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NUMERICAL RESOLUTION OF AN INVERSE 2D STEFAN PROBLEM

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Abstract - The present work deals with a numerical resolution of an inverse Stefan problem in 2D case. It consists in identifying the moving solid-liquid interface in a melting material from temperature measurements performed only on the solid phase. The space profile and time evolution of this interface are simultaneously estimated by minimizing a penalized output least square criterion on the whole time domain measurements. Fully discrete approach is adopted to establish the criterion gradient expression and a quasi-Newtonian optimization method is used. Numerical results are presented to illustrate the feasibility and efficiency of the proposed method with respect to the classical sequential method.

1. INTRODUCTION

It is known that the control of solid-liquid interface motions and the interface fluxes, in many industrial applications of material processing (casting, welding, crystal growth,....), can lead to desired cast structures and mechanical properties in the final cast product [6]. Therefore the problem of determining the interface position is of great interest. Direct measurement of this solid-liquid interface, is not realizable in many situations, since the temperature sensors cannot be installed into the material. Also, an accurate estimation of this interface, by resolution of the heat and mass transfer equations in both solid and liquid phases is not possible, because many phenomena occurring in the liquid phase are complex to model and partially unknown.

One way to obtain the time dependent interface is to identify it with an inverse approach from the modeled solid phase only. While based on this idea, this identification problem has been solved in some papers ([1], [5], [7]) in a sequential way, where the space profile of the interface is estimated for each time step. In [2] a global identification of this interface, on the whole measurements time interval, is proposed. It is numerically established in that work, that the proposed method is faster and more accurate than the sequential one for the 1D case. For the 2D case, some theoretical results are presented in [3], but without any numerical validation. However, the proposed continuous approach is not easy to implement numerically. Also it cannot lead to satisfactory results in 2D or 3D cases since the discretization of the continuous expression of the gradient does not lead to the discrete form of this gradient.

The aim of the present work is to propose a feasible method able to estimate simultaneously space and time interface variations in 2D case. The method we suggest is based on the discrete Lagrangian approach. We begin by discretizing the model equations and the penalized output least square criterion. Then a discrete Lagrangian and discrete adjoint state are introduced and by means of some derivations, the exact expression of discrete criterion gradient is established. A quasi-Newtonian method can be used to minimize the regularized criterion on the whole time horizon.

The layout of this paper is as follows. In Section 2, we set and formulate the identification problem. In Section 3, we transform the initial problem into a fixed domain. In Section 4, we present the discretization scheme for the model equations and the criterion gradient. In Section 5, we define a discrete Lagrangian and we deduce the discrete gradient expression. In section 6, a test example is presented and the proposed method is tested for various situations. In Section 7, the proposed method is compared with the classical sequential method.

2. PROBLEM SETTING

A rectangular enclosure (width $L_x = 1$, height L_y) is filled with a material at uniform initial temperature which is below the melting temperature of the material T_f. At time $t = 0$, the temperature $T(x, y = L_y, t)$ is suddenly increased above T_f; therefore the solid begins to melt.
The moving solid-liquid interface position is characterized by the function $s(x,t)$. Then the solid region is: $\Omega_s(t) = \{(x,y) : 0 < x < 1;\ 0 < y < s(x,t)\}$ with boundary $\partial\Omega_s(t) = \Gamma_0 \cup \Gamma_1 \cup \Gamma_2 \cup \Gamma(t)$ where $\Gamma_0 = \{(x,0) : 0 < x < 1\}$, $\Gamma_1 = \{(1,y) : 0 < y < L_y\}$, $\Gamma_2 = \{(0,y) : 0 < y < L_y\}$ and $\Gamma(t) = \{(x, s(x,t)) : 0 < x < 1\}$.

Using dimensionless variables, one gets the heat conduction equation in the time dependent solid domain:

$$u_t - \Delta u = 0 \qquad \text{in } \Omega_s(t) \times (0,T). \tag{1}$$

The boundary and initial conditions are:

$$u_x = 0 \qquad \text{on } (\Gamma_1 \cup \Gamma_2) \times (0,T), \tag{2}$$
$$u_y = \phi(x,t) \qquad \text{on } \Gamma_0 \times (0,T), \tag{3}$$
$$u(x,y,0) = T_0 \qquad \text{in } \Omega_s(0), \tag{4}$$

on the moving interface:

$$u = 0 \qquad \text{on } \Gamma(t) \times (0,T). \tag{5}$$

The inverse problem, we are dealing with, consists in finding the solid-liquid interface position $s(x,t)$ from temperature measurements $\varphi(x,t)$ performed on the side Γ_0 during the time interval $(0,T)$.
As mentioned in the introduction, this problem has been considered in [1] [5] [7]. In all these works, the time dependent interface position is estimated in a sequential way for the cited reason that the time and space discretization of $s(x,t)$ produce a large number of unknowns. To determine all these variables will require an important time computing. However, the results obtained in [2] for the 1D case, shows that it is possible to globally identify $s(x,t)$ on the whole time horizon (0,T), in a time computing less than that the sequential identification one. This is essentially due to the use of sensitivity equations to establish the criterion gradient whereas in the sequential method case, this gradient is numerically calculated by variations of the criterion.

In view of these results, we formulate the identification problem as follows:
minimize, with respect to $s(x,t)$, the penalized least square criterion:

$$J_1 = \int_0^T \int_0^1 (u(x,0,t) - \varphi(x,t))^2 dxdt + \frac{\sigma}{2} \int_0^T \int_0^1 (\frac{\partial^2 s}{\partial x \partial t}(x,t))^2 dxdt.$$

The first term represents the distance between the output model and the observed temperature φ and the second term represents a weighted regularizing term introduced to deal with the ill-posedeness nature of the inverse problem.

The problem is a nonlinear constrained one and posed it on a moving domain and solve it in this form, is hard to do. The major difficulty comes from the fact that, in order to use a speedy optimization method, we have to derive the criterion with respect to the moving boundary of domain. To overcome this difficulty, we begin by transforming it in a fixed domain by means of an appropriate transformation.

3. PROBLEM TRANSFORMATION

The so-called Landau transformation allows us to map the physical moving domain into a fixed domain. It consists in the variables change: $z = \frac{y}{s(x,t)}$.
Let:

$$v(x,z,t) = u(x,y,t) \text{ and } \Omega = \{(x,z) : 0 < x < 1; 0 < z < 1\}.$$

Assuming that:

$$s_x(0,t) = s_x(1,t) = 0,$$

we obtain, for eqns (1)-(5), the transformed system:

$$\begin{array}{ll} v_t + a v_z + b v_{xz} + c v_{zz} - v_{xx} = 0 & \text{in } \Omega \times (0,T) \\ v(x,1,t) = 0 & 0 < x < 1, \\ v_x(0,z,t) = v_x(1,z,t) = 0 & 0 < z < 1, \\ v_z(x,0,t) = s(x,t)\phi(x,t) & \text{on } \Gamma_0, \\ v(x,z,0) = T_0 & \text{in } \Omega. \end{array} \tag{6}$$

where the coefficients a, b, c are given by:

$$a = z_t - z_{xx} = \frac{z}{s}(-s_t + s_{xx} - 2\frac{s_x^2}{s}),$$
$$b = 2z\frac{s_x}{s},$$
$$c = -\frac{1}{s^2}(1 + z^2 s_x^2).$$

Thus the criterion J_1 becomes :

$$J_1 = \int_0^T \int_0^1 (v(x,0,t) - \varphi(x,t))^2 dxdt + \frac{\sigma}{2} \int_0^T \int_0^1 (\frac{\partial^2 s}{\partial x \partial t}(x,t))^2 dxdt.$$

Now, J_1 has to be minimized with respect to a function appearing in the coefficients of the model equations.

Most numerical optimization methods require the gradient of the function to be minimized. The continuous expression of the gradient of J_1 can be established like in [3]. However, using a discretization of this continuous expression does not lead, numerically to a satisfactory results. Thus we opt for the fully discrete approach. We discretize the model eqns(6) and the criterion J_1 and then we seek for the gradient of the discrete criterion.

4. PROBLEM DISCRETIZATION

Using an implicit scheme in time with a step dt, and a central finite difference scheme for space derivatives with steps $dx(=\frac{1}{n_x})$ and $dz(=\frac{1}{n_z})$, the discretization of the system (6) leads to:

$$\begin{aligned}
&\frac{v_{ij}^n - v_{ij}^{n-1}}{dt} + a_{ij}^n (v_z)_{ij}^n + b_{ij}^n (v_{xz})_{ij}^n + c_{ij}^n (v_{zz})_{ij}^n - (v_{xx})_{ij}^n = 0, \quad i = 2,...,n_x;\ j = 2,...,n_z, \\
&v_{i(n_z+1)}^n = 0, && i = 1,...,n_x+1 \\
&\frac{v_{2j}^n - v_{1j}^n}{dx} = \frac{v_{(n_x+1)j}^n - v_{n_x j}^n}{dx} = 0, && j = 1,...,n_z, \\
&\frac{v_{i2}^n - v_{i1}^n}{dz} = s_i^n \phi_i^n, && i = 2,...,n_x, \\
&v_{ij}^0 = T_0, && i = 1,...,n_x+1,\ j = 1,...,n_z+1,
\end{aligned} \tag{7}$$

for: $n = 1,...,m\,(T = mdt)$, $(.)_{ij}^n$ denotes $(.)(ndt,(i-1)dx,(j-1)dz)$, and the coefficients in the discretization are given by:

$$\begin{aligned}
a_{ij}^n &= \frac{z_j}{s_i^n}[\frac{s_i^{n-1} - s_i^n}{dt} + \frac{s_{i+1}^n - 2s_i^n + s_{i-1}^n}{(dx)^2} - \frac{2}{s_i^n}(\frac{s_{i+1}^n - s_{i-1}^n}{2dx})^2], \\
b_{ij}^n &= \frac{2z_j}{s_i^n}[\frac{s_{i+1}^n - s_{i-1}^n}{2dx}], \\
c_{ij}^n &= -\frac{1}{(s_i^n)^2}(1 + z_j^2(\frac{s_{i+1}^n - s_{i-1}^n}{2dx})^2).
\end{aligned}$$

Letting:

$$\underline{v}^n = (v_{11}^n,...,v_{(n_x+1)(n_z+1)}^n)^T, \underline{v} = (\underline{v}^0,...,\underline{v}^m)^T,$$

$$\underline{s}^n = (s_1^n,...,s_{n_x+1}^n)^T, \underline{s} = (\underline{s}^0,...,\underline{s}^m)$$

the system of eqns (7) can be written in the following matrix form:

$$\begin{cases} A_n \underline{v}^n = \underline{r}^n, & n = 1,...,m \\ \underline{v}^0 = T_0. \end{cases} \tag{8}$$

where

$$r_{(i-1)(n_z+1)+j}^n = \begin{cases} v_{ij}^{n-1}, & i = 2,...,n_x, j = 2,...,n_z \\ s_i^n \phi_i^n(dz), & i = 2,...,n_x, j = 1 \\ 0, & otherwise \end{cases}$$

For simplicity, we do not give the detailed expression of the matrix A_n. It is an $(n_x+1)(n_z+1)$ matrix depending of $\underline{s}^{n-1}$ and $\underline{s}^n$.
Finally, we associate to J_1 the discrete criterion:

$$J(\underline{s}) = \sum_{n=1}^m \sum_{i=2}^{n_x} (v_{i1}^n - \varphi_i^n)^2 + \frac{\varepsilon}{2} \sum_{n=1}^m \sum_{i=2}^{n_x} (s_{i+1}^n - s_{i-1}^n - s_{i+1}^{n-1} + s_{i-1}^{n-1})^2. \tag{9}$$

where ε is the regularization parameter.

Now we have to minimize J with respect to $s_i^n, i = 2, ..., n_x;\ n = 1, ..., m$.

5. LAGRANGIAN AND DISCRETE GRADIENT

The discrete criterion J depends implicitly on the interface $\underline{s}$ by means of the state $\underline{v}$. To get the gradient of this criterion, we introduce a discrete Lagrangian L and an adjoint state $\underline{p}$ independent of the s and v. The Lagrangian is defined by the following expression:

$$L(\underline{v}, \underline{s}, \underline{p}) = J(\underline{s}) + \sum_{n=1}^{m} (\underline{p}^{n-1})^T (A_n \underline{v}^n - \underline{r}^n). \tag{10}$$

We assume that: $\underline{p}^m = 0$.

According to the well known Lagrangian's calculus, the adjoint state $\underline{p}$ must verify:

$$\frac{\partial L}{\partial \underline{v}^n}(\underline{v}, \underline{s}, \underline{p}) = 0, \quad n = 1, ..., m.$$

Thus we have the adjoint system:

$$\begin{cases} A_n^T \underline{p}^{n-1} = -\dfrac{\partial J}{\partial \underline{v}^n}(\underline{s}) + \dfrac{\partial}{\partial \underline{v}^n}(\underline{p}^{nT} . \underline{r}^{n+1}) = \underline{w}^n, \quad n = m, ..., 1 \\ \underline{p}^m = 0. \end{cases} \tag{11}$$

where:

$$w^n_{(i-1)(n_z+1)+j} = \begin{cases} -2(v_{i1}^n - \varphi_i^n), & i = 2, ..., n_x, j = 1 \\ p_{ij}^n, & i = 2, ..., n_x, j = 2, ..., n_z \\ 0 & otherwise \end{cases}$$

Since $\underline{v}$ is solution of discrete system (8) and $\underline{p}$ is solution of (11), the gradient of the discrete criterion J is obtained by setting:

$$(\nabla J)_i^n = \frac{\partial L}{\partial s_i^n}; \quad i = 2, ..., n_x, \ \ n = 1, ..., m.$$

Let:

$$\alpha = \frac{\varepsilon}{2} \frac{\partial}{\partial s_i^n} \sum_{k=1}^{m} \sum_{i=2}^{n_x} (s_{i+1}^k - s_{i-1}^k - s_{i+1}^{k-1} + s_{i-1}^{k-1})^2$$

Then, the gradient is expressed as follows :

$$(\nabla J)_i^n = \begin{cases} \alpha + \underline{p}^{n-1T} (\dfrac{\partial A_n}{\partial s_i^n}) \underline{v}^n + \underline{p}^{nT} (\dfrac{\partial A_{n+1}}{\partial s_i^n}) \underline{v}^{n+1} - (dz) \phi_i^n p_{i1}^{n-1}, & n = 1, ..., m-1, \\ \alpha + \underline{p}^{n-1T} (\dfrac{\partial A_n}{\partial s_i^n}) \underline{v}^n - (dz) \phi_i^n p_{i1}^{n-1}, & n = m, \end{cases} \tag{12}$$

for: $i = 2, ..., n_x$.

It is easy to establish that α and the $(n_x + 1)(n_z + 1)$ matrices $(\frac{\partial A_n}{\partial s_i^n})$ and $(\frac{\partial A_{n+1}}{\partial s_i^n})$ are obtained by deriving, term by term, respectively, A_n and A_{n+1}, with respect to s_i^n.

6. NUMERICAL EXPERIENCE

6.1. Test Example

The proposed identification method is tested numerically with the following specifications: $T_0 = -1$, $dx = 0.1$ $(n_x = 10)$, $dz = 0.04$ $(n_z = 10)$, $\phi(x, t) = 10$, $T = 1$, $dt = 0.01 (m = 100)$.

With the interface: $s(x, t) = 0.4 - 0.16(1 - e^{-t})(1 - \cos(2\pi x))/2$ we solve the discrete system of eqns(8) to obtain the temperature $v(x, 0, t)$ which will be taken as $\varphi(x, t)$ in the identification algorithm. Thus we will expect to recover $s(x, t)$ by inverse resolution with the proposed method.

Let us underline that we have set: $s(0, t) = s(dx, t) = s(n_x dx, t) = s(1, t) = 0.4$ to satisfy numerically the conditions $s_x(0, t) = s_x(1, t) = 0$. However, in the identification algorithm, the interface at the points $x = dx$ and $x = 1 - dx$ is supposed unknown and must be, also, estimated. Thus 900 unknowns have to be determined.

6.2. Optimization method

The mimimization of J is done using a quasi-Newtonian method implemented in MATLAB as a subroutine called "fminu". The Hessian is updated at each iteration using Davidon-Fletcher-Powell formula. A Cubic interpolation is used to estimate the minimum in the line search direction. The subroutine "fminu" requires: an initialization function noted s_0, the expression (9) of J and expression (12) of gradient ∇J. The latter intervenes in the adjoint state system (11).

All computations are performed with the help of MATLAB on a PC (500Mhz, RAM=32Mbits). To check the identification quality, the relative error between the computed interface s_c and the exact interface s, is defined as:

$$Erm = \sqrt{\frac{\sum_{n=1}^{n=m}\sum_{i=2}^{i=n_x}(s_{ci}^n - s_i^n)^2}{\sum_{n=1}^{n=m}\sum_{i=2}^{i=n_x}(s_i^n)^2}} \tag{13}$$

Let's denote by T_c the computing time required by the proposed method to achieve the identification.

6.3. Results

First we take the initialization function $s_0(x,t) = s(x,0)/2 = 0.2$ (mean value of the initial domain). The convergence of the identification algorithm requires an $\varepsilon \neq 0$. The behaviour of Erm as function of ε, shown in Table 1, is typical of a regularization method. We observe that $\varepsilon = 1$ gives a good compromise between accuracy and weak computing time.

ε	Erm	$T_c(min)$
0.5	$2.68\ 10^{-4}$	38.7
1	$2.57\ 10^{-4}$	35
1.5	$3.74\ 10^{-4}$	34.5

Table 1. Errors and computing time versus ε.

Figure 1 compares the calculated interface and the exact one for different instants. It shows, that the estimated interface agrees well with the exact one except near the initial time where a weak oscillation of the computed interface is observed. The latter remark is traditional ([2], [4]) and related to the temperature discountinuities on the interface at the initial time.

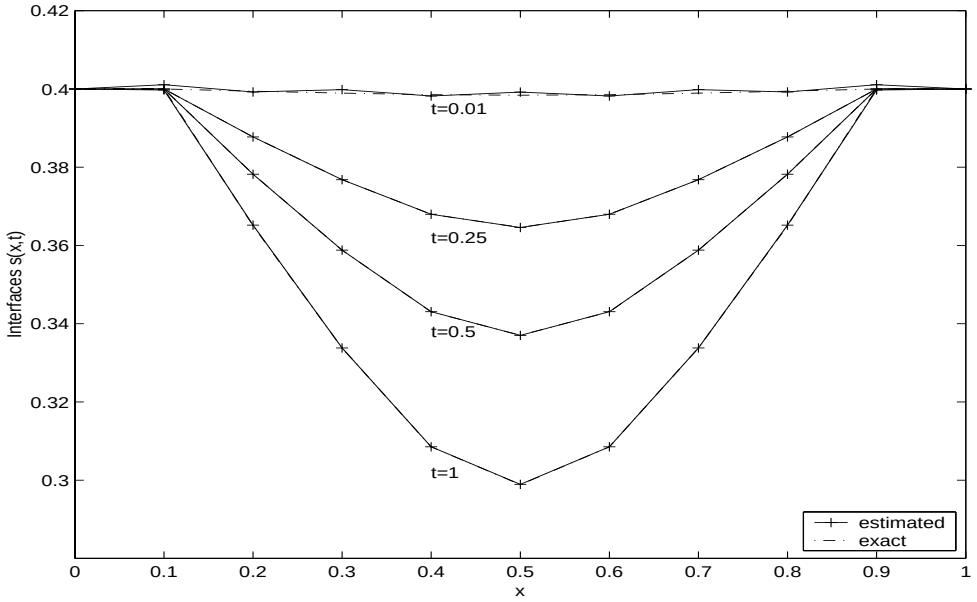

Figure 1. Estimated and exact interfaces: $\varepsilon = 1$, $s_0(x,t) = 0.2$.

If the identification algorithm is initiated by a function even further from the exact interface ($s_0(x,t) = 0.01$ for example), the algorithm convergence always requires regularization and the same results obtained above remain valid.

When the initialization function is the initial interface ($s_0(x,t) = s(x,0) = 0.4$) or very close to the exact interface ($s_0(x,t) = s(x,t) - 0.01$ for example), the identification algorithm can converge without regularization. This is due to the fact that the inverse problem used exact data generated by the direct system. With a regularization $\varepsilon = 1$, the accuracy of identification is increased and the time computing is reduced. Figure 2 shows clearly the very good agreement.

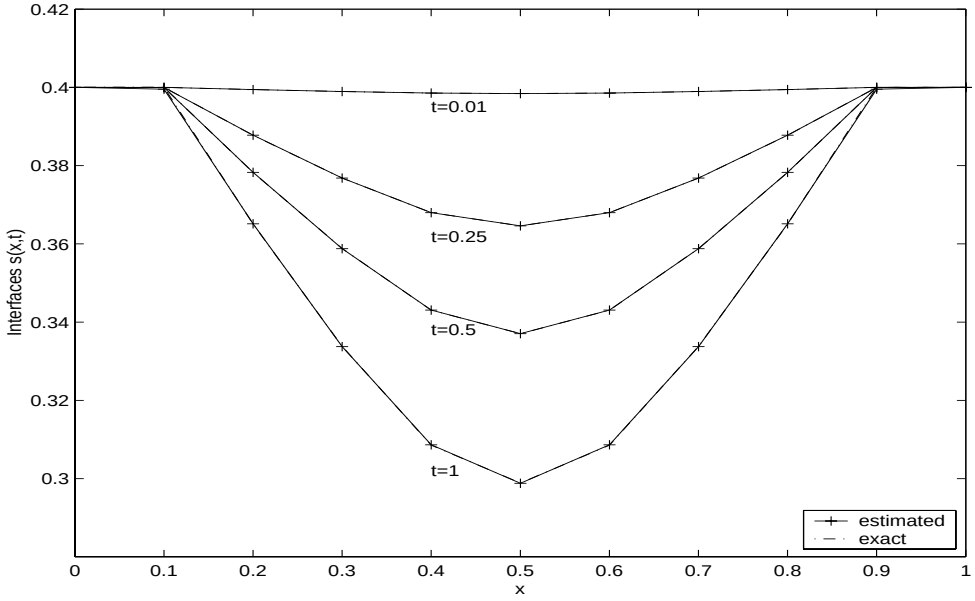

Figure 2. Estimated and exact interfaces: $\varepsilon = 1$, $s_0(x,t) = 0.4$.

7. COMPARISON WITH THE SEQUENTIAL METHOD

The aim of this section is to compare the method proposed here, denoted by Whole Time method (WTM), with the classical sequential one.

The classical sequential method (SM) used in works ([1], [5], [7]) to identify the interface $s(x,t)$ proceeds as follows: at time $t = (n+1)dt$, the interface s is assumed to be time independent, its space profile is obtained by minimizing J defined only on the time horizon $[t_{n+1}, t_{n+r}]$. The optimization procedure is then resumed on the next time interval $[t_{n+2}, t_{n+1+r}]$ to get $s(x, t_{n+2})$. So, the identification of s on the whole time $[0,T]$ will require much computing time. Moreover, the gradient is evaluated by means of numerical finite differences which increases the computing time.

7.1. Noiseless comparison

The WTM method is started with $s_0(x,t) = s(x,0) = 0.4$. We take the horizon length $r = 10$ in the SM.

We note according to Table 2, Figure 2 and Figure 3, that the WTM overrides the SM as well in accuracy (10^{-5} compared to 10^{-3}) as in speed where it saves a very important time computing.

Methods	Erm	$T_c(min)$
SM	$7.7\ 10^{-3}$	120
WTM	$7.73\ 10^{-5}$	26

Table 2. Comparison of the methods, noiseless case.

7.2. Noisy case comparison

To avoid "inverse crimes phenomena", we add to the simulated measurements φ, a noise with 0.01% as amplitude.

Table 3 indicates that always the WTM needs a computer time much less than the SM to estimate the interface with approximately the same precision.

While comparing the noisy and noiseless cases, it can be observed that the WTM is more sensitive to the noise (Errors passed from 10^{-5} to 10^{-3}) than the SM where the errors remain of the same order

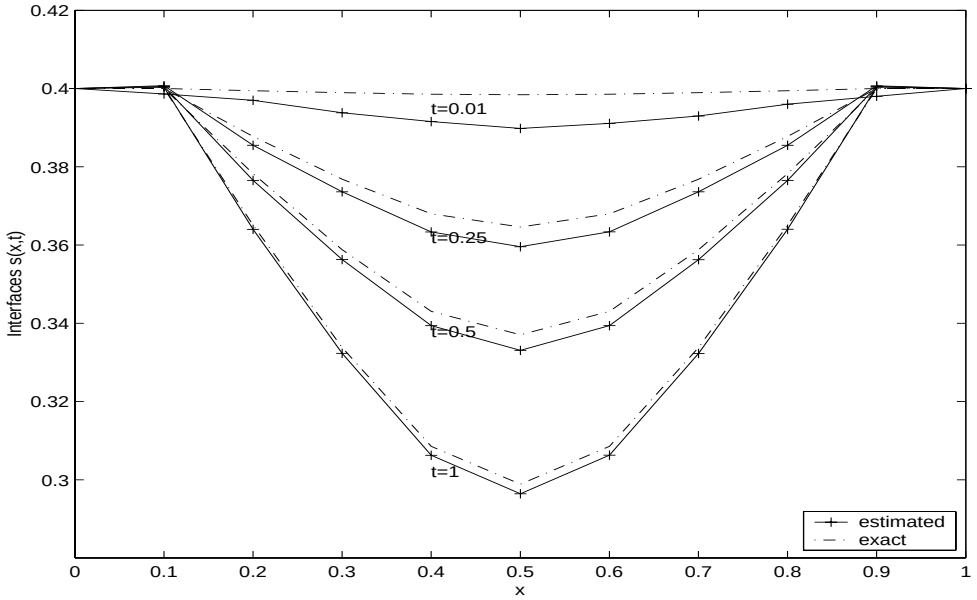

Figure 3. Sequential Method results.

of magnitude. Note from Figure 4, that it is difficult to correctly recover the interface near to the fixed boundaries.

Methods	Erm	$T_c(min)$
(SM)	$7.8\ 10^{-3}$	109
(WTM)	$7.3\ 10^{-3}$	27

Table 3. Comparison of the methods, 0.01% noisy case.

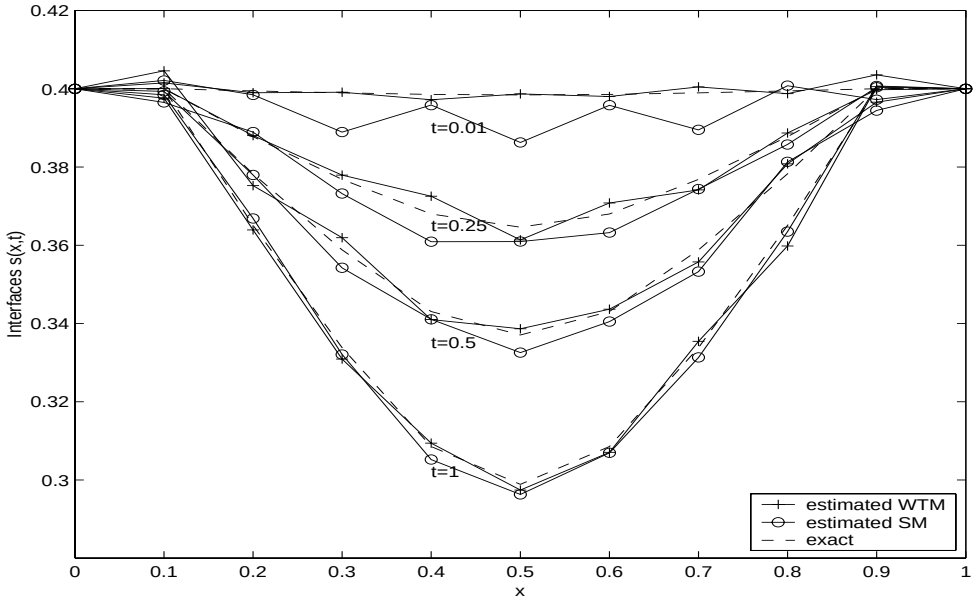

Figure 4. Whole Time and Sequential Methods, noisy case.

8. CONCLUSIONS

Computational results show that the proposed whole time method is able to simultaneously estimate time and space variation of the melting front and saves much computer time compared with the usual sequential method. It is also more accurate. However, in the present work, the interface is identified only on the discretization space and time points since all computations are carried out on the discrete problem. The attempt to use an appropriate method such as the boundary element method to solve the direct system (1)-(5) will be a future work.

REFERENCES

1. A. Afshari, *Identification de l'Evolution d'un Front de Fusion/Solidification par Résolution Inverse de l'Equation de la Chaleur dans le Domaine Solide*, Thèse d'Université Paris-Sud, Orsay, France, 1990.
2. A. El Badia and F. Moutazaim, A one-phase inverse Stefan problem. *Inverse Problems* (1999) **15**, 1507-1522.
3. A. El Badia, On an inverse phase change problem, *Inverse Problems in Engineering Mechanics II*, 2000, pp.529-535.
4. N. L. Gold'man, *Inverse Stefan Problems*, Dordrecht, Kluwer, 1997.
5. B. Guerrier, H. Liu and C. Bénard, Estimation of the time-dependent profile of a melting front by inverse resolution. *J. Dynamic Syst. Meas. Control* (1997) **119**, 574-578.
6. W. Kurz and D. J. Fisher, *Fundamentals of Solidification*, Trans. Tech. Publications, Switzerland, 1989.
7. X. Wang, M. Rosset-Louerat and C. Bénard, Inverse problem identification of a melting front in 2D case, *Int. Ser. Numer. Math.*, 1992, Vol.**107**, pp.99-110.