ in (3.1), where $\varphi_{h,P}$ is the function defined by (3.4); it is of the form

$$L_P u_h = L'_P u_h , \tag{A1}$$

where L_P is a linear functional which involves the values of u_h corresponding to the time indices $n + 0$, $n + 1/2$ and $n + 1$, and where L'_P is a linear functional which involves the computed values of u_h corresponding to the time index n. The functional L_P corresponds to the first three integrals of the bilinear form (2.8) and the functional L'_P corresponds to the fourth integral.

Let us consider first the functional L_P. It can be written in the form:

$$L_P u_h = \sum_{P' \in \mathscr{S}'^n} \gamma_P(P')\, u_h^*(P'), \tag{A2}$$

with the notation $u_h^*(P) = u_{i+\mu}^{n+\nu}$ for $P = P_{i+\mu}^{n+\nu}$ (note that $u_h^*(P) \neq u_h(P)$ for $\nu = 0$ since $u_h^*(P) = u_{i+\mu}^{n+0}$ and $u_h(P) = u_{i+\mu}^n$). The values of $u_h^*(P')$ which appear in (A2) are unknown except at the nodes $P' \in \mathscr{S}'^n - \mathscr{S}^n$ (which are located on the boundary $x = 0$).

The coefficients $\gamma_P(P')$ can be written in the form

$$\gamma_P(P') = \sum_K \sum_{m=1}^{3} \gamma_{P,K,m}(P'),$$

where the sum is taken for all elements K in $\bar{G}_h^n$ which contain both P and P' (there are at most two such elements for each pair of points P and P') and where the index m corresponds to each of the first three integrals of (2.8). Each coefficient $\gamma_{P,K,m}(P')$ is obtained by approximating the mth integral of (2.8) on the element K by means of the corresponding quadrature formula of Section 3.4 Explicit formulae for computing these coefficients are given below. The notations are the same as in Section 3.1: the points $\hat{P}$, $\hat{P}'$ and $\hat{M}$ are the points of the unit square $\hat{K}$ which correspond to the points P, P' and M of the element K; a point $\hat{P} \in \hat{\Sigma}$ is determined by its indices μ and ν. All the functions defined on $\hat{K}$ and independent of the element K are denoted $\hat{\cdot}$ where the dot stands for an arbitrary symbol. Finally, $x(M)$ denotes the x-coordinate of a point M.

The explicit expression of the shape functions is:

$$\hat{\varphi}_P(\hat{M}) = \hat{\varphi}(\hat{M}; \hat{P}) = \hat{\rho}_\mu(\xi)\, \hat{\rho}_\nu(\eta),$$

with $\hat{M} = (\xi, \eta)$, $\hat{P} = (\mu, \nu)$ and

$$\begin{aligned} \hat{\rho}_0(s) &= (1 - s)(1 - 2s), \\ \hat{\rho}_{1/2}(s) &= 4s(1 - s), \\ \hat{\rho}_1(s) &= s(2s - 1). \end{aligned}$$

Let

$$\begin{aligned} \hat{\alpha}(\hat{P}, \hat{P}') &= (\partial\hat{\varphi}_P/\partial\xi)(\hat{P}'), \\ \hat{\beta}(\hat{P}, \hat{P}') &= (\partial\hat{\varphi}_P/\partial\eta)(\hat{P}'), \\ \hat{\epsilon}_1(\hat{P}) &= \hat{e}(\mu),\ \hat{\epsilon}_2(\hat{P}) = \hat{e}(\nu), \qquad \text{for } \hat{P} = (\mu, \nu), \qquad \text{with} \\ \hat{e}(0) &= \hat{e}(1) = 1/6 \qquad \text{and} \qquad \hat{e}(1/2) = 2/3, \\ \hat{\epsilon}(\hat{P}) &= \hat{\epsilon}_1(\hat{P})\, \hat{\epsilon}_2(\hat{P}), \\ \hat{\delta}(\hat{P}, \hat{P}', \hat{M}) &= \hat{\epsilon}(\hat{P}')(\hat{\alpha}(\hat{P}, \hat{P}')\hat{\beta}(\hat{M}, \hat{P}') - \hat{\beta}(\hat{P}, \hat{P}')\hat{\alpha}(\hat{M}, \hat{P}')), \end{aligned}$$

$$\sigma(M) = \sum_{M' \in \Sigma(K)} \hat{\alpha}(\hat{M}', \hat{M})\, x(M').$$

Then,

$$\gamma_{P,K,1}(P') = \sum_{M\in\Sigma(K)} \hat{\delta}(\hat{P}, \hat{P}', \hat{M})\, x(M),$$

$$\gamma_{P,K,2}(P') = (t^{n+1} - t^n) \sum_{M\in\Sigma(K)} \hat{\epsilon}(\hat{M})\, \hat{\alpha}(\hat{P}, \hat{M})\, \hat{\alpha}(\hat{P}', \hat{M})/\sigma(M),$$

$$\gamma_{P,K,3}(P') = \begin{cases} \hat{\epsilon}_1(\hat{P}')\, \hat{\varphi}_P(\hat{P}')\, \sigma(P') & \text{if } P' \in \mathscr{S}'^n \cap \Omega^{n+1}, \\ 0 & \text{if } P' \notin \mathscr{S}'^n \cap \Omega^{n+1}. \end{cases}$$

Let us now consider the functional L'_P. Let $\mathscr{S}'^n_0 = \mathscr{S}'^n \cap \Omega^n$ = the set of all nodes of $\mathscr{S}'^n$ which lie on the line $t = t^n$. Then,

$$L'_P u_h = \sum_{P'\in\mathscr{S}'^n_0} \gamma'_P(P')\, u_h(P'),$$

with

$$\gamma'_P(P') = \sum_K \gamma_{P,K,4}(P'),$$

$$\gamma_{P,K,4}(P') = \hat{\epsilon}_1(\hat{P}')\, \hat{\varphi}_P(\hat{P}')\, \sigma(P') \qquad \text{for } P' \in \mathscr{S}'^n_0.$$

Remarks. The values of the coefficients $\hat{\alpha}$, $\hat{\beta}$, $\hat{\epsilon}$ and $\hat{\delta}$ are independent of the element K and are computed once and for all.

The function $\sigma(M)$ which appears at the denumerator of the expression of $\gamma_{P,K,2}$ is equal to $\mathscr{J}(M)/(t^{n+1} - t^n)$, where $\mathscr{J}(M)$ denotes the Jacobian of the mapping $\mathscr{F}$. The conditions $x_i^{n+\nu} \leqslant x_{i+1}^{n+\nu}$, $x_{i+1/2}^{n+\nu} = (x_i^{n+\nu} + x_{i+1}^{n+\nu})/2$, imply that $\mathscr{J}(M)$ is strictly positive for all $M \in \Sigma(K)$.

The foregoing formulae are general; they do not assume that the point $P_{i+1/2}^{n+\nu}$ is the midpoint of the segment $[P_i^{n+\nu} P_{i+1}^{n+\nu}]$; the only condition is that the Jacobian of the mapping $\mathscr{F}$ must not vanish.

APPENDIX 2.

(1) *Isoparametric numerical integration*

In Section 3.4, we have described how the integrals involved in the integral relation (3.1) are computed by means of Simpson's rule. It is easy to check that the use of Simpson's rule is in accordance with the general theory of numerical integration for isoparametric finite elements (see [3, 15]).

On the unit square $\hat{K}$, the coefficients of the quadrature formula at the points $\hat{P}_\mu{}^\nu$ are equal to

$$\hat{\omega}_\mu{}^\nu = \hat{e}(\mu)\hat{e}(\nu),$$

with $\hat{e}(0) = \hat{e}(1) = 1/6$ and $\hat{e}(1/2) = 2/3$.

On an element $K = K_i^n$, the coefficients of the corresponding quadrature formula at the points $P_{i+\mu}^{n+\nu}$ are equal to

$$\omega_{i+\mu}^{n+\nu} = \hat{\omega}_\mu{}^\nu \hat{\mathscr{J}}_i^n(\hat{P}_\mu{}^\nu),$$

where $\hat{\mathscr{J}}_i^n(\hat{P})$ is the value at the point $\hat{P}$ of the Jacobian of the mapping $\mathscr{F}: \hat{K} \to K_i^n$.

We have

$$\hat{\mathscr{J}}_i^n(\hat{P}_\mu{}^\nu) = (t^{n+1} - t^n)(x_{i+1}^{n+\nu} - x_i^{n+\nu}),$$

which yields the formula of Section 3.4.

(2) *Monotonicity of the Function $f(p)$*

In Section 5.1.a, we have considered the function $f(p) = ((r_1)^p - 1)/((r_2)^p - 1)$ with $r_1 > r_2 > 1$ and we have used the fact that it is strictly increasing from $+1$ to $+\infty$ as p increases from $-\infty$ to $+\infty$. This property is easy to prove by studying the sign of the derivative $f'(p)$.

For simplicity, we will write a and b instead of r_1 and r_2 and use some further notation which is independent of the notation used in the other parts of this paper. We have:

$$f(p) = y(p)/z(p), \qquad \text{with} \quad y(p) = a^p - 1,\ z(p) = b^p - 1,\ a > b > 1.$$

The function $f(p)$ is defined for all $p \in \mathbb{R}$, except for $p = 0$ since $y(0) = z(0) = 0$. But, as $p \to 0$, $f(p)$ converges to $y'(0)/z'(0) = \operatorname{Log} a/\operatorname{Log} b$; hence, we can extend the definition of the function $f(p)$ to all of $\mathbb{R}$ by continuity.

We have

$$y(p) < z(p) < 0 \qquad \text{for} \quad p < 0,$$
$$y(p) > z(p) > 0 \qquad \text{for} \quad p > 0.$$

Hence,

$$f(p) > 1, \qquad \text{for all} \quad p.$$

For $p \neq 0$, we have

$$\frac{f'(p)}{f(p)} = \frac{y'(p)}{y(p)} - \frac{z'(p)}{z(p)} = g(a, p) - g(b, p),$$

with

$$g(s, p) = \frac{s^p \cdot \operatorname{Log} s}{s^p - 1} = \frac{\operatorname{Log} s}{1 - s^{-r}}.$$

Let us show that the function $g(s, p)$ is strictly increasing with respect to s for $s > 1$ and for any fixed $p \neq 0$. We have:

$$\frac{\partial}{\partial s} g(s, p) = \left(\frac{1}{s}(1 - s^{-p}) - ps^{-p-1} \operatorname{Log} s\right) \Big/ (1 - s^{-p})^2$$
$$= (s^p - 1 - p \operatorname{Log} s)/s^{p+1}(1 - s^{-p})^2$$

For $s > 1$ and $p \neq 0$, $(\partial/\partial s)g(s, p)$ has the same sign as $h(s, p) = s^p - p \operatorname{Log} s - 1$.

But, we have:

$$h(s, p) = 0 \qquad \text{for} \quad s = 1,$$

$$\frac{\partial h}{\partial s}(s, p) = ps^{p-1} - p/s = p(s^p - 1)/s > 0 \qquad \text{for} \quad s > 1$$

and for $p \neq 0$.
Hence, $h(s, p) > 0$ for $s > 1$ and $p \neq 0$.

It follows

$$\frac{\partial}{\partial s} g(s, p) > 0 \qquad \text{for} \quad s > 1 \quad \text{and} \quad p \neq 0,$$

$$g(a, p) - g(b, p) > 0 \qquad \text{for} \quad a > b > 1 \qquad \text{and} \qquad p \neq 0,$$

$$f'(p) > 0 \qquad \text{for} \quad p \neq 0, \text{ and therefore,}$$

$f(p)$ is increasing for all $p \in \mathbb{R}$.

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