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THE ITERATIVE TRANSFORMATION METHOD: NUMERICAL SOLUTION OF ONE-DIMENSIONAL PARABOLIC MOVING BOUNDARY PROBLEMS

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The main contribution of this paper is the application of the iterative transformation method to the numerical solution of the sequence of free boundary problems obtained from one-dimensional parabolic moving boundary problems *via* the implicit Euler's method. The combination of the two methods represents a numerical approach to the solution of those problems. Three parabolic moving boundary problems, two with explicit and one with implicit moving boundary conditions, are solved in order to test the validity of the proposed approach. As far as the moving boundary position is concerned the obtained numerical results are found to be in agreement with those available in literature.

Keywords: Iterative transformation method; Implicit Euler's method; Parabolic moving boundary problems

AMS Subject Classifications: 65L10, 65M06, 35R35

C. R. Category: G1.8

1. INTRODUCTION

A moving boundary problem is a nonlinear initial-boundary value problem with a moving boundary whose position has to be determined as part of the solution. Parabolic moving boundary problems describe many phenomena of interest arising in physical and biological sciences, engineering,

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metallurgy, soil mechanics, decision and control theory, *etc.* (see [6]). We consider the following class of moving boundary problems of the parabolic type

$$
\begin{aligned}
&\frac{\partial^2 u}{\partial x^2} = \frac{\partial u}{\partial t} + f(x,t) \quad \text{on } t>0,\ 0<x<s(t) \\
&\alpha(t)u(0,t) + \beta(t)\frac{\partial u}{\partial x}(0,t) = \gamma(t), \quad \alpha^2+\beta^2 \neq 0,\ \gamma \neq 0 \\
&u(s(t),t) = p\frac{ds}{dt}(t) \\
&\frac{\partial u}{\partial x}(s(t),t) = q\frac{ds}{dt}(t) \\
&s(0)=a, \quad u(x,0) = \begin{cases} r(x) & \text{for } 0 \leq x \leq a \\ 0 & \text{for } a<x \end{cases}
\end{aligned}
\tag{1.1}
$$

where $f(\cdot,\cdot)$ and $r(\cdot)$ are given functions of their arguments, p and q are given constants and $s(t)$ is the unknown moving boundary. For a more general class of problems see the last section. The problem (1.1) is nonlinear because $s(t)$ depends on the initial and boundary data so that a superposition principle cannot be valid (that was pointed out by Landau [15]). As a consequence obtaining analytical solutions for problems belonging to the class (1.1) is a difficult task (see [6, pp. 101 – 139]).

Several numerical methods have been proposed for the solution of moving boundary problems. Let us list here those of more frequent use: finite difference, finite element, isotherm migration, of lines, enthalpy, truncation (alternating phase) and variational inequalities. For the fundamental aspects of those methods, as well as for an extended bibliography, we refer the interested reader to [6, pp. 163 – 282]. As far as the performance of different methods is concerned the introductory remark in a survey paper by Fox [13] is pertinent: "Problems of the same general nature can differ enough in detail to make a good method for one problem less satisfactory and even mediocre for another almost similar problem". This point of view justifies the development of so many different numerical methods.

At a more general level the numerical approaches for the solution of moving boundary problems belong to three main classes, namely front-tracking, fixing-domain and fixed-domain. In a front-tracking approach the position of the moving boundary is computed explicitly by the numerical algorithm. The method of lines is an example of the front-tracking strategy. On the other hand in a fixed-domain or in a fixing-domain approach the moving boundary can be recovered *a posteriori* from the solution properties. For a fixing-domain approach a variable transformation is used in order to reduce the problem to a computational domain. The isotherm migration method belongs to the fixing-domain class. A weak formulation of the problem is usually used for the fixed-domain approach. The enthalpy method is within the fixed-domain class.

Our approach belongs to the front-tracking class. We reduce a moving boundary problem to a sequence of free boundary problems by an implicit Euler's method and we apply the iterative transformation method in order to transform each free boundary problem to initial value problems. The combination of the two methods represents a numerical approach to the solution of one-dimensional moving boundary parabolic problems.

The iterative transformation method was introduced within the similarity analysis of moving boundary problems in [7, 9]. A constructive formulation of the method is given in [10]. The iterative method was introduced as an extension of the non-iterative transformation method defined in [12]. In several cases of interest, the similarity analysis allows us to reduce a moving boundary problem to a free boundary problem governed by ordinary differential equations. As an example the application of the iterative transformation method to a hyperbolic moving boundary problem is considered in [8]. Here, instead of working out a preliminary similarity analysis, which has a limited range of application, we apply the implicit Euler's method. We have a strong motivation for using an implicit method: for explicit methods stability arguments become important and that restricts the choice of space and time steps and thus the achievable accuracy.

A different application of the iterative transformation method, namely to the numerical solution of boundary value problems on infinite intervals, is developed in [11].

The moving boundary conditions in (1.1) are called explicit when $p \neq 0$ or $q \neq 0$ (implicit otherwise). In the case of explicit moving boundary conditions it is possible to apply a finite difference formula to find a first approximation of the moving boundary position at the next time step. Of course that is not possible when implicit moving boundary conditions are prescribed. Moreover, existence and uniqueness of solution is easier to prove for problems with explicit boundary conditions than for problems with implicit ones (see [20]). Problems with implicit moving boundary conditions arise in diffusion of oxygen and lactic acid in tissues [14], in the theory of diffusion flames [3], and in statistical decision theory [2].

Our numerical approach, which is defined in the next section, can be applied to problems with either explicit or implicit moving boundary conditions. The three test problems considered in Section 3 concern with two problems involving explicit and with a problem involving implicit moving boundary conditions. In Section 4 we discuss the details of a positive numerical test of convergence for the classical Stefan's problem. There, by using the second and third test problems, we point out the role played by the truncation error. Moreover, the numerical results obtained by our approach are found to be in agreement with those reported in literature. Finally, in the last section, we propose the extension of our approach to a wide class of parabolic moving boundary problems where the governing differential equation and the moving boundary conditions are also nonlinear and may depend on the free boundary and its derivative.

2. THE NUMERICAL APPROACH

An implicit Euler's approximation of the time derivatives allows us to reduce the problem (1.1) to the following sequence of free boundary problems

$$\begin{aligned}
&\frac{d^2U_n}{dx^2} = \frac{U_n - U_{n-1}}{\Delta t} + f(x, n\Delta t) \\
&\alpha U_n(0) + \beta \frac{dU_n}{dx}(0) = \gamma, \quad U_n(s_n) = p\frac{s_n - s_{n-1}}{\Delta t} \\
&\frac{dU_n}{dx}(s_n) = q\frac{s_n - s_{n-1}}{\Delta t} \\
&s_0 = a, \quad U_0(x) = \begin{cases} r(x) & \text{for } 0 \le x \le a \\ 0 & \text{for } a < x \end{cases}
\end{aligned} \tag{2.1}$$

where $U_n(x) \approx u(x, n\Delta t)$ and $s_n \approx s(n\Delta t)$ for $n = 1, \ldots, N$. Here and in the following Δt (Δx) is the time (space) step size. It is not difficult to ascertain that for each value of $n = 1, \ldots, N$ (2.1) represents, besides the term U_{n-1}, a particular case of the class of free boundary problems considered in [9]. As a consequence the numerical solution of (2.1) can be obtained by an appropriate use of the iterative transformation method defined there (see also [10]).

Let us define an *ad hoc* application of the iterative transformation method to the numerical solution of (2.1). First, we introduce the modified sequence of free boundary problems

$$\begin{aligned}
&\frac{d^2U_n}{dx^2} = \frac{h^{-2\delta/\sigma}U_n - h^{(1-2\delta)/\sigma}U_{n-1}}{\Delta t} + h^{(1-2\delta)/\sigma}f(h^{-\delta/\sigma}x,\ n\Delta t) \\
&\alpha U_n(0) + \beta h^{\delta/\sigma}\frac{dU_n}{dx}(0) = \gamma
\end{aligned}$$

$$U_n(s_n) = h^{1/\sigma} p \frac{h^{-\delta/\sigma} s_n - s_{n-1}}{\Delta t}$$
$$\frac{dU_n}{dx}(s_n) = h^{(1-\delta)/\sigma} q \frac{h^{-\delta/\sigma} s_n - s_{n-1}}{\Delta t} \tag{2.2}$$
$$s_0 = a, \quad U_0(x) = \begin{cases} r(x) & \text{for } 0 \le x \le a \\ 0 & \text{for } a < x \end{cases}$$

where h is a numerical parameter. The sequence of free boundary problems (2.1) is recovered from (2.2) by setting $h=1$. Moreover, in (2.2) the governing differential equation and the two boundary conditions at s_n are invariant with respect to the stretching group of transformations

$$x^* = \lambda^\delta x, \quad s_n^* = \lambda^\delta s_n, \quad U_n^* = \lambda U_n, \quad h^* = \lambda^\sigma h \tag{2.3}$$

where $\ln \lambda$ is the group parameter and δ and σ are arbitrary (but non-zero) constants.

In order to solve (2.1) numerically we consider a value h^*, set $s_n^* = s_{n-1}$ (but $s_1^* = 0.5$ if $s_0 = 0$), fix values of δ and σ and integrate inwards on $[0, s_n^*]$ the governing differential equation with the invariant endpoint conditions in (2.2) in order to find the values $U_n^*(0)$ and $(dU_n^*/dx^*)(0)$. As a consequence of the partial invariance of (2.2) with respect to (2.3) we can easily obtain

$$\lambda = \frac{\alpha(n\Delta t) U_n^*(0) + \beta(n\Delta t) h^{*\delta/\sigma} (dU_n^*/dx^*)(0)}{\gamma(n\Delta t)}$$
$$U_n(0) = \lambda^{-1} U_n^*(0), \quad \frac{dU_n}{dx}(0) = \lambda^{\delta-1} \frac{dU_n^*}{dx^*}(0) \tag{2.4}$$
$$s_n = \lambda^{-\delta} s_n^*, \quad h = \lambda^{-\delta} h^*.$$

The method is iterative because we iterate different values of h^* until we find (from (2.4)) the value of $|h-1|$ to be zero within a prefixed tolerance. To this end a root-finding method can be used. A further numerical integration allows us to define U_n on $[0, s_n]$. We remark that in the application of the iterative transformation method to the numerical solution of the sequence of free boundary problems (2.1) we are allowed to consider $U_{n-1}(x)$ and s_{n-1} at the n-th time step as invariants with respect to (2.3). Moreover, the choice $s_n^* = s_{n-1}$ is useful because $U_{n-1}(x)$ is defined only on $[0, s_{n-1}]$. However, if $s_n > s_{n-1}$, then in order to define U_n on $[0, s_n]$ it is necessary to extend $U_{n-1}(x)$ outside of $[0, s_{n-1}]$ and this can be done in the standard way by setting $U_{n-1}(x) = U_{n-1}(s_{n-1})$ for $s_{n-1} < x \le s_n$.

3. THREE TEST PROBLEMS

In this section we report three test problems that have been used in literature in order to validate different numerical methods. The first is the classical Stefan's problem

$$\begin{aligned}&\frac{\partial^2 u}{\partial x^2}=\frac{\partial u}{\partial t}, \quad u(0,t)=1, \quad u(s(t),t)=0\\ &\frac{\partial u}{\partial x}(s(t),t)=-\frac{1}{S}\frac{ds}{dt}(t), \quad s(0)=0, \quad u(x,0)=0 \quad \text{for } 0<x\end{aligned} \tag{3.1}$$

where S is the Stefan's number. A reliable approximate similarity solution for (3.1) is available in [9]. The moving boundary is given by $s(t)=At^{1/2}$. If $S=0.1$ then $A=0.440033$; this value of A is in agreement up to four decimal places with that obtained analytically (by an asymptotic expansion). The following variant of the Stefan's problem

$$\begin{aligned}&\frac{\partial^2 u}{\partial x^2}=\frac{\partial u}{\partial t}, \quad u(0,t)=-1, \quad u(s(t),t)=0\\ &\frac{\partial u}{\partial x}(s(t),t)=\frac{ds}{dt}(t), \quad s(0)=0.25, \quad u(x,0)=\begin{cases}4x-1 & \text{for } 0\le x\le 0.25\\ 0 & \text{for } 0.25<x\end{cases}\end{aligned} \tag{3.2}$$

was considered by Rubinstein [19, pp. 380–387]. The test problem (3.2) was used by Rubinstein [19, pp. 380–387] and by Asaithambi [1] to validate, respectively, the method of integral equations and the Galerkin method. In (3.1) and (3.2) explicit boundary conditions at the moving boundary are given.

As a third test problem we consider the Meyer's formulation [17] of a problem from decision theory [21]

$$\begin{aligned}&\frac{\partial^2 u}{\partial x^2}=\frac{\partial u}{\partial t}+\frac{1}{2t^2}, \quad \frac{\partial u}{\partial x}(0,t)=-\frac{1}{2}\\ &u(s(t),t)=0, \quad \frac{\partial u}{\partial x}(s(t),t)=0, \quad s(0)=0, \quad u(x,0)=0 \quad \text{for } 0<x\end{aligned} \tag{3.3}$$

Meyer used this problem to validate the combination of the method of lines and of the invariant imbedding method. The original formulation of the problem (3.3) considered by Sackett has a singularity in the boundary data at the initial time. To overcome this difficulty Sackett used a sophisticated similarity transformation whereas Meyer applied a simple subtracting of the singularity from the boundary data. In (3.3) the governing differential equation is singular at the initial time and the moving boundary conditions are implicit.

4. NUMERICAL RESULTS

In this section in order to simplify the exposition, we limit ourselves to report only the numerical results related to the moving boundary position.

Concerning the numerical solution of (3.1) we used the available similarity solution in order to perform a test of convergence as reported in Table I.

Here the D notation indicates a double precision arithmetic and in the following the E notation a simple one. Of course the results listed in Table I were obtained with a constant ratio $\Delta t/\Delta x$. The convergence of the numerical solution to the similarity solution as Δx goes to zero is evident. Moreover, the last line of Table I reports the errors measured in the root mean square (rms) norm defined by

$$\|e\|_{\mathrm{rms}} = \left(\sum_{n=1}^{N} (s(n\Delta t) - s_n)^2/N \right)^{1/2}.$$

This is of interest because we can see that the rate of convergence is nearly linear and that 1% of accuracy is achieved by the results obtained with $\Delta t = 0.0125$.

TABLE I Convergence test for the numerical solution of (3.1) with $S=0.1$. We used $\delta=1$, $\sigma=1$ and $s_1^*=0.5$

	Δx				*Similarity*
t	$1D-2$	$5D-3$	$2.5D-3$	$1.25D-3$	*solution*
0.025				0.0496	0.069575
0.05			0.0701	0.0806	0.098394
0.1		0.0992	0.1139	0.1245	0.139151
0.2	0.1403	0.1611	0.1761	0.1860	0.196789
0.3		0.2089	0.2234	0.2326	0.241016
0.4	0.2277	0.2489	0.2629	0.2717	0.278301
0.5		0.2841	0.2976	0.3061	0.311150
0.6	0.2953	0.3157	0.3288	0.3372	0.340848
0.7		0.3447	0.3575	0.3658	0.368158
0.8	0.3519	0.3716	0.3841	0.3925	0.393577
0.9		0.3968	0.4091	0.4175	0.417452
1.	0.4016	0.4206	0.4327	0.4413	0.440033
$\|e\|_{\mathrm{rms}}$	0.0470	0.0282	0.0157	0.0080	

As far as the numerical solution of (3.2) is concerned some representative numerical results are reported in Table II. For this particular problem we decided to solve the free boundary problem at the first time step for several values of Δt instead of proceeding further in the numerical integration. This because the non-zero initial conditions for the moving boundary problem represent a test problem for the applicability of the iterative transformation method already at the first time step. For this problem reliable numerical results are obtained anyway. That holds because of a negligible truncation error in the considered range of time steps (*cf.* the last three columns of Tab. III below).

The values listed by Rubinstein were determined with the maximum relative error of 1%. In relation to problem (3.2) Rubinstein was also interested in the determination of the time T defined by the equation $s(T)=0.5$. A simple linear extrapolation of our results in Table II provides the value $T=0.122699$, which can be compared with $T=0.12092$ obtained in [19, p. 386].

As far as the problem (3.3) is concerned the most significant numerical results obtained by our approach are listed in Table III.

TABLE II Comparison of numerical results for the problem (3.2). We used $\delta=1/2$, $\sigma=2$, $s_1^*=0.25$ and $\Delta x=1E-3$

Rubinstein [19, *p.* 386]		*This work*	
t	$s(t)$	Δt	$s(\Delta t)$
0.01	0.281347	0.01	0.285078
0.02	0.307925	0.02	0.313744
0.04	0.354519	0.04	0.360851
0.06	0.395471	0.06	0.399998
0.08	0.432581	0.08	0.434228
0.1	0.466754	0.1	0.465035

TABLE III Comparison of numerical results for the problem (3.3). We used $\delta=1/2$, $\sigma=2$, $s_1^*=0.5$ and $\Delta x=1E-4$

	Sackett [21]	*Meyer* [17]	*This work*		
t	$s(t)$	$s(t)$	$s(t)$	Δt	$s(\Delta t)$
0.05		0.0025	0.0025	0.05	0.0025
0.1	0.009994	0.0100	0.0100	0.1	0.0100
0.2	0.039805	0.0398	0.0399	0.2	0.0399
0.3	0.088548	0.0886	0.0893	0.3	0.0900
0.4	0.154261	0.1543	0.1571	0.4	0.1583
0.5	0.234175	0.2343	0.2420	0.5	0.2451

From the last three columns of Table III we notice that the first three determinations of the moving boundary position obtained with different values of the first time step coincide with those computed by proceeding further in the numerical integration. However, owing to the truncation error the difference in the two approximations increases at greater values of time.

For the numerical solution of the initial value problems involved in the application of the iterative transformation method we used the classical fourth order Runge-Kutta method. Moreover, we applied appropriate termination criteria [18] in order to stop the iterations obtained by the secant method. We always identified a particular interval where the function $\lambda^{-\sigma}h^* - 1$ changes sign (bracketing). Therefore, some preliminary numerical experiments were used for the results reported in the tables above.

5. EXTENSION AND DISCUSSION

The numerical approach proposed so far can be extended to a class of parabolic moving boundary problems more general than (1.1). In fact, let us consider the following class of problems

$$\frac{\partial^2 u}{\partial x^2} = f\left(x, t, s, \frac{ds}{dt}, u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial t}\right) \quad \text{on } t > 0,\ 0 < x < s(t)$$

$$\begin{aligned} \alpha(t)u(0,t) + \beta(t)\frac{\partial u}{\partial x}(0,t) &= \gamma(t), \quad \alpha^2 + \beta^2 \neq 0,\ \gamma \neq 0 \\ u(s(t),t) &= p\left(t, s(t), \frac{ds}{dt}(t)\right) \\ \frac{\partial u}{\partial x}(s(t),t) &= q\left(t, s(t), \frac{ds}{dt}(t)\right) \\ s(0) = a, \quad u(x,0) &= \begin{cases} r(x) & \text{for } 0 \le x \le a \\ 0 & \text{for } a < x \end{cases} \end{aligned} \tag{5.1}$$

where $f(\cdot,\cdot,\cdot,\cdot,\cdot,\cdot,\cdot)$, $p(\cdot,\cdot,\cdot,)$ and $q(\cdot,\cdot,\cdot)$ are given functions of their arguments. The class (5.1) encompasses several problems of interest; not only problems governed by a nonlinear differential equation (see, as an example, [16]), but also problems where the free boundary or its derivative are involved in the governing equation (see, for instance, [4, 5]).

The implicit Euler's method allows us to obtain from (5.1) the following sequence of free boundary problems

$$\frac{d^2U_n}{dx^2} = f\left(x, n\Delta t, s_n, \frac{s_n - s_{n-1}}{\Delta t}, U_n, \frac{dU_n}{dx}, \frac{U_n - U_{n-1}}{\Delta t}\right) \quad \text{on } 0 < x < s_n$$

$$\alpha(n\Delta t)U_n(0) + \beta(n\Delta t)\frac{dU_n}{dx}(0) = \gamma(n\Delta t)$$

$$U_n(s_n) = p\left(n\Delta t, s_n, \frac{s_n - s_{n-1}}{\Delta t}\right)$$

$$\frac{dU_n}{dx}(s_n) = q\left(n\Delta t, s_n, \frac{s_n - s_{n-1}}{\Delta t}\right)$$

$$s_0 = a, \quad U_0(x) = \begin{cases} r(x) & \text{for } 0 \leq x \leq a \\ 0 & \text{for } a < x \end{cases} .$$

As far as the application of the iterative transformation method is concerned we have to consider instead of (2.2) the following modified sequence of free boundary problems

$$\frac{d^2U_n}{dx^2} = h^{(1-2\delta)/\sigma} f\left(h^{-\delta/\sigma}x, n\Delta t, h^{-\delta/\sigma}s_n, \frac{h^{-\delta/\sigma}s_n - s_{n-1}}{\Delta t}, h^{-1/\sigma}U_n, h^{(\delta-1)/\sigma}\frac{dU_n}{dx}, \frac{h^{-1/\sigma}U_n - U_{n-1}}{\Delta t}\right)$$

$$\alpha(n\Delta t)U_n(0) + \beta(n\Delta t)h^{\delta/\sigma}\frac{dU_n}{dx}(0) = \gamma(n\Delta t)$$

$$U_n(s_n) = h^{1/\sigma} p\left(n\Delta t, h^{-\delta/\sigma}s_n, \frac{h^{-\delta/\sigma}s_n - s_{n-1}}{\Delta t}\right)$$

$$\frac{dU_n}{dx}(s_n) = h^{(1-\delta)/\sigma} q\left(n\Delta t, h^{-\delta/\sigma}s_n, \frac{h^{-\delta/\sigma}s_n - s_{n-1}}{\Delta t}\right)$$

$$s_0 = a, \quad U_0(x) = \begin{cases} r(x) & \text{for } 0 \leq x \leq a \\ 0 & \text{for } a < x \end{cases}$$

for which the iterative transformation method is defined exactly as in Section 2. Hence, it can be easily realized that our approach doesn't depend on the linearity of the governing differential equation and of the moving boundary conditions.

On the other hand, it is easily seen that the proposed approach, in its present form, is applicable only to one-phase one-dimensional parabolic moving boundary problems. The proposed approach is not suitable for the numerical treatment of two-phase, multi-dimensional or mushy regions problems.

As a conclusion we have shown the applicability of the iterative transformation method to solving the sequence of free boundary problems obtained *via* the application of the implicit Euler's method to one-dimensional parabolic moving boundary problems.

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