

Highly Accurate Computation of Spatial-Dependent Heat Conductivity and Heat Capacity in Inverse Thermal Problem

Chein-Shan Liu¹, Li-Wei Liu² and Hong-Ki Hong²

Abstract: In this paper we are concerned with the parameters identification of the inverse heat conduction problems governed by linear parabolic partial differential equations (PDEs). It is the first time that one can construct a closed-form estimation method for the inverse thermal problems of estimating the spatial-dependent thermophysical parameters. The key points hinge on an establishment of a one-step group preserving scheme (GPS) for the semi-discretization of PDEs, as well as a closed-form solution of the resulting algebraic equations. The new method, namely the Lie-group estimation method, has four advantages: it does not require any prior information on the functional forms of thermal conductivity and heat capacity; no initial guesses are required; no iterations are required; and the inverse problem can be solved in closed-form. Numerical examples were examined to convince that the new approach is highly accurate and efficient with the maximum estimation error very small even for identifying the highly discontinuous and oscillatory parameters. Although the estimation is carried out under a large measurement noise, our method is also stable.

Keyword: Inverse problem, One-step group preserving scheme, Inverse thermal problem, Estimation of thermophysical parameters, Lie-group estimation method, Closed-form estimation.

1 Introduction

In this paper we propose a new method for the identification of unknown coefficients $c(x)$ and

$k(x)$ in the following heat conduction problem:

$$c(x)u_t - \nabla \cdot (k(x)\nabla u) = h(x,t) \text{ in } \Omega, \quad (1)$$

$$u = u_B \text{ on } \Gamma_B, \quad (2)$$

$$u = u^0 \text{ on } \Gamma_0, \quad (3)$$

$$u = u^T \text{ on } \Gamma_T, \quad (4)$$

where u is a scalar temperature field of heat distribution, $h(x,t)$ is a heat source term, and $c(x)$ and $k(x)$ are heat capacity and heat conductivity functions of x , reflecting the nonhomogeneity of the materials to be identified. We take a bounded domain D in \mathbb{R}^m , $m \leq 3$, and a spacetime domain $\Omega = D \times (0, T)$ in \mathbb{R}^{m+1} for a final time $T > 0$, and write three surfaces $\Gamma_B = \partial D \times [0, T]$, $\Gamma_0 = D \times \{0\}$ and $\Gamma_T = D \times \{T\}$ of the boundary $\partial\Omega$. ∇ denotes the m -dimensional gradient operator. Eqs. (1)-(4) constitute an m -dimensional inverse heat conduction problem for a given boundary data $u_B : \Gamma_B \mapsto \mathbb{R}$, an initial data $u^0 : \Gamma_0 \mapsto \mathbb{R}$ and a final data $u^T : \Gamma_T \mapsto \mathbb{R}$ to identify the two unknown functions of $c(x)$ and $k(x)$.

The identification problem in Eqs. (1)-(4) can find a wide range engineering and science applications. For new materials, it is often easier to measure the temperature at some points in the medium at a certain time, rather than to directly measure the thermophysical parameters $k(x)$ and $c(x)$ themselves. The inverse heat conduction problem considered here is to retrieve the heat conductivity $k(x)$ and the heat capacity $c(x)$ in Eq. (1) for a given measured data $u(x, T)$ at a time T . This parameters identification problem is known to be highly ill-posed in the sense that small disturbances of the measured temperature may result in a tremendous error on the parameters' estimation. In order to overcome this problem, there have appeared many studies, for example, Keung

¹Department of Mechanical and Mechatronic Engineering, Taiwan Ocean University, Keelung, Taiwan, E-mail: cslu@mail.ntou.edu.tw

²Department of Civil Engineering, Taiwan University, Taipei, Taiwan

and Zou (1998), Engl and Zou (2000), Ben-yu and Zou (2001), Jia and Wang (2004), and references therein.

Ito and Kunisch (1990, 1996) have proposed very stable and efficient Lagrangian method for the identification of only $k(x)$ under a steady-state condition of Eq. (1) and with a smooth assumption on $k(x)$. Then, Chen and Zou (1999) extended the Lagrangian method to non-smooth case in the steady-state elliptic system. In practical applications we may encounter the inverse thermal problems for composite materials or highly heterogeneous materials with a requirement to estimate the discontinuous and oscillatory thermophysical parameters in a transient state. For this inverse problem, it remains a great challenge due to the lack of efficient, accurate and stable method.

Our approach of the above inverse problem is based on the numerical method of line, which is a well-developed numerical method that transforms the partial differential equations (PDEs) into a system of ordinary differential equations (ODEs), together with the group preserving scheme (GPS) developed previously by Liu (2001) for ODEs. The GPS method is very effective to treat ODEs with special structures as shown by Liu (2005, 2006a) for stiff equations and ODEs with constraints. It is also extended to the calculations of backward heat conduction problem by Liu (2004) and Liu, Chang and Chang (2006), and the sideways heat conduction problem by Chang, Liu and Chang (2005).

Recently, Liu (2006b) has extended the GPS technique to solve the boundary value problems (BVPs), and the numerical results reveal that the GPS is a rather promising method to effectively calculate the two-point BVPs. In the construction of the Lie group method for the calculations of BVPs, Liu (2006b) has introduced the idea of the one-step GPS by utilizing the closure property of Lie group, and hence, the new shooting method has been named by Liu (2006b) the Lie-group shooting method (LGSM). The LGSM is also shown effective on the second order general boundary value problems [Liu (2006c)], the singularly perturbed BVPs [Liu (2006d)], and the

backward heat conduction problems [Chang, Liu and Chang (2007)].

On the other hand, in order to effectively solve the backward in time problems of parabolic PDEs, a past cone structure and a backward group preserving scheme have been successfully developed, such that the new one-step Lie-group numerical methods have been used to solve the backward in time Burgers equation by Liu (2006e), and the backward in time heat conduction equation by Liu, Chang and Chang (2006).

Liu (2006f, 2006g, 2007) has used the concept of one-step GPS to develop the numerical estimation method for the unknown temperature-dependent heat conductivity and heat capacity of one-dimensional heat conduction equation. Because the Lie-group method possesses a certain advantage than other numerical methods due to its group structure, the Lie-group estimation method (LGEM) is believed to be a powerful technique to solve the inverse problems of parameters identification. However, the methodology of LGEM is not yet applied to the identification of parabolic type linear PDEs with nonhomogeneous coefficients in the open literature. It thus deserves our attention to develop an effective, accurate and stable numerical method for this specific inverse problem and to investigate the numerical behavior of this new method based on the group properties. This paper is arranged as follows. In Section 2 for a self-content reason we give a brief sketch of the GPS for ODEs. While the GPS seems useful for the integration of ODEs since its initial development at five years ago, the combination of it with the semi-discretization technique as to be demonstrated in Section 3 for the heat conduction equation really provides us a feasible link to solving the evolutionary type PDEs by the GPS. Due to the good property of Lie group, we will propose an integration technique with a large time stepsize, such that we can use the one-step GPS technique to identify the parameters appeared in the PDEs. The resulting algebraic equations are derived in Section 4 when we apply the one-step GPS to identify the heat conductivity $k(x)$. Again, we demonstrate that how the Lie group theory can help us to solve these parameter estimation equa-

tions with closed-form. Several numerical examples are examined to test our Lie-group estimation method (LGEM). In Section 5 we turn to the estimation of both $k(x)$ and $c(x)$, where we introduce a coordinate transformation technique, which together with the one-step GPS method render again the closed-form solutions of $k(x)$ and $c(x)$ simultaneously. In this section we also consider the measurement noise effect on the numerical results obtained from the new LGEM. Finally, we emphasize some positive results of the new computing method in Section 6.

2 GPS for differential equations system

Group-preserving scheme (GPS) can preserve the internal symmetry group of the considered system. Although we do not know previously the symmetry group of nonlinear differential equations systems, Liu (2001) has embedded them into the augmented dynamical systems, which concern with not only the evolution of state variables but also the evolution of the magnitude of the state variables vector. That is, we can embed

$$\dot{\mathbf{u}} = \mathbf{f}(\mathbf{u}, t), \quad \mathbf{u} \in \mathbb{R}^n, \quad t \in \mathbb{R}, \quad (5)$$

into the following $n + 1$ -dimensional augmented dynamical system:

$$\frac{d}{dt} \begin{bmatrix} \mathbf{u} \\ \|\mathbf{u}\| \end{bmatrix} = \begin{bmatrix} \mathbf{0}_{n \times n} & \frac{\mathbf{f}(\mathbf{u}, t)}{\|\mathbf{u}\|} \\ \frac{\mathbf{f}^T(\mathbf{u}, t)}{\|\mathbf{u}\|} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \|\mathbf{u}\| \end{bmatrix}. \quad (6)$$

It is obvious that the first row in Eq. (6) is the same as the original equation (5), but the inclusion of the second row in Eq. (6) gives us a Minkowskian structure of the augmented state variables of $\mathbf{X} := (\mathbf{u}^T, \|\mathbf{u}\|)^T$ to satisfy the cone condition:

$$\mathbf{X}^T \mathbf{g} \mathbf{X} = 0, \quad (7)$$

where

$$\mathbf{g} = \begin{bmatrix} \mathbf{I}_n & \mathbf{0}_{n \times 1} \\ \mathbf{0}_{1 \times n} & -1 \end{bmatrix} \quad (8)$$

is a Minkowski metric, \mathbf{I}_n is the identity matrix of order n , and the superscript τ stands for the transpose. In terms of $(\mathbf{u}, \|\mathbf{u}\|)$, Eq. (7) becomes

$$\mathbf{X}^T \mathbf{g} \mathbf{X} = \mathbf{u} \cdot \mathbf{u} - \|\mathbf{u}\|^2 = \|\mathbf{u}\|^2 - \|\mathbf{u}\|^2 = 0, \quad (9)$$

where the dot between two n -dimensional vectors denotes their Euclidean inner product. The cone condition is thus the most natural constraint that we can impose on the dynamical system (6).

Consequently, we have an $n + 1$ -dimensional augmented system:

$$\dot{\mathbf{X}} = \mathbf{A} \mathbf{X} \quad (10)$$

with a constraint (7), where

$$\mathbf{A} := \begin{bmatrix} \mathbf{0}_{n \times n} & \frac{\mathbf{f}(\mathbf{u}, t)}{\|\mathbf{u}\|} \\ \frac{\mathbf{f}^T(\mathbf{u}, t)}{\|\mathbf{u}\|} & 0 \end{bmatrix}, \quad (11)$$

satisfying

$$\mathbf{A}^T \mathbf{g} + \mathbf{g} \mathbf{A} = \mathbf{0}, \quad (12)$$

is a Lie algebra $so(n, 1)$ of the proper orthochronous Lorentz group $SO_o(n, 1)$. This fact prompts us to devise the group-preserving scheme (GPS), whose discretized mapping \mathbf{G} must exactly preserve the following properties:

$$\mathbf{G}^T \mathbf{g} \mathbf{G} = \mathbf{g}, \quad (13)$$

$$\det \mathbf{G} = 1, \quad (14)$$

$$G_0^0 > 0, \quad (15)$$

where G_0^0 is the 00th component of \mathbf{G} .

Although the dimension of the new system is raising one more, it has been shown that under the Lipschitz condition of

$$\|\mathbf{f}(\mathbf{u}, t) - \mathbf{f}(\mathbf{y}, t)\| \leq \mathcal{L} \|\mathbf{u} - \mathbf{y}\|, \quad \forall (\mathbf{u}, t), (\mathbf{y}, t) \in \mathbb{D}, \quad (16)$$

where \mathbb{D} is a domain of $\mathbb{R}^n \times \mathbb{R}$, and \mathcal{L} is known as a Lipschitz constant, the new system has an advantage to permit the GPS given as follows [Liu (2001)]:

$$\mathbf{X}_{\ell+1} = \mathbf{G}(\ell) \mathbf{X}_\ell, \quad (17)$$

where \mathbf{X}_ℓ denotes the numerical value of \mathbf{X} at the discrete time t_ℓ , and $\mathbf{G}(\ell) \in SO_o(n, 1)$ is the group value of \mathbf{G} at time t_ℓ . If $\mathbf{G}(\ell)$ satisfies the properties in Eqs. (13)-(15), then \mathbf{X}_ℓ satisfies the cone condition in Eq. (7).

The Lie group can be generated from $\mathbf{A} \in so(n, 1)$ by an exponential mapping,

$$\mathbf{G}(\ell) = \exp[\Delta t \mathbf{A}(\ell)] = \begin{bmatrix} \mathbf{I}_n + \frac{(a_\ell - 1)}{\|\mathbf{f}_\ell\|^2} \mathbf{f}_\ell \mathbf{f}_\ell^T & \frac{b_\ell \mathbf{f}_\ell}{\|\mathbf{f}_\ell\|} \\ \frac{b_\ell \mathbf{f}_\ell^T}{\|\mathbf{f}_\ell\|} & a_\ell \end{bmatrix}, \quad (18)$$

where

$$a_\ell := \cosh\left(\frac{\Delta t \|\mathbf{f}_\ell\|}{\|\mathbf{u}_\ell\|}\right), \quad (19)$$

$$b_\ell := \sinh\left(\frac{\Delta t \|\mathbf{f}_\ell\|}{\|\mathbf{u}_\ell\|}\right). \quad (20)$$

Substituting Eq. (18) for $\mathbf{G}(\ell)$ into Eq. (17), we obtain

$$\mathbf{u}_{\ell+1} = \mathbf{u}_\ell + \eta_\ell \mathbf{f}_\ell, \quad (21)$$

$$\|\mathbf{u}_{\ell+1}\| = a_\ell \|\mathbf{u}_\ell\| + \frac{b_\ell}{\|\mathbf{f}_\ell\|} \mathbf{f}_\ell \cdot \mathbf{u}_\ell, \quad (22)$$

where

$$\eta_\ell := \frac{b_\ell \|\mathbf{u}_\ell\| \|\mathbf{f}_\ell\| + (a_\ell - 1) \mathbf{f}_\ell \cdot \mathbf{u}_\ell}{\|\mathbf{f}_\ell\|^2} \quad (23)$$

is an adaptive factor. From $\mathbf{f}_\ell \cdot \mathbf{u}_\ell \geq -\|\mathbf{f}_\ell\| \|\mathbf{u}_\ell\|$ we can prove that

$$\eta_\ell \geq \left[1 - \exp\left(-\frac{\Delta t \|\mathbf{f}_\ell\|}{\|\mathbf{u}_\ell\|}\right)\right] \frac{\|\mathbf{u}_\ell\|}{\|\mathbf{f}_\ell\|} > 0, \quad \forall \Delta t > 0. \quad (24)$$

This scheme is group properties preserved for all $\Delta t > 0$.

3 Solving heat conduction problems by one-step GPS

3.1 Semi-Discretization

The semi-discrete procedure of PDE yields a coupled system of ODEs. For the one-dimensional heat conduction equation

$$\frac{\partial u}{\partial t} = k \frac{\partial^2 u}{\partial x^2}, \quad (25)$$

we adopt the numerical method of line to discretize the spatial coordinate x by

$$\left. \frac{\partial^2 u(x, t)}{\partial x^2} \right|_{x=i\Delta x} = \frac{u_{i+1}(t) - 2u_i(t) + u_{i-1}(t)}{(\Delta x)^2},$$

where Δx is a uniform discretization spacing length, and $u_i(t) = u(i\Delta x, t)$ for simple notation. Such that Eq. (25) can be approximated by

$$\dot{u}_i(t) = \frac{k}{(\Delta x)^2} [u_{i+1}(t) - 2u_i(t) + u_{i-1}(t)]. \quad (27)$$

The next step is to advance the solution from the initial condition to a desired time T . Really, Eq. (27) has totally n coupled linear ODEs for the n variables $u_i(t), i = 1, 2, \dots, n$, which can be numerically integrated to obtain the solutions.

3.2 One-step GPS

Applying scheme (21) to Eq. (27) we can compute the heat conduction equation by the GPS. Assume that the total time T is divided by K steps, that is, the time stepsize we use in the GPS is $\Delta t = T/K$.

Starting from an initial augmented condition $\mathbf{X}_0 = \mathbf{X}(0)$ we want to calculate the value $\mathbf{X}(T)$ at a desired time $t = T$. By Eq. (17) we can obtain

$$\mathbf{X}_T = \mathbf{G}_K(\Delta t) \cdots \mathbf{G}_1(\Delta t) \mathbf{X}_0, \quad (28)$$

where \mathbf{X}_T approximates the real $\mathbf{X}(T)$ within a certain accuracy depending on Δt . However, let us recall that each $\mathbf{G}_i, i = 1, \dots, K$, is an element of the Lie group $SO_o(n, 1)$, and by the closure property of the Lie group, $\mathbf{G}_K(\Delta t) \cdots \mathbf{G}_1(\Delta t)$ is also a Lie group denoted by $\mathbf{G}(T)$. Hence, we have

$$\mathbf{X}_T = \mathbf{G}(K\Delta t) \mathbf{X}_0 = \mathbf{G}(T) \mathbf{X}_0. \quad (29)$$

This is a one-step transformation from $\mathbf{X}(0)$ to $\mathbf{X}(T)$. The most simple method to calculate $\mathbf{G}(T)$ is given by

$$\mathbf{G}(T) = \begin{bmatrix} \mathbf{I}_n + \frac{(a-1)}{\|\mathbf{f}_0\|^2} \mathbf{f}_0 \mathbf{f}_0^T & \frac{b \mathbf{f}_0}{\|\mathbf{f}_0\|} \\ \frac{b \mathbf{f}_0^T}{\|\mathbf{f}_0\|} & a \end{bmatrix}, \quad (30)$$

where

$$a := \cosh\left(\frac{T \|\mathbf{f}_0\|}{\|\mathbf{u}_0\|}\right), \quad (31)$$

$$b := \sinh\left(\frac{T \|\mathbf{f}_0\|}{\|\mathbf{u}_0\|}\right). \quad (32)$$

That is, we use the initial values of $\mathbf{u}(0)$ to calculate $\mathbf{G}(T)$. Then from Eqs. (21) and (22) we obtain a one-step GPS:

$$\begin{aligned} \mathbf{u}_T &= \mathbf{u}_0 + \eta \mathbf{f}_0 \\ &= \mathbf{u}_0 + \frac{(a-1)\mathbf{f}_0 \cdot \mathbf{u}_0 + b\|\mathbf{u}_0\|\|\mathbf{f}_0\|}{\|\mathbf{f}_0\|^2} \mathbf{f}_0, \end{aligned} \quad (33)$$

$$\|\mathbf{u}_T\| = a\|\mathbf{u}_0\| + \frac{b\mathbf{f}_0 \cdot \mathbf{u}_0}{\|\mathbf{f}_0\|}. \quad (34)$$

The accuracy and efficiency are demonstrated below by numerical examples.

3.3 Example 1

Let us consider the one-dimensional heat conduction equation

$$u_t = u_{xx}, \quad 0 < x < 1, \quad 0 < t < T, \quad (35)$$

with the boundary conditions

$$u(0, t) = 0, \quad u(1, t) = 1,$$

and the initial condition

$$u(x, 0) = \sin \pi x + x.$$

The exact solution is given by

$$u(x, t) = e^{-\pi^2 t} \sin \pi x + x. \quad (36)$$

Liu (2004) has applied the GPS on the above equation by using very small time stepsize. The numerical solution was summarized in Table 1 to show the numerical values at point $x = 0.5$ for different times, where $n = 20$ and $\Delta t = 0.001$ sec were used in the calculation by Liu (2004). In the same table the Galerkin solutions given by Fletcher (1984) with $N = 2, 3$ orders are also included to compare with the exact solution (36) as well as with the GPS solutions. It can be seen that the GPS solutions are more accurate than that of the Galerkin solutions. Our scheme is more easy to implement than that of the Galerkin method, which requires to do a lot of integrals before obtaining the N ordinary differential equations for the N variable coefficients.

In order to apply the one-step GPS to this problem, by a variable transformation $v(x, t) = u(x, t) - x$ let us write Eq. (35) to be

$$v_t = v_{xx}, \quad 0 < x < 1, \quad 0 < t < T, \quad (37)$$

with the boundary conditions

$$v(0, t) = 0, \quad v(1, t) = 0,$$

and the initial condition

$$v(x, 0) = \sin \pi x.$$

We apply the one-step GPS for this problem by solving v , and then $u(x, t) = v(x, t) + x$ is available. In Table 1 we compare the numerical solutions of the one-step GPS at point $x = 0.5$ for different times with the exact solutions. In the calculations by the one-step GPS we were fixed $\Delta x = 1/200$ and let the time stepsizes equal to the times which we carry out the comparison. Very surprisingly, the numerical one-step GPS solutions are very good and almost equal to the exact solutions. If we increase the grid numbers the one-step GPS may produce the same exact solutions.

When $T = 0.4$ sec, we compare three different computations in Fig. 1(a) by the one-step Euler method, the one-step fourth-order Runge-Kutta method (RK4) and the one-step GPS, where $\Delta x = 1/100$ and $\Delta t = 0.4$ sec were fixed. It can be seen that while the one-step GPS provides very accurate solution, the one-step Euler method and the one-step RK4 method both gave invalid solutions. In order to get a solution as accurate as that obtained by the one-step GPS, the RK4 method requires 40000 steps, i.e., $\Delta t = 0.00001$ sec, as shown in Fig. 1(b) for the comparison of numerical errors.

4 Identifying $k(x)$ by the LGEM

The above numerical example supports that the one-step GPS can be very accurate when the time stepsize employed in the calculation is reasonably large. In this section we will start to estimate the nonhomogeneous coefficient functions in the heat conduction equation through an extra measurement of the temperature at a final time. By using the one-step GPS we also suppose that the initial temperature is given, which must be nonzero.

Table 1: The comparison of numerical solutions with exact solutions of Example 1

Time (sec)	Galerkin (N=2)	Galerkin (N=3)	GPS	One-step GPS	Exact
0.02	1.32611	1.32020	1.32083	1.32087	1.32087
0.04	1.18389	1.17278	1.17373	1.17383	1.17383
0.06	1.06757	1.05188	1.05296	1.05312	1.05312
0.08	0.97242	0.95274	0.95382	0.95405	0.95404
0.10	0.89461	0.87144	0.87243	0.87272	0.87271
0.12	0.83096	0.80477	0.80563	0.80595	0.80594
0.14	0.77890	0.75009	0.75080	0.75115	0.75114
0.16	0.73632	0.70526	0.70580	0.70616	0.70615
0.18	0.70150	0.66849	0.66886	0.66923	0.66922
0.20	0.67301	0.63833	0.63856	0.63892	0.63891

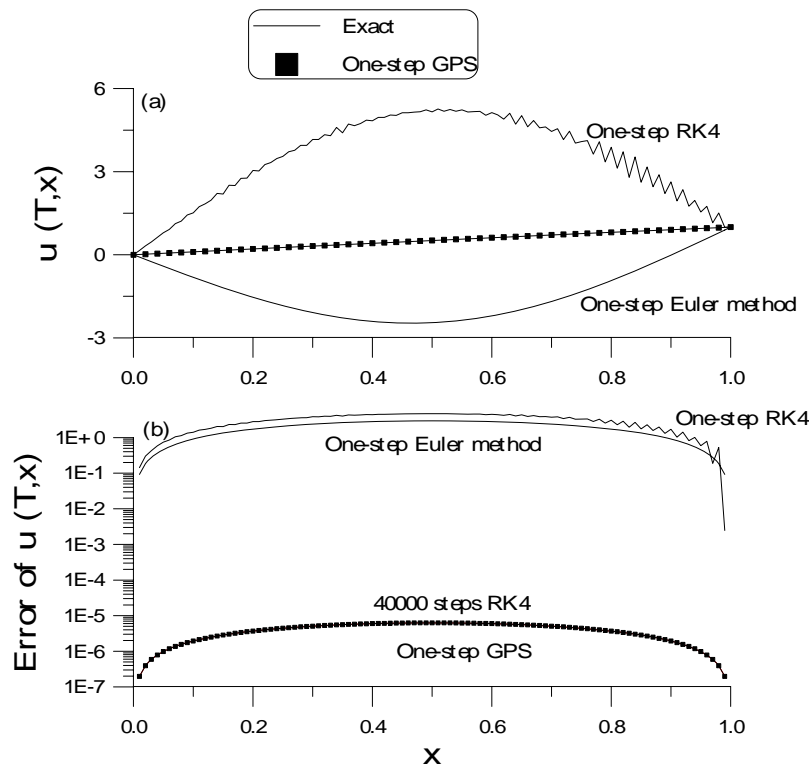


Figure 1: Comparing numerical solutions of one-step GPS, RK4 and Euler methods for Example 1 in (a), and (b) the numerical errors.

4.1 Semi-Discretization

We first assume that $c(x) = 1$, and consider a heat conducting slab composed of nonhomogeneous material with only a variable heat conductivity function $k(x)$ to be identified:

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left[k(x) \frac{\partial u}{\partial x} \right] + h(x, t). \quad (38)$$

In order to identify the heat conductivity $k(x)$, let us impose the following conditions:

$$u(0, t) = u_0(t), \quad u(1, t) = u_r(t), \quad (39)$$

$$u(x, 0) = u^0(x), \quad u(x, T) = u^T(x), \quad (40)$$

where $u_0(t)$ and $u_r(t)$ are boundary conditions at two ends of the slab, and $u^0(x)$ and $u^T(x)$ are two temperature distributions of the slab measured at two different times $t = 0$ and $t = T$.

Let us consider the following difference:

$$\begin{aligned} & \frac{\partial}{\partial x} \left[k(x) \frac{\partial u}{\partial x} \right] \Big|_{x=i\Delta x} \\ &= \frac{1}{(\Delta x)^2} \{ k_{i+1} [u_{i+1} - u_i] - k_i [u_i - u_{i-1}] \}, \end{aligned} \quad (41)$$

and Eq. (38) becomes n coupled ODEs:

$$\begin{aligned} \frac{\partial u_i(t)}{\partial t} &= \frac{1}{(\Delta x)^2} \{ k_{i+1} [u_{i+1}(t) - u_i(t)] \\ &\quad - k_i [u_i(t) - u_{i-1}(t)] \} + h(x_i, t) \end{aligned} \quad (42)$$

with unknown coefficient $k_i = k(x_i) = k(i\Delta x)$, $i = 1, \dots, n$. Here, $k_{n+1} = k(x_{n+1})$ is the boundary value of k , which can be directly measured as a known value.

4.2 One-step GPS equation

When apply the one-step GPS to Eq. (42) from time $t = 0$ to time $t = T$ we obtain a nonlinear equation for k_i :

$$\begin{aligned} u_i^T &= u_i^0 + \frac{\eta}{(\Delta x)^2} \{ k_{i+1} [u_{i+1}^0 - u_i^0] - k_i [u_i^0 - u_{i-1}^0] \} \\ &\quad + \eta h(x_i, 0), \end{aligned} \quad (43)$$

where u_i^T and u_i^0 are two measured temperatures at the i -th grid point. However, η in the above is not a constant but a nonlinear function of k_i .

It is not difficult to rewrite Eq. (43) as

$$\begin{aligned} k_i &= \frac{1}{u_i^0 - u_{i-1}^0} \left[k_{i+1} (u_{i+1}^0 - u_i^0) \right. \\ &\quad \left. - \frac{(\Delta x)^2}{\eta} [u_i^T - u_i^0 - \eta h(x_i, 0)] \right]. \end{aligned} \quad (44)$$

In order to solve k_i , let us return to Eq. (33):

$$\mathbf{f}_0 = \frac{1}{\eta} [\mathbf{u}_T - \mathbf{u}_0]. \quad (45)$$

Substituting it for \mathbf{f}_0 into Eq. (34) we obtain

$$\frac{\|\mathbf{u}_T\|}{\|\mathbf{u}_0\|} = a + \frac{b[\mathbf{u}_T - \mathbf{u}_0] \cdot \mathbf{u}_0}{\|\mathbf{u}_T - \mathbf{u}_0\| \|\mathbf{u}_0\|}, \quad (46)$$

where

$$a := \cosh \left(\frac{T \|\mathbf{u}_T - \mathbf{u}_0\|}{\eta \|\mathbf{u}_0\|} \right), \quad (47)$$

$$b := \sinh \left(\frac{T \|\mathbf{u}_T - \mathbf{u}_0\|}{\eta \|\mathbf{u}_0\|} \right). \quad (48)$$

Let

$$\cos \theta := \frac{[\mathbf{u}_T - \mathbf{u}_0] \cdot \mathbf{u}_0}{\|\mathbf{u}_T - \mathbf{u}_0\| \|\mathbf{u}_0\|}, \quad S := \frac{T \|\mathbf{u}_T - \mathbf{u}_0\|}{\|\mathbf{u}_0\|}, \quad (49)$$

and from Eqs. (46)-(48) it follows that

$$\frac{\|\mathbf{u}_T\|}{\|\mathbf{u}_0\|} = \cosh \left(\frac{S}{\eta} \right) + \cos \theta \sinh \left(\frac{S}{\eta} \right). \quad (50)$$

Upon defining

$$Z := \exp \left(\frac{S}{\eta} \right), \quad (51)$$

from Eq. (50) we obtain a quadratic equation for Z :

$$(1 + \cos \theta) Z^2 - \frac{2 \|\mathbf{u}_T\|}{\|\mathbf{u}_0\|} Z + 1 - \cos \theta = 0. \quad (52)$$

The solution is found to be

$$Z = \frac{\frac{\|\mathbf{u}_T\|}{\|\mathbf{u}_0\|} + \sqrt{\left(\frac{\|\mathbf{u}_T\|}{\|\mathbf{u}_0\|} \right)^2 - (1 - \cos^2 \theta)}}{1 + \cos \theta}, \quad (53)$$

and from Eq. (51) we obtain a closed-form solution of η :

$$\eta = \frac{T \|\mathbf{u}_T - \mathbf{u}_0\|}{\|\mathbf{u}_0\| \ln Z}. \quad (54)$$

Up to here we must point out that for a given T , η is fully determined by \mathbf{u}_0 and \mathbf{u}_T , which are supposed to be known. Therefore, the original nonlinear equation (44) becomes a linear equation for k_i .

Therefore, if we substitute the above η into Eq. (44) and start from a given $k_{n+1} = k(x_{n+1})$ we can proceed to find k_n, \dots, k_1 sequentially. This solution is closed-form for k_i .

In the above we have mentioned that η is a nonlinear function of k_i ; however, by viewing Eqs. (49), (53) and (54) it is known that η is fully determined by \mathbf{u}_0 and \mathbf{u}_T , which are given (or measured) at two different times. This point is very important for our closed-form solution of the parameter. The key points rely on the construction of the method by using the one-step GPS for the estimation of parameter, and the full use of the $n +$

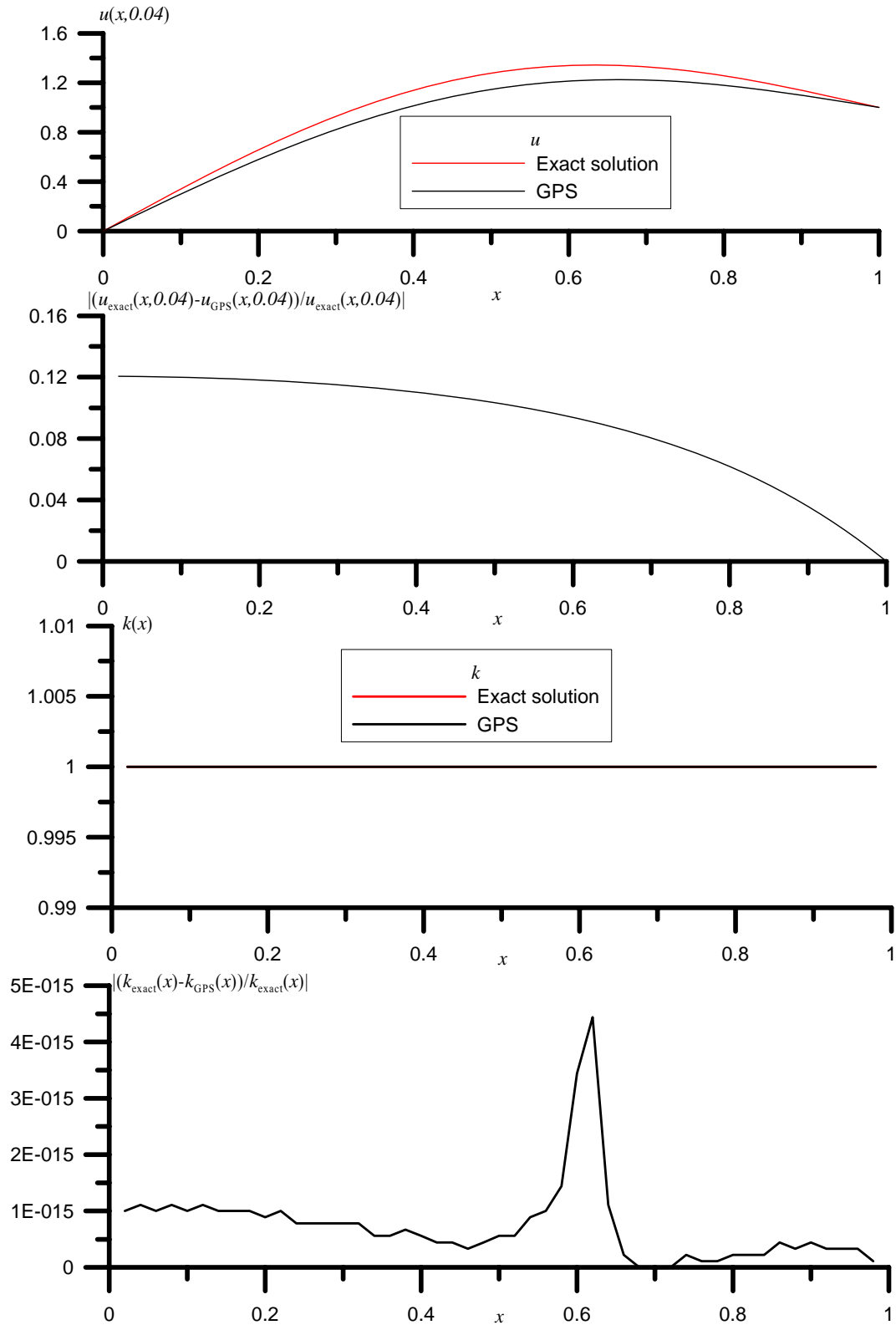


Figure 2: Comparing numerical solution of one-step GPS with exact solution for Example 1 and the error in the estimation of $k(x)$.

1 equations (33) and (34), which are the Lie group transformation between initial temperature and final temperature in the augmented Minkowski space. To distinguish the present method by a combined use of the one-step GPS and the closed-form solution with the aid of Eq. (34), we may call the new method a Lie-group estimation method (LGEM). In order to test our estimation method by the LGEM, let us first consider a simple Example 1 given in Section 3.3, where the exact $k(x)$ is $k(x) = 1$. In this identification of $k(x)$ we have fixed $\Delta x = 1/50$ and $T = 0.04$ sec. Applying Eq. (44), the solutions of k_i is almost equal to 1 with the maximum relative error 4.441×10^{-15} as shown in Fig. 2.

4.3 Example 2

Let us consider a one-dimensional heat conduction problem with [Yeung and Lam (1996)]

$$k(x) = 1 + 0.25e^{-4}(x - 0.3)^2, \quad (55)$$

$$h(x, t) = (x - 0.6)^2(1 - t)e^{-t} - \left\{ 2 + [0.5 - 4(x - 0.3)(x - 0.6)e^{-4(x - 0.3)^2}] \right\} te^{-t}. \quad (56)$$

Under the boundary conditions

$$u(0, t) = 0.36te^{-t}, \quad u(1, t) = 0.16te^{-t}, \quad (57)$$

and the initial condition

$$u(x, 0.1) = 0.090484(x - 0.6)^2, \quad (58)$$

the exact solution is given by

$$u(x, t) = (x - 0.6)^2 te^{-t}. \quad (59)$$

The one-dimensional domain $[0, 1]$ is discretized by $N = n + 2$ points including two end points, at which the two boundary conditions $u_0(t) = 0.36te^{-t}$ and $u_{n+1}(t) = 0.16te^{-t}$ are imposed on the totally n differential equations obtained from Eq. (42). In this identification of $k(x)$ we have fixed $\Delta x = 1/40$, i.e., $n = 39$, and $T = 0.101$ sec. Applying Eq. (44), the solutions of k_i is almost equal to the exact one with the maximum relative error 6.18×10^{-13} as shown in Fig. 3. The above maximum relative error is much smaller than the one 0.0004 obtained by Yeung and Lam (1996).

4.4 Example 3

Let us consider a one-dimensional heat conduction problem with [Yeung and Lam (1996)]

$$k(x) = (x - 3)^2, \quad (60)$$

$$h(x, t) = -7(x - 3)^2 e^{-t}. \quad (61)$$

Under the boundary conditions

$$u(0, t) = 9e^{-t}, \quad u(1, t) = 4e^{-t}, \quad (62)$$

and the initial condition

$$u(x, 0) = (x - 3)^2, \quad (63)$$

the exact solution is given by

$$u(x, t) = (x - 3)^2 e^{-t}. \quad (64)$$

In this identification of $k(x)$ we have fixed $\Delta x = 1/40$ and $T = 0.01$ sec. Applying Eq. (44), the solutions of k_i is almost equal to the exact one with the maximum relative error 2.92×10^{-11} as shown in Fig. 4. The above maximum relative error is much smaller than the one 0.0025 obtained by Yeung and Lam (1996).

4.5 Example 4

Let us consider a one-dimensional heat conduction problem with [Keung and Zou (1998)]

$$k(x) = \begin{cases} 2 - x & x \in [0, 0.3], \\ 1 - x + 4x^2 & x \in (0.3, 0.70), \\ 3 & x \in [0.7, 1], \end{cases} \quad (65)$$

$$h(x, t) = \begin{cases} \{ \pi \cos \pi t (0.5 - |x - 0.5|) + 1 \} \\ \quad \cdot \exp[\sin \pi t] & x \in [0, 0.3], \\ \{ \pi \cos \pi t (0.5 - |x - 0.5|) + (1 - 8x) \} \\ \quad \cdot \exp[\sin \pi t] & x \in (0.3, 0.5), \\ \{ \pi \cos \pi t (0.5 - |x - 0.5|) - (1 - 8x) \} \\ \quad \cdot \exp[\sin \pi t] & x \in [0.5, 0.7), \\ \pi \cos \pi t \exp[\sin \pi t] (0.5 - |x - 0.5|) & x \in [0.7, 1]. \end{cases} \quad (66)$$

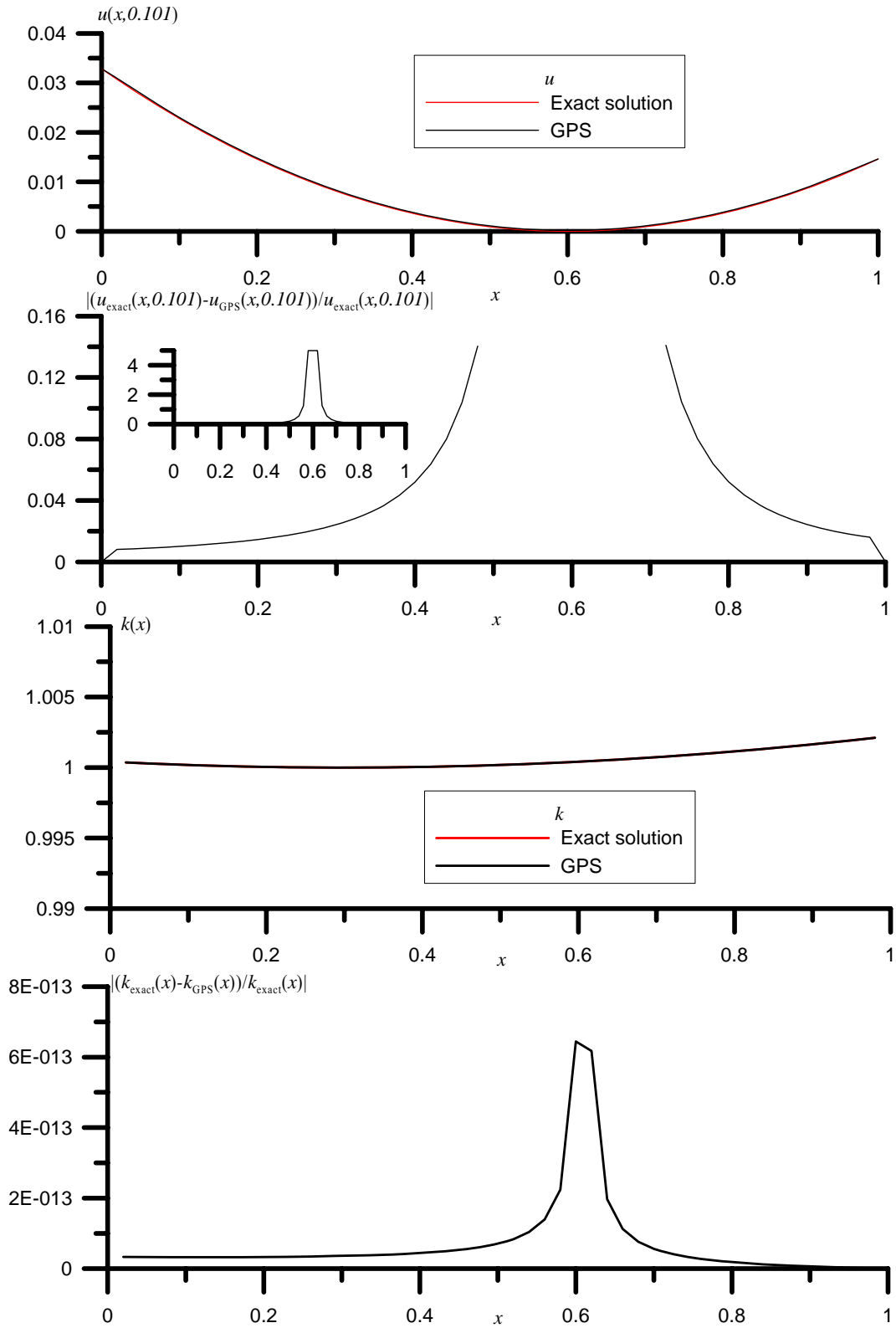


Figure 3: Comparing numerical solution of one-step GPS with exact solution for Example 2 and the error in the estimation of $k(x)$.

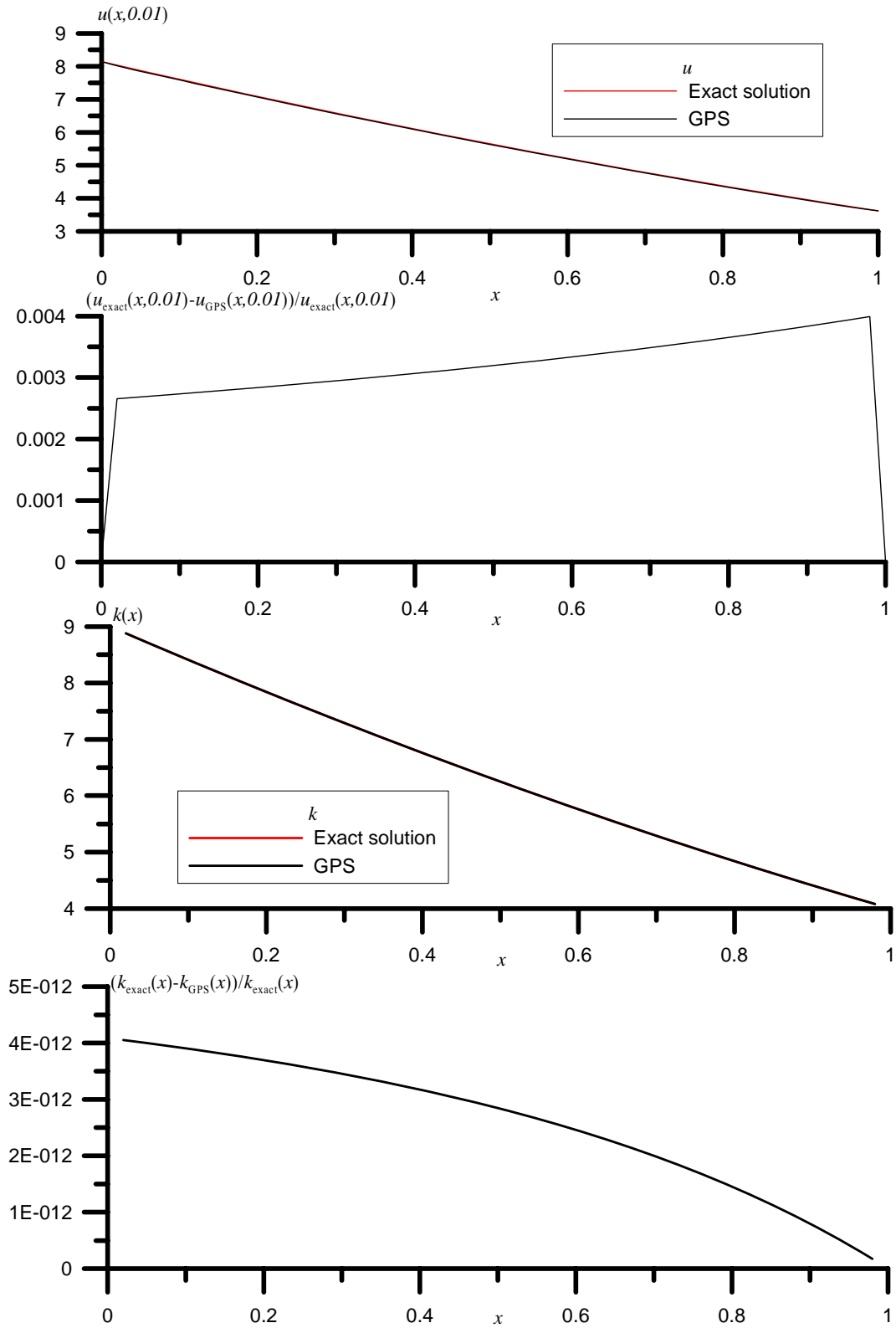


Figure 4: Comparing numerical solution of one-step GPS with exact solution for Example 3 and the error in the estimation of $k(x)$.

Under the boundary conditions

$$u(0,t) = u(1,t) = 0, \quad (67)$$

and the initial condition

$$u(x,0) = 0.5 - |x - 0.5|, \quad (68)$$

the exact solution is given by

$$u(x,t) = (0.5 - |x - 0.5|) \exp[\sin \pi t]. \quad (69)$$

In this identification of $k(x)$ we have fixed $\Delta x = 1/260$ and $T = 0.5$ sec. Applying Eq. (44), the solutions of k_i is almost equal to the exact one with a maximum error 8.882×10^{-16} as shown in Fig. 5. The error is much smaller than the one 0.026 calculated by Keung and Zou (1998). From this example one may appreciate the high accuracy of our estimation method of LGEM even for identifying a highly discontinuous parameter of the above one $k(x)$ in Eq. (65).

4.6 Example 5

This problem is with the following observed data

$$u^T(x) = \sin \pi x, \quad T = 1, \quad (70)$$

which is obtained from the following exact solution:

$$u(x,t) = \sin \pi x \exp[\sin \pi t]. \quad (71)$$

But the identifying function $k(x)$ is highly discontinuous and oscillatory given as follows:

$$k(x) = \begin{cases} 2 & x \in [0, 0.3], \\ 4 & x \in (0.3, 0.6), \\ 2 + \sin(10\pi x) & x \in [0.6, 1]. \end{cases} \quad (72)$$

The function $h(x,t)$ is calculated as

$$h(x,t) = \begin{cases} \{ \pi \cos \pi t + 2\pi^2 \} \exp[\sin \pi t] \sin \pi x & x \in [0, 0.3], \\ \{ \pi \cos \pi t + 4\pi^2 \} \exp[\sin \pi t] \sin \pi x & x \in (0.3, 0.6), \\ \{ \pi \cos \pi t + (2 + \sin 10\pi x)\pi^2 \} \\ \cdot \exp[\sin \pi t] \sin \pi x \\ - 10\pi^2 \cos \pi x \cos 10\pi x \exp[\sin \pi t] & x \in [0.6, 1]. \end{cases}$$

(73)

In this identification of $k(x)$ we have fixed $\Delta x = 1/100$ and $T = 1$ sec. Applying Eq. (44), the solutions of k_i is almost equal to the exact one with the maximum error 6.484×10^{-14} as shown in Fig. 6. The error is much smaller than the one 0.054 calculated by Keung and Zou (1998). From this example it can be seen that our method is also applicable to the estimation of highly discontinuous and oscillatory parameter. It should be stressed that the final time $T = 1$ used here is no more a small quantity. Through these identifications of $k(x)$ in Examples 1-5, it can be seen that our estimations are very accurate in the orders of $10^{-16} - 10^{-11}$, no matter the function $k(x)$ is constant, smooth or non-smooth. To our best knowledge, there appears no report in the open literature that in the estimation of thermophysical parameter one can obtain the closed-form estimating solution. It is clear that the accuracy and efficiency of our LGEM is much better than other methods.

5 Identifying $k(x)$ and $c(x)$ simultaneously

Encouraging by the success of the Lie-group estimation method (LGEM) developed in the previous section for estimating $k(x)$, we will extend the LGEM to both the estimations of $k(x)$ and $c(x)$.

5.1 Semi-Discretization

Let us consider a heat conducting slab with spatial-dependent $c(x) > 0$ and $k(x) > 0$:

$$c(x) \frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left[k(x) \frac{\partial u}{\partial x} \right]. \quad (74)$$

If we consider the central difference as that given by Eq. (41), then Eq. (74) becomes n -coupled linear ODEs:

$$\dot{u}_i(t) = \frac{1}{(\Delta x)^2 c_i} \left\{ k_{i+1} [u_{i+1}(t) - u_i(t)] - k_i [u_i(t) - u_{i-1}(t)] \right\} \quad (75)$$

with unknown coefficients $c_i = c(x_i)$, $k_i = k(x_i)$, $i = 1, \dots, n$.

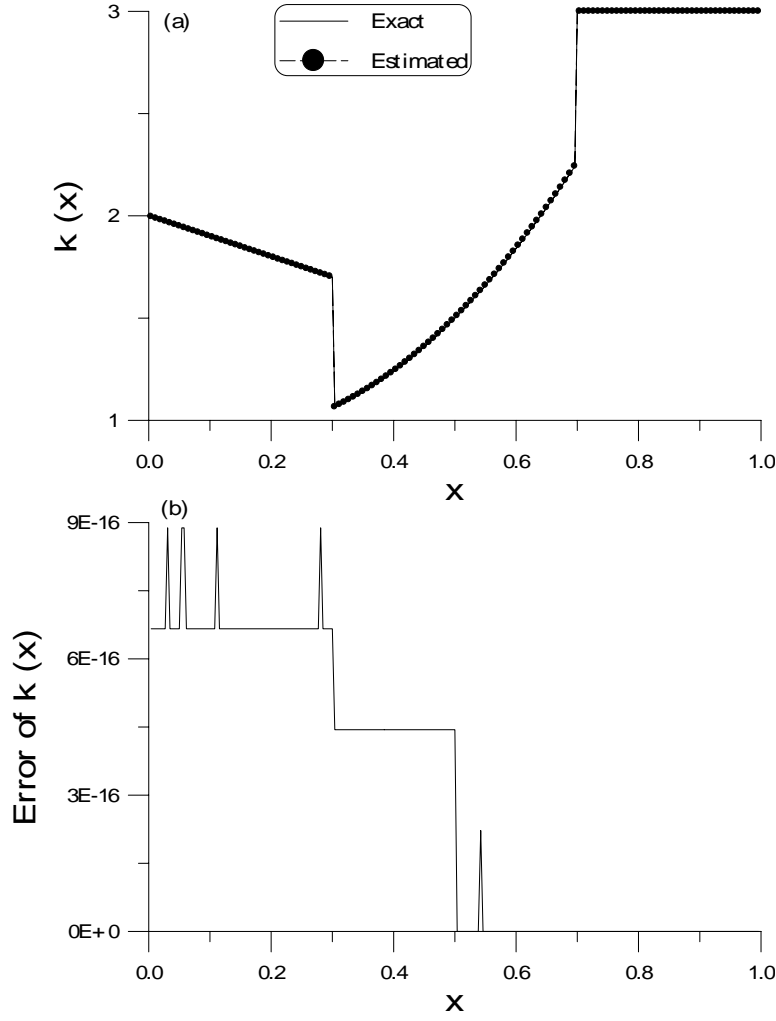


Figure 5: Comparing exact and estimated $k(x)$ for Example 4 in (a), and (b) the estimation error.

5.2 One-step GPS equation

When apply the one-step GPS to Eq. (75) from time $t = 0$ to time $t = T$ we obtain

$$u_i^T = u_i^0 + \frac{\eta_a}{(\Delta x)^2 c_i} \{k_{i+1}[u_{i+1}^0 - u_i^0] - k_i[u_i^0 - u_{i-1}^0]\}. \quad (76)$$

Let $y_i := k_i/c_i$ and suppose that $c(x)$ is a slowly changing function of x , then we can further approximate Eq. (76) by

$$u_i^T = u_i^0 + \frac{\eta_a}{(\Delta x)^2} \{y_{i+1}[u_{i+1}^0 - u_i^0] - y_i[u_i^0 - u_{i-1}^0]\}, \quad (77)$$

which can be rearranged to

$$y_i = \frac{1}{u_i^0 - u_{i-1}^0} \left[y_{i+1}[u_{i+1}^0 - u_i^0] - \frac{(\Delta x)^2}{\eta_a} (u_i^T - u_i^0) \right], \quad (78)$$

where

$$\cos \theta_a := \frac{[\mathbf{u}_T - \mathbf{u}_0] \cdot \mathbf{u}_0}{\|\mathbf{u}_T - \mathbf{u}_0\| \|\mathbf{u}_0\|}, \quad (79)$$

$$Z_a = \frac{\frac{\|\mathbf{u}_T\|}{\|\mathbf{u}_0\|} + \sqrt{\left(\frac{\|\mathbf{u}_T\|}{\|\mathbf{u}_0\|}\right)^2 - (1 - \cos^2 \theta_a)}}{1 + \cos \theta_a}, \quad (80)$$

$$\eta_a = \frac{T \|\mathbf{u}_T - \mathbf{u}_0\|}{\|\mathbf{u}_0\| \ln Z_a}. \quad (81)$$

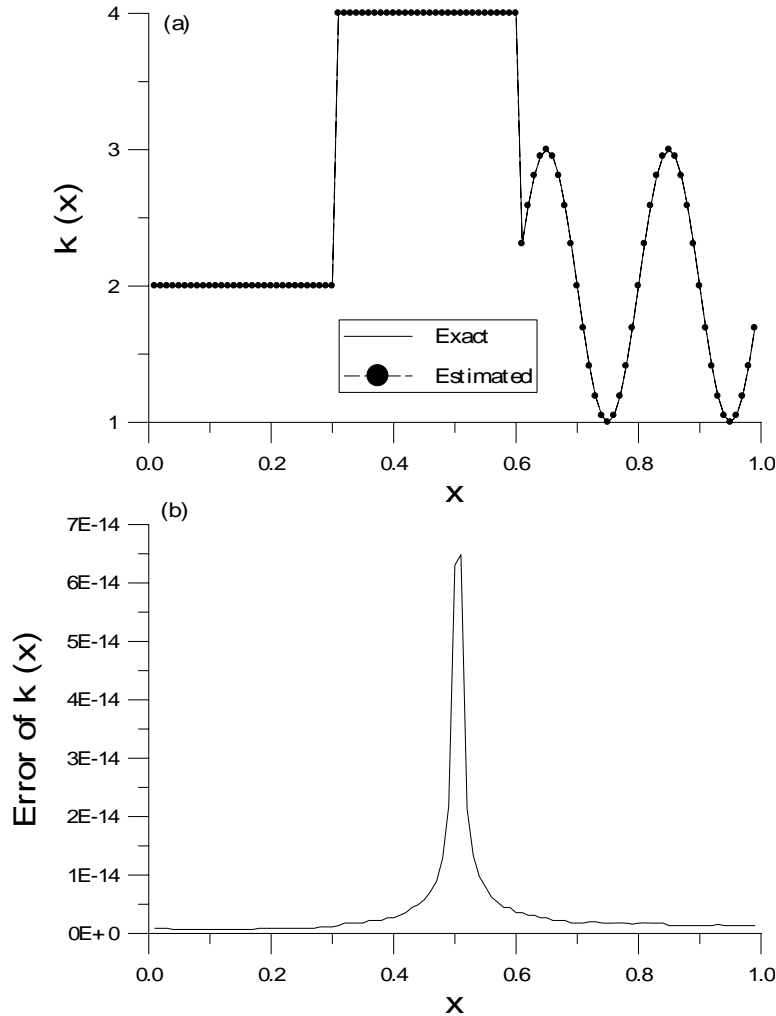


Figure 6: Comparing exact and estimated $k(x)$ for Example 5 in (a), and (b) the estimation error.

Therefore, if we start from a given $y_{n+1} = k(x_{n+1})/c(x_{n+1})$ we can proceed to find y_n, \dots, y_1 sequentially by Eq. (78).

From the above process we can estimate $y(x) = k(x)/c(x)$ but not $c(x)$ or $k(x)$ alone. However, let us consider the following coordinate transformation:

$$z(x) = \int_0^x y(\xi) d\xi = \int_0^x \frac{k(\xi)}{c(\xi)} d\xi, \quad (82)$$

and z is a monotonic function of x because of $y(x) = k(x)/c(x) > 0$. With this transformation, y can be expressed as a function of z , and Eq. (74) can be written as

$$\frac{\partial u}{\partial t} = y^2 \frac{\partial}{\partial z} \left(y \frac{\partial u}{\partial z} \right) + y^3 \frac{k'}{k} \frac{\partial u}{\partial z}. \quad (83)$$

Here k is also supposed to be a function of z and the prime denotes the differentiation with respect to z .

If we consider the following central difference:

$$\begin{aligned} & \frac{\partial}{\partial z} \left[y(z) \frac{\partial u}{\partial z} \right] \Big|_{z=i\Delta z} \\ &= \frac{1}{(\Delta z)^2} \{ y_{i+1} [u_{i+1} - u_i] - y_i [u_i - u_{i-1}] \}, \quad (84) \end{aligned}$$

then Eq. (83) becomes n -coupled linear ODEs:

$$\begin{aligned} \dot{u}_i(t) = & \frac{y_i^2}{(\Delta z)^2} \left\{ y_{i+1} [u_{i+1}(t) - u_i(t)] \right. \\ & \left. - y_i [u_i(t) - u_{i-1}(t)] \right\} \\ & + \frac{y_i^3}{(\Delta z)^2} \left(\frac{k_{i+1}}{k_i} - 1 \right) [u_{i+1}(t) - u_i(t)] \end{aligned} \quad (85)$$

with unknown coefficients $k_i = k(z_i)$, $i = 1, \dots, n$. Notice that y_i were already calculated previously. When Δz is calculated from Eq. (82) as by $\Delta z = y_i \Delta x$, the above equation can be further reduced to

$$\begin{aligned} \dot{u}_i(t) = & \frac{1}{(\Delta x)^2} \left\{ y_{i+1} [u_{i+1}(t) - u_i(t)] \right. \\ & \left. - y_i [u_i(t) - u_{i-1}(t)] \right\} \\ & + \frac{y_i}{(\Delta x)^2} \left(\frac{k_{i+1}}{k_i} - 1 \right) [u_{i+1}(t) - u_i(t)]. \end{aligned} \quad (86)$$

When apply the one-step GPS to Eq. (86) from time $t = 0$ to time $t = T$ we obtain

$$\begin{aligned} u_i^T = u_i^0 + & \frac{\eta_b}{(\Delta x)^2} \left\{ y_{i+1} [u_{i+1}^0 - u_i^0] - y_i [u_i^0 - u_{i-1}^0] \right\} \\ & + \frac{y_i \eta_b}{(\Delta x)^2} \left(\frac{k_{i+1}}{k_i} - 1 \right) [u_{i+1}^0 - u_i^0], \end{aligned} \quad (87)$$

which can be written as

$$\begin{aligned} k_i = k_{i+1} \left[1 + \left\{ (\Delta x)^2 [u_i^T - u_i^0] \right. \right. \\ \left. \left. - \eta_b \left\{ y_{i+1} \cdot [u_{i+1}^0 - u_i^0] - y_i [u_i^0 - u_{i-1}^0] \right\} \right\} \right. \\ \left. \left. / \left\{ \eta_b y_i [u_{i+1}^0 - u_i^0] \right\} \right]^{-1}, \end{aligned} \quad (88)$$

where

$$\cos \theta_b := \frac{[\mathbf{u}_T - \mathbf{u}_0] \cdot \mathbf{u}_0}{\|\mathbf{u}_T - \mathbf{u}_0\| \|\mathbf{u}_0\|}, \quad (89)$$

$$Z_b = \frac{\frac{\|\mathbf{u}_T\|}{\|\mathbf{u}_0\|} + \sqrt{\left(\frac{\|\mathbf{u}_T\|}{\|\mathbf{u}_0\|} \right)^2 - (1 - \cos^2 \theta_b)}}{1 + \cos \theta_b}, \quad (90)$$

$$\eta_b = \frac{T \|\mathbf{u}_T - \mathbf{u}_0\|}{\|\mathbf{u}_0\| \ln Z_b}. \quad (91)$$

If we start from a given $k_{n+1} = k(x_{n+1})$ we can proceed to find k_n, \dots, k_1 sequentially by Eq. (88). When both y and k are estimated we can calculate the heat capacity by $c = k/y$.

5.3 Example 6

Let us apply the above LGEM to estimate the following thermophysical parameters:

$$k(x) = \begin{cases} 2 & x \in [0, 0.3], \\ 4 & x \in (0.3, 0.6), \\ 2 + \sin(10\pi x) & x \in [0.6, 1], \end{cases} \quad (92)$$

$$c(x) = \begin{cases} 2 - x & x \in [0, 0.3], \\ 1 - x + 4x^2 & x \in (0.3, 0.6), \\ 3 & x \in [0.6, 1]. \end{cases} \quad (93)$$

Subjecting to the boundary conditions:

$$u(0, t) = u(1, t) = 0, \quad (94)$$

and the initial condition

$$u(x, 0) = x, \quad (95)$$

we can apply the one-step GPS to calculate the required data.

In this identification of $k(x)$ and $c(x)$ we have fixed $\Delta x = 1/200$ and $T = 0.1$ sec. We first apply Eq. (78) to estimate y_i , which is with the maximum error 3.954×10^{-6} . Then we use Eq. (88) to estimate k_i , the maximum error of which is 1.11×10^{-15} . Then $c_i = k_i/y_i$ is calculated, the maximum error of which is 3.558×10^{-5} . In Fig. 7 we compare the numerical solutions of $k(x)$ and $c(x)$ with the exact solutions. The errors are very small in the order of 10^{-15} for $k(x)$, and in the order of 10^{-5} for $c(x)$. From this example one may appreciate the highly accurate LGEM we provided here even identifying the highly discontinuous and oscillatory parameters of the above $k(x)$ and $c(x)$. As mentioned in Section 1 the inverse thermal problem is sensitive to the measurement error. In the case when the final measured data are contaminated by the random noise,

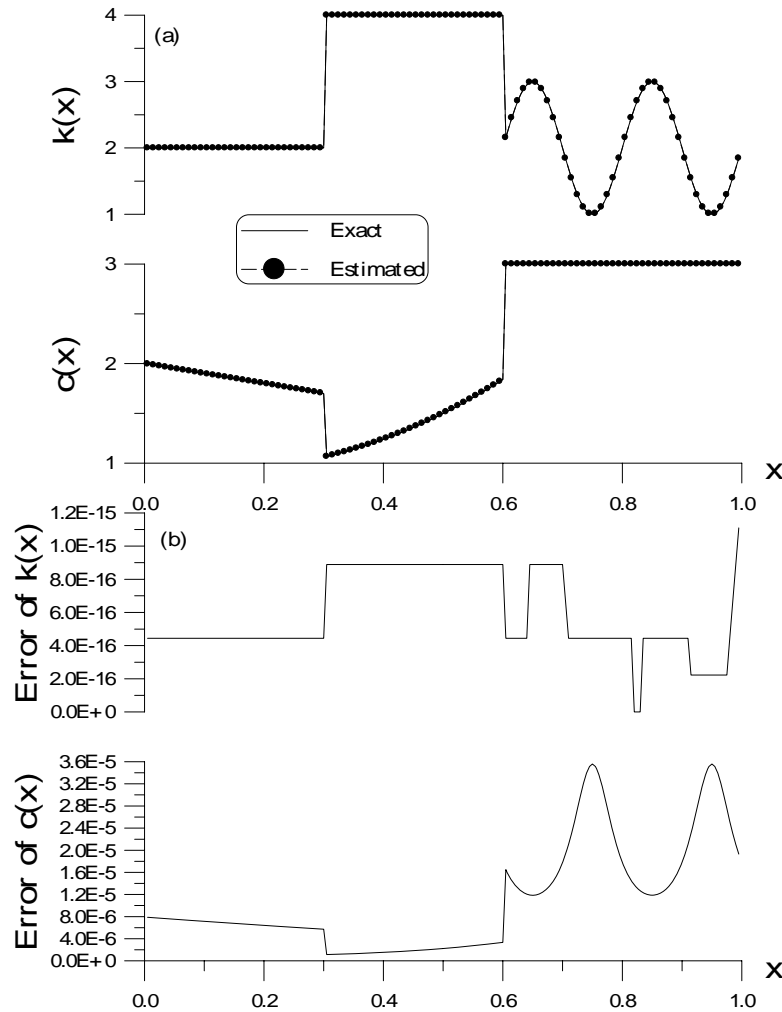


Figure 7: Comparing exact and estimated $k(x)$ and $c(x)$ for Example 6 in (a), and (b) the estimation errors.

we are concerned with the stability of our estimation method, which is investigated by adding random noise on the final data. We use the function `RANDOM_NUMBER` given in Fortran to generate the noisy data $R(i)$, where $R(i)$ are random numbers in $[-1, 1]$. The noise is obtained by multiplying $R(i)$ by a factor s , and we let $u_i^T [1 + sR(i)]$ replace the u_i^T in our estimation equations.

The numerical results with noise were compared with the exact solutions in Fig. 8, where we use $\Delta x = 1/100$ and $T = 0.1$ sec. It can be seen that the noise level with $s = 0.01$ disturbs the numerical solutions deviating from the exact solutions very small, and it appears that the measurement noise makes no obvious effect of our estimation even at the two singular points $x = 0.3$ and

$x = 0.6$.

6 Conclusions

In order to estimate the spatial-dependent thermal conductivity and heat capacity under a given initial temperature and a measured temperature at a final time, we have employed the LGEM to derive algebraic equations and solved them in closed-form. The key points were the construction of one-step group preserving scheme and the full use of the $n + 1$ equations (33) and (34), which are the Lie group transformation between initial temperature and final temperature in the augmented Minkowski space.

Numerical examples were worked out, which show that our LGEM is applicable even under

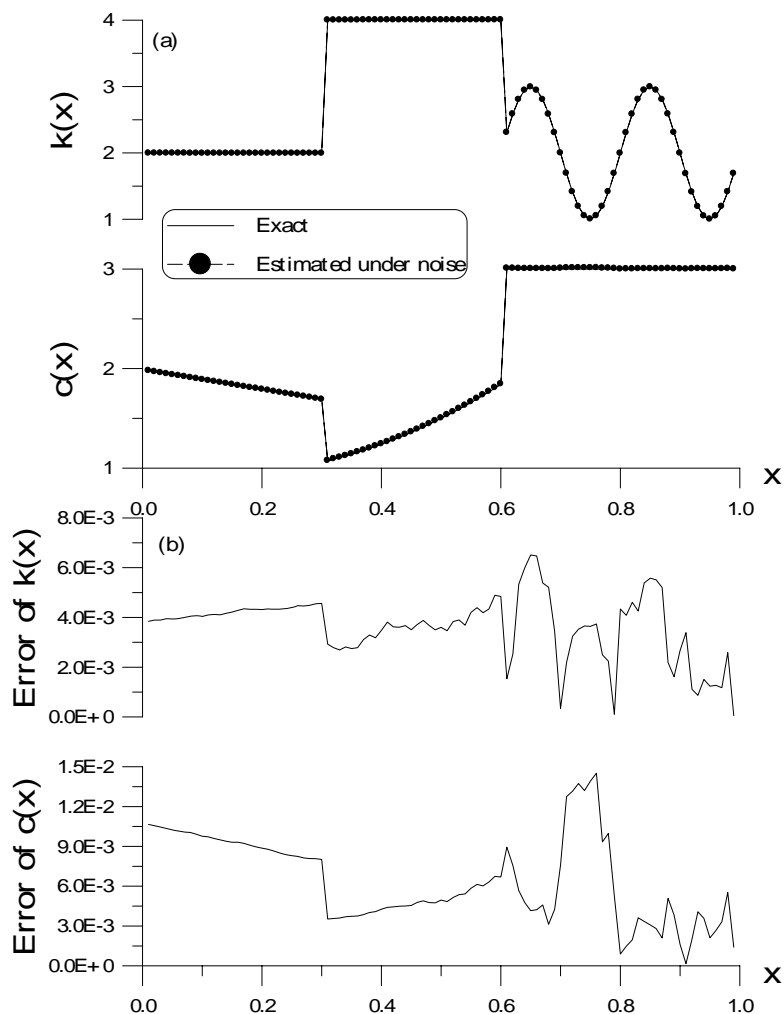


Figure 8: Comparing exact and estimated $k(x)$ and $c(x)$ under noise for Example 6 in (a), and (b) the estimation errors.

a large noise on the measured final temperature. Through this study, it can be concluded that the new estimation method is accurate, effective and stable. Its numerical implementation is very simple and the computational speed is very fast.

In contrast to other parameter estimation methods, the advantages of the new method are that it does not need any prior information on the functional forms of thermal conductivity and heat capacity, no initial guesses are required, no iterations are required and the closed-form solutions are available. It is the first time that one can construct a closed-form estimation method for the inverse problems of estimating the spatial-dependent thermophysical parameters. According to these facts, we may claim that the present

LGEM is highly accurate and effective.

References

- Ben-yu G.; Zou, J.** (2001): An augmented Lagrangian method for parameter identifications in parabolic systems. *J. Math. Anal. Appl.*, vol. 263, pp. 49-68.
- Chang, C.-W.; Liu, C.-S.; Chang, J.-R.** (2005): A group preserving scheme for inverse heat conduction problems. *CMES: Computer Modeling in Engineering & Sciences*, vol. 10, pp. 13-38.
- Chang, J.-R.; Liu, C.-S.; Chang, C.-W.** (2007): A new shooting method for quasi-boundary regularization of backward heat conduction problems. *Int. J. Heat Mass Transf.*, in press.

- Chen, Z. M.; Zou, J.** (1999): An augmented Lagrangian method for identifying discontinuous parameters in elliptic systems. *SIAM J. Contr. Optim.*, vol. 37, pp. 892-910.
- Engl, H. W.; Zou, J.** (2000): A new approach to convergence rate analysis of Tikhonov regularization for parameter identification in heat conduction. *Inv. Prob.*, vol. 16, pp. 1907-1923.
- Fletcher, C. A. J.** (1984): Computational Galerkin Methods. Springer-Verlag, New York.
- Ito, K.; Kunisch, K.** (1990): The augmented Lagrangian method for parameter estimation in elliptic systems. *SIAM J. Contr. Optim.*, vol. 28, pp. 113-136.
- Ito, K.; Kunisch, K.** (1996): Augmented Lagrangian-SQR-methods in Hilbert spaces and applications to control in the coefficients problems. *SIAM J. Optim.*, vol. 6, pp. 96-125.
- Jia, C.; Wang, G.** (2004): Identifications of parameters in ill-posed linear parabolic equations. *Nonlinear Anal.*, vol. 57, pp. 677-686.
- Keung, Y. L.; Zou, J.** (1998): Numerical identifications of parameters in parabolic systems. *Inv. Prob.*, vol. 14, pp. 83-100.
- Liu, C.-S.** (2001): Cone of non-linear dynamical system and group preserving schemes. *Int. J. Non-Linear Mech.*, vol. 36, pp. 1047-1068.
- Liu, C.-S.** (2004): Group preserving scheme for backward heat conduction problems. *Int. J. Heat Mass. Transf.*, vol. 47, pp. 2567-2576.
- Liu, C.-S.** (2005): Nonstandard group-preserving schemes for very stiff ordinary differential equations. *CMES: Computer Modeling in Engineering & Sciences*, vol. 9, pp. 255-272.
- Liu, C.-S.** (2006a): Preserving constraints of differential equations by numerical methods based on integrating factors. *CMES: Computer Modeling in Engineering & Sciences*, vol. 12, pp. 83-107.
- Liu, C.-S.** (2006b): The Lie-group shooting method for nonlinear two-point boundary value problems exhibiting multiple solutions. *CMES: Computer Modeling in Engineering & Sciences*, vol. 13, pp. 149-163.
- Liu, C.-S.** (2006c): Efficient shooting methods for the second order ordinary differential equations. *CMES: Computer Modeling in Engineering & Sciences*, vol. 15, pp. 69-86.
- Liu, C.-S.** (2006d): The Lie-group shooting method for singularly perturbed two-point boundary value problems. *CMES: Computer Modeling in Engineering & Sciences*, vol. 15, pp. 179-196.
- Liu, C.-S.** (2006e): An efficient backward group preserving scheme for the backward in time Burgers equation. *CMES: Computer Modeling in Engineering & Sciences*, vol. 12, pp. 55-65.
- Liu, C.-S.** (2006f): One-step GPS for the estimation of temperature-dependent thermal conductivity. *Int. J. Heat Mass Transf.*, vol. 49, pp. 3084-3093.
- Liu, C.-S.** (2006g): An efficient simultaneous estimation of temperature-dependent thermophysical properties. *CMES: Computer Modeling in Engineering & Sciences*, vol. 14, pp. 77-90.
- Liu, C.-S.** (2007): Identification of temperature-dependent thermophysical properties in a partial differential equation subject to extra final measurement data. *Num. Meth. Partial Diff. Eq.*, in press.
- Liu, C.-S.; Chang, C.-W.; Chang, J.-R.** (2006): Past cone dynamics and backward group preserving schemes for backward heat conduction problems. *CMES: Computer Modeling in Engineering & Sciences*, vol. 12, pp. 67-81.
- Yeung, W. K.; Lam, T. T.** (1996): Second-order finite difference approximation for inverse determination of thermal conductivity. *Int. J. Heat Mass. Transf.*, vol. 39, pp. 3685-3693.