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A Mollified Gradient Approach for Solving an Inverse Moving Boundary Problem

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Abstract. In this paper a numerical procedure based on mollification approach and conjugate gradient method is established to solve a one dimensional inverse moving boundary value problem. The problem is considered with noisy data. A regularized problem using mollification approach is considered and the conjugate gradient method is used to solve the proposed problem. Some numerical examples are considered to show the ability of this method. These examples show that the accurate and stable results can be obtained efficiently for these kind of problems.

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1. Introduction

A large number of situations in heat and mass transfer appear as moving boundary problems. These are associated with phase change when

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one phase keeps growing at the expense of the other phase and the two-phase interface moves as a function of time. Heat transfer problems with phase-change are very common in physics and engineering. Typical examples include the production or melting of ice, solidification of castings, and aerodynamic heating of missiles. All of these problems share the characteristic of an interface boundary which moves toward either the solid (melting) or the liquid region (solidification). In these problems, the thermal behavior is assumed to be governed by a well known partial differential equation of heat conduction [1,4,6,7,8]. During recent years, much interest has been devoted to the numerical analysis of nonlinear phase change problems. The main feature of such problems is the moving interface at which the phase change occurs.

These problems often known as direct and inverse Stefan problems. The direct Stefan problem requires determining both the temperature and the moving boundary interface when the initial and boundary conditions, and the thermal properties of the heat conducting body are known. Conversely, inverse Stefan problems require determining the initial and/or boundary conditions, and/or thermal properties from additional information which may involve the partial knowledge or measurement of the moving boundary interface position, its velocity in a normal direction, or the temperature at selected interior thermocouple of the domain [1,4,6,8]. Moreover, inverse Stefan problems belong to a very important class of improperly posed problems of control theory which have many engineering applications. For example, in the technology of refining a material by means of recrystallization one is interested in solving the inverse Stefan problem which consists of finding the temperature and heat flux at the fixed surface which guarantee the flatness of the crystallization front, see [3, 4, 6]. Various numerical methods have been developed to solve the Stefan problems. These methods need to be able to efficiently solve the heat equation on irregular domains and keep track of a moving interface that may undergo complex topological changes [3,4,6].

In this work we investigate the inverse problem of parameter identification in a one-phase ablation-type moving boundary problems numerically. Such a problem can be regarded as discovering the cause from the known result. These inverse problems are ill-posed in the sense that

small perturbations in the observed functions may result in large changes in the corresponding solutions [1,8,6]. The ill-posed nature requires special numerical techniques having regularization properties to stabilize the results of calculations. Recently the filtration based methods such mollification method and the iterative regularization methods such as conjugate gradient methods have been employed in the solution of inverse heat transfer problems and found to be very efficient [2,9,10]. In this study a regularization procedure based on discrete mollification approach and conjugate gradient method (CGM) is established to solve an inverse moving boundary problem. To handle the input data errors, first the mollified version of our interest problem is achieved and then the CGM is used to recover the unknown parameters.
The outline of this paper is as follows: In Section 2, the mathematical formulation of our interest inverse problem is introduced. In Section 3, a numerical procedure based on marching and mollification methods is developed to solve the proposed problem. Section 4 contains the convergence and stability analysis of the introduced numerical method and finally in Section 5 some numerical examples are given and solved with the proposed method.

2. A Brief Review of Discrete Mollification

Let $\delta > 0$, $p' > 0$, $A_p = (\int_{-p'}^{p'} \exp(-s^2)ds)^{-1}$, $I = [0,1]$ and $I_\delta = [p'\delta, 1-p'\delta]$. Notice that the interval I_δ is nonempty whenever $p' < 1/2\delta$. Furthermore suppose $K = \{x_j : j \in Z, 1 \leqslant j \leqslant M\} \subset I$, satisfying

$$x_{j+1} - x_j > d > 0, j \in Z,$$

and

$$0 \leqslant x_1 < x_2 < \cdots < x_M \leqslant 1,$$

where Z is the set of integers and d is a positive constant. Now if $G = \{g_j\}_{j\in Z}$ be a discrete function defined on K and $s_j = (1/2)(x_j + x_{j+1}), j \in Z$, Then the discrete $\delta-$mollification of G is defined by [2,9,10]

$$J_\delta G(x) = \sum_{j=1}^{M} \left(\int_{s_{j-1}}^{s_j} \rho_\delta(x-s)ds \right) g_j,$$

where

$$\rho_{\delta,p'}(x) = \begin{cases} A_p \delta^{-1} \exp\left(-\frac{x^2}{\delta^2}\right), & |x| \leqslant p'\delta, \\ 0, & |x| > p'\delta. \end{cases}$$

Notice that, $\sum_{j=1}^{M} (\int_{s_{j-1}}^{s_j} \rho_\delta(x-s)ds) = \int_{-p'\delta}^{p'\delta} \rho_\delta(s)ds = 1$.
Let $\Delta x = \sup_{j\in Z}(x_{j+1} - x_j)$, some useful results of the consistency, stability, and convergence of discrete δ-mollification are as follows [9].

Theorem 2.1. *If $g(x)$ is uniformly Lipschitz in I and $G = \{g_j = g(x_j) : j \in Z\}$ is the discrete version of g, then there exists a constant C, independent of δ, such that*

$$\| J_\delta G - g \|_{\infty, I_\delta} \leqslant C(\delta + \Delta x).$$

Moreover, if $g'(x) \in C(I)$ then,

$$\| (J_\delta G)' - g' \|_{\infty, I_\delta} \leqslant C\left(\delta + \frac{\Delta x}{\delta}\right).$$

If the discrete functions $G = \{g_j : j \in Z\}$ and $G^\varepsilon = \{g_j^\varepsilon : j \in Z\}$, which are defined on K, satisfy $\| G - G^\varepsilon \|_{\infty,K} \leqslant \varepsilon$, then we have

$$\| J_\delta G - J_\delta G^\varepsilon \|_{\infty, I_\delta} \leqslant \varepsilon,$$

$$\| (J_\delta G)' - (J_\delta G^\varepsilon)' \|_{\infty, I_\delta} \leqslant \frac{C\varepsilon}{\delta}.$$

If $g(x)$ is uniformly Lipschitz on I, let $G = \{g_j = g(x_j) : j \in Z\}$ be the discrete version of g and $G^\varepsilon = \{g_j^\varepsilon : j \in Z\}$ be the perturbed discrete version of g satisfying $\| G - G^\varepsilon \|_{\infty,K} \leqslant \varepsilon$. then,

$$\| J_\delta G^\varepsilon - J_\delta g \|_{\infty, I_\delta} \leqslant C(\varepsilon + \Delta x),$$

and

$$\| J_\delta G^\varepsilon - g \|_{\infty, I_\delta} \leqslant C(\varepsilon + \delta + \Delta x).$$

Moreover, if $g'(x) \in C(I)$ then,

$$\| (J_\delta G^\varepsilon)' - (J_\delta g)' \|_{\infty, I_\delta} \leqslant \frac{C}{\delta}(\varepsilon + \Delta x),$$

$$\| (J_\delta G^\varepsilon)' - g' \|_{\infty, I_\delta} \leqslant C \left(\delta + \frac{\varepsilon}{\delta} + \frac{\Delta x}{\delta} \right).$$

Denoting the centered difference operator by $\boldsymbol{D}$, *i.e.,* $\boldsymbol{D} f(x) = \frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x}$. *Then we have the following results [5,12].*

Theorem 2.2. *If* $g' \in C^1(R^1)$, *and* $G = \{g_j = g(x_j) : j \in Z\}$ *is the discrete version of* g, *with* G, G^ε *satisfying* $\| G - G^\varepsilon \|_{\infty,K} \leqslant \varepsilon$, *then,*

$$\| \boldsymbol{D}(J_\delta G^\varepsilon) - (J_\delta g)' \|_\infty \leqslant \frac{C}{\delta}(\varepsilon + \Delta x) + C_\delta (\Delta x)^2,$$

$$\| \boldsymbol{D}(J_\delta G^\varepsilon) - g' \|_\infty \leqslant C \left(\delta + \frac{\varepsilon}{\delta} + \frac{\Delta x}{\delta} \right) + C_\delta (\Delta x)^2.$$

Suppose $G = \{g_j : j \in Z\}$ *is a discrete function defined on a set* K, *and* $\boldsymbol{D}_0^\delta$ *is a differentiation operator defined by* $\boldsymbol{D}_0^\delta(G) = \boldsymbol{D}(J_\delta G)(x) \mid_K$, *then*

$$\| \mathbf{D}_0^\delta(G) \|_{\infty,K} \leqslant \frac{C}{\delta} \| G \|_{\infty,K} .$$

3. Governing Equations

3.1 Problem definition

To illustrate the methodology for developing expressions for use in determining an unknown boundary function in a nonhomogeneous medium with constant thermal properties, we consider the following one dimensional inverse moving boundary heat conduction problem

$$C\frac{\partial T}{\partial t} = K\frac{\partial^2 T}{\partial x^2} + h\frac{\partial T}{\partial x} + f(x,t),\ 0 < x < s(t),\ \ 0 < t < T_f, \quad (1)$$

$$T(x,0) = \varphi_1(x), \quad 0 \leqslant x \leqslant s(0), \quad (2)$$

$$T(0,t) = q(t), \quad 0 < t < T_f, \quad (3)$$

$$T(s(t),t) = p(t), \quad 0 < t < T_f, \quad (4)$$

$$\frac{\partial}{\partial x} T(s(t),t)|_{t=t_j} = \overline{\phi}_j, \quad j = 1,2,...,N, \quad (5)$$

where the coefficients K, C and h show the thermophysical properties of our interest environment and supposed to be constants, $f(x,t)$ shows

the nonhomogeneous or source term and $s(t) > 0$ represents the moving boundary.
In the problem (1)-(5) it is supposed that $s(t)$ is a known function and the surface of the slab at $x = 1$ is exposed to an unknown transient heat $p(t)$. Our interest problem consists of determining two functions $u(x, t)$ and $p(t)$ satisfying these equations. This one-dimensional moving boundary problem can be transformed to a fixed boundary problem by a simple stretching of the spatial coordinate according $\zeta = x/s(t)$. Introducing dimensionless variables and parameters, the problem (1)-(5) is transformed into the following dimensionless form

$$\begin{aligned}
Cs^2(t)u_t(\zeta,t) &= Ku_{\zeta\zeta}(\zeta,t) + s(t)\left(h + Cs(t)\zeta\frac{ds}{dt}\right)u_\zeta(\zeta,t) \\
&+ F(\zeta,t), \quad 0 < \zeta < 1,\ 0 < t < T_f, \qquad (6)\\
u(\zeta,0) &= \varphi(\zeta), \quad 0 < \zeta < 1, \qquad (7)\\
u(0,t) &= q(t), \quad 0 < t < T_f, \qquad (8)\\
u(1,t_j) &= p(t), \quad 0 < t < T_f, \qquad (9)\\
u_\zeta(1,t_j) &= \phi_j, \quad j = 1,2,...,N, \qquad (10)
\end{aligned}$$

where $u(\zeta,t) = T(\zeta s(t),t)$, $F(\zeta,t) = s^2(t)f(\zeta s(t),t)$, $\varphi(\zeta) = \varphi_1(\zeta s(0))$ and $\phi_j = \overline{\phi}_j s(t_j)$. It is assumed that $q(t)$, $\varphi(t)$ and ϕ_j, $j = 1,2,....,N$, are only known approximately as $p^\varepsilon(t)$, $\varphi^\varepsilon(t)$ and ϕ_j^ε such that

$$\begin{aligned}
\|\varphi(t) - \varphi^\varepsilon(t)\|_\infty &\leqslant \varepsilon \\
\|q(t) - q^\varepsilon(t)\|_\infty &\leqslant \varepsilon \\
\|\phi_j - \phi_j^\varepsilon\|_\infty &\leqslant \varepsilon.
\end{aligned}$$

Because of the presence of the noise in the problem's data, we first stablize the problem using the mollification method.

3.2 Regularized problem

The regularized problem is formulated as follows. Determine $v(x,t)$ and $p(t) = v(1,t)$ from the following problem

$$
\begin{aligned}
Cs^2(t)v_t(\zeta,t) &= Kv_{\zeta\zeta}(\zeta,t) + s(t)\left(h + Cs(t)\zeta\frac{ds}{dt}\right)v_\zeta(\zeta,t) \\
&+ s^2(t)F(\zeta,t), \quad 0<\zeta<1,\ 0<t<T_f, &(11)\\
v(\zeta,0) &= J_{\delta'}(\varphi(\zeta)), \quad 0<\zeta<1. &(12)\\
v(0,t) &= J_{\delta_0}(q(t)), \quad 0<t<T_f, &(13)\\
v(1,t) &= J_{\delta_0}(p(t)), \quad 0<t<T_f, &(14)
\end{aligned}
$$

with respect to the following overspecified data

$$v_\zeta(1,t) = J_{\delta_0^*}(\phi_j), \quad j=1,2,...,N, \tag{15}$$

where $J_\delta(.)$ shows the mollified function with respect to the mollification radii δ and the radii of mollifications, δ_0, δ_0^* and δ' are chosen automatically using the GCV method [2, 9].

We use the variational formulation of the inverse heat conduction problem under analysis. In such a case, the solution of the inverse problem based on the minimization of the residual functional defined by the following equation

$$J_1 = \frac{1}{2}\sum_{i=1}^{N}(v(1,t_i;p) - J_{\delta_0^*}(\phi_i))^2, \tag{16}$$

where $v(1,t;p)$ is the temperature computed at $\zeta = 1$ by the solving direct problem (11)-(14) at the $t = t_j,\ j = 1,2,...,N$. The conjugate gradient method with an adjoint problem is used for the minimization of the objective functional. Such minimization procedure requires the solution of auxiliary problems, known as sensitivity and adjoint problems. This inverse problem is recast as an optimum control problem of finding the unknown control function p such that minimizes the functional (16).

4. Method of Optimization by Conjugate Gradient

4.1 Sensitivity problem

The sensitivity function, solution of the sensitivity problem, is defined as the directional derivative of $v(x,t)$ in the direction of the perturbation of the unknown function $p(t)$ [3,5,11,12]. The sensitivity problem for $v(x,t)$ is obtained by assuming that dependent variable $v(x,t)$ is perturbed by $\varepsilon\Delta v(x,t)$ when the coefficient $p(t)$ is perturbed by $\varepsilon\Delta p(t)$, where ε is a real number. The sensitivity problem is then obtained by applying the following limiting process

$$\lim_{\varepsilon\to 0}\frac{L_\varepsilon(p_\varepsilon)-L(p)}{\varepsilon} \tag{17}$$

where $L_\varepsilon(p_\varepsilon)$ and $L(p)$ are the direct problem formulations written in operator form for perturbed and unperturbed quantities, respectively. The application of the limiting process given by equation (17) results in the following sensitivity problem

$$\begin{aligned} Cs^2(t)\Delta v_t(\zeta,t) &= K\Delta v_{\zeta\zeta}(\zeta,t)+s(t)\left(h+Cs(t)\zeta\frac{ds}{dt}\right)\Delta v_\zeta(\zeta,t), \\ &\quad 0<\zeta<1,\ 0<t<T_f, && (18)\\ \Delta v(\zeta,0) &= 0, \quad 0<\zeta<1. && (19)\\ \Delta v(0,t) &= 0, \quad 0<t<T_f, && (20)\\ \Delta v(1,t) &= J_{\delta_0}(\Delta p(t)), \quad 0<t<T_f. && (21)\end{aligned}$$

4.2 Adjoint problem

In order to derive the adjoint problem, the governing equation of the direct problem (11) is multiplied by the Lagrange multiplier $\lambda(\zeta,t)$, integrated in the corresponded space and time domains and added to the original functional (16) [3]. The following extended functional is obtained

$$\begin{aligned} J &= \frac{1}{2}\int_0^{T_f}\sum_{i=1}^{N}(v(1,t_i;p)-J_{\delta_0^*}(\phi_i))^2\delta(\tau-t_i)d\tau \\ &+ \int_0^{T_f}\int_0^1\{Kv_{\zeta\zeta}(\zeta,\tau)+s(\tau)\left(h+Cs(\tau)\zeta\frac{ds}{d\tau}\right)v_\zeta(\zeta,\tau) \\ &- Cs^2(\tau)v_t(\zeta,\tau)\}\lambda(\zeta,\tau)d\zeta d\tau, \qquad (22)\end{aligned}$$

where $\delta(.)$ is the Dirac delta function. Direction derivative of $J(p)$ in the direction of perturbation in $p(t)$ is defined by

$$\lim_{\varepsilon \to 0} \frac{J(p_\varepsilon) - J(p)}{\varepsilon}, \tag{23}$$

where $J(p_\varepsilon)$ denotes the extended functional (23) written for perturbed $p(t)$. The following adjoint problem for the Lagrange multiplier $\lambda(x,t)$ is obtained after some lengthy manipulation and letting the directional derivative of $J(p)$ go to zero

$$K\lambda_{\zeta\zeta}(\zeta,t) - s(t)\left(h + Cs(t)\zeta\frac{ds}{dt}\right)\lambda_\zeta(\zeta,t) + Cs(t)\zeta\frac{ds}{dt}\lambda + Cs^2(t)\lambda_t(\zeta,t) = 0,$$

$$0 < \zeta < 1,\ 0 < t < T_f, \tag{24}$$

$$\lambda(\zeta, T_f) = 0, \quad 0 < \zeta < 1. \tag{25}$$

$$\lambda(0,t) = 0, \quad 0 < t < T_f, \tag{26}$$

$$\lambda(1,t) = -\sum_{i=1}^{N}(v(1,t_i;q) - J_{\delta_0^*}(\phi_i))\delta(t-t_i), \quad 0 < t < T_f. \tag{27}$$

The adjoint problem is different from the standard initial value problem in that the final time condition at time $t = T_f$, is specified instead of the customary initial condition. However, this problem can be transformed to an initial value problem by the transformation of the time variables as $\tau = T_f - t$. Then the classical methods such as finite differences methods can be used to solve the above adjoint problem.

During the limiting process used to obtain the adjoint problem, applied to the directional derivatives of $J(p)$, in the direction of perturbation in $p(t)$, the following integral term is obtained

$$\Delta J = \int_0^{T_f} \{s(t)(h + C\frac{ds}{dt})\lambda(1,t) - \lambda_\zeta(1,t)\}\Delta q(t)dt \tag{28}$$

In the other hand, we supposed that $p(t) \in L_2[0,1]$. Therefore ΔJ might be written as [3,5,12]

$$\Delta J = \int_0^{T_f} \nabla J(p)\Delta p(t)dt. \tag{29}$$

Now, by comparing equations (28) and (29) we obtain the gradient components of $J(p)$ with respect to $p(t)$ as

$$\nabla J(p) \equiv J'(p) = s(t)(h + C\frac{ds}{dt})\lambda(1,t) - \lambda_\zeta(1,t). \tag{30}$$

4.3 Iterative regularization procedure

For the estimation of $p(t)$, the iterative procedure of the CGM is written as follows [3,5,12]

$$p^{n+1}(t) = p^n(t) - \beta^n d^n(t), \quad n = 0, 1, \dots . \tag{31}$$

where $d^n(t)$ is the direction of descent, β is the search step size, and n is the number of iterations. For the iterative procedure, the direction of descent is obtained as a linear combination of the gradient direction with directions of descent of the previous iterations. The direction of descent for the conjugate gradient method can be written as

$$d^0(t) = \nabla J(p(t)), \tag{32}$$

$$d^n(t) = \nabla J^n(p(t)) + \gamma^n \nabla J^{n-1}(p(t)) \quad n = 0, 1, \dots . \tag{33}$$

where γ^n is the conjugation coefficient. Different versions of the conjugate gradient method can be found in literature, depending on how the conjugation coefficient are computed [3]. Here, these parameters are obtained as follows

$$\gamma^0(t) = 0, \tag{34}$$

$$\gamma^n(t) = \frac{\int_0^1 J^n(q(t)^2 dt}{\int_0^1 J^{n-1}(q(t)^2 dt}, \quad n = 1, \dots . \tag{35}$$

The search step size β^n, appearing in the expression of the iterative procedure for estimation of $p(t)$ are obtained by minimizing the objective functional at each iteration along the specified directions of descent. If the objective functional given by (16) is linearized with respect to β^n, the following expression is obtained for determining the search step size

$$\beta^n = \frac{\sum_{i=1}^N (v(1, t_i; p) - J_{\delta_0^*}(\phi_i))\Delta v(1, t_i; p)}{\sum_{i=1}^N (\Delta v(1, t_i; p))^2}, \tag{36}$$

where $v(1, t_i; p)$ and $\Delta v(1, t_i; p)$ are the solutions of direct and sensitivity problems respectively, at the n iteration obtained by setting $p(t) = p^n(t)$ and $\Delta p(t) = d^n(t)$.

As shown in this section, the conjugate gradient method of function estimation belongs to the class of iterative regularization methods. In such class of methods, the stopping criterion for the computational procedure is used as a regularization parameter, so that sufficiently accurate and smooth solution is obtained for the unknown functions. For the stopping criterion, we illustrate in this work the use of the discrepancy principle [3]. With the use of the discrepancy principle, the iterative procedure of the conjugate gradient method is stopped when the difference between the measured and the estimated variables is of the order of the standard deviation,$\overline{\delta}$ of the measurements. Therefore, the iterative procedure is stopped when

$$J(p(t)) < \zeta, \tag{37}$$

where a standard way to determine this tolerance is as follows [3]

$$\zeta = \frac{1}{2}N\overline{\delta}^2. \tag{38}$$

5. Computational Tests

The purpose of this section is to numerically validate the proposed numerical procedure. An excellent way to check the accuracy of the numerical calculations is to compare them to the analytical solutions. In all cases, without loss of generality, we set $p' = 3$ (see [10]). The radii of mollification are always chosen automatically using the mollification and GCV methods. Discretized measured approximations of boundary data are modeled by adding random errors to the exact data functions [3,5].

The errors between exact and approximate solutions are measured by the relative weighted l_2-norm given by

$$\frac{\left[\int_0^1 \int_0^{T_f} |v_{ex}(\zeta,t) - v_{app}(\zeta,t)|^2 dt d\zeta\right]^{1/2}}{\left[\int_0^1 \int_0^{T_f} |v_{ex}(\zeta,t)|^2 dt d\zeta\right]^{1/2}}.$$

All numerical results has been produced by MATLAB software.

Example 5.1. As the first test-case, in the problem (6)-(10) consider The exact solution may be derived as

$$u(\zeta,t) = -\frac{1}{2} - t + 2(2-\sqrt{3-2t})\zeta - \frac{1}{2}(2-\sqrt{3-2t})^2\zeta^2. \tag{39}$$

The relative l_2 errors between numerical and analytical results are shown in Table 1 for two different noise levels. In addition Figure 1 demonstrates the exact and computed $p(t)$.

Table 1: Relative l_2 error norms for Example 1.

ε	u	u_t	u_ζ
0.001	0.0066421	0.01619	0. 0043352
0.01	0.074694	0.014971	0.0030744

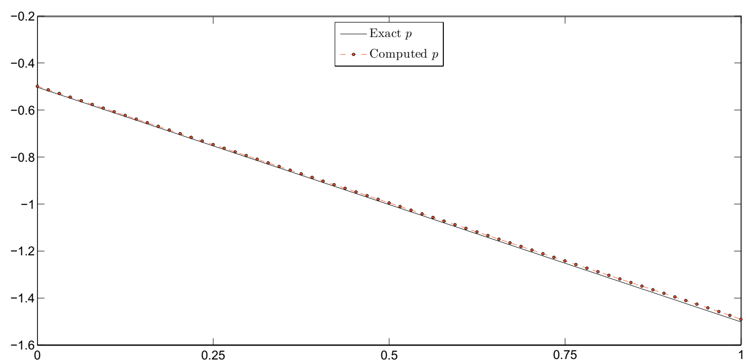

Figure 1: The analytical and numerical solutions for the boundary functions $p(t)$ for Example 1.

Example 5.2. In this example in the problem (6)-(10) we consider The exact solution for $u(\zeta,t)$ can be obtained as

$$u(\zeta,t) = \tanh\left(t + \frac{\zeta}{t+2} + 1\right), \quad (\zeta,t) \in [0,1]\times[0,1].$$

In this example we consider three noise levels to show the behavior of numerical solution. The relative l_2 errors between the numerical and analytical results are shown in Table 2. This table shows that when the noise level approach to zero, the accuracy of the computed results is increased.

Table 2: Relative l_2 error norms for Example 2.

ε	u	u_t	u_ζ
0.0001	0.000399	0.013452	0.024209
0.001	0.002896	0.0135	0.025954
0.01	0.035195	0.016291	0.027758

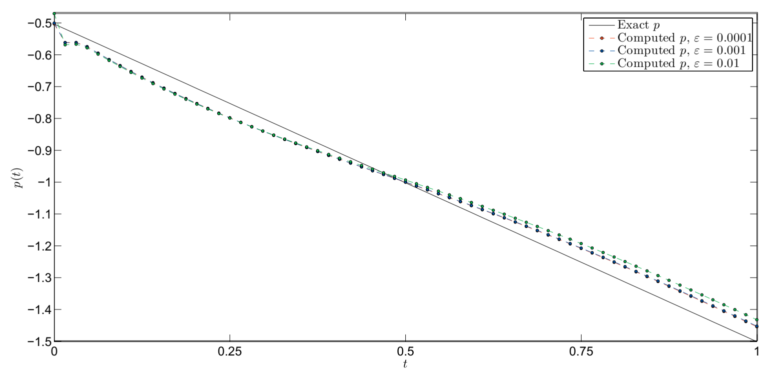

Figure 2: The analytical and numerical solutions for the boundary functions $p(t)$ for Example 2.

6. Conclusion

Overall, from the numerical results presented in this paper, it can be concluded that the marching scheme approximations show good accuracy and stability in comparison with the available exact solutions, even for relatively high noise levels being applied to the boundary input data. Changing the noise level did not seem to change the shape of the approximation, except for t close to the final time T and for the approximation of the flux along the fixed boundary, with errors usually of the same order as those applied in the input data. This conclusion is consistent with the previous studies on the inverse heat conduction problems.

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