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One-step GPS for the estimation of temperature-dependent thermal conductivity

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Abstract

In this paper we are concerned with the estimation of temperature-dependent thermal conductivity of a one-dimensional inverse heat conduction problem. First, we construct a one-step group-preserving scheme (GPS) for the semi-discretization of quasilinear heat conduction equation, and then derive a quasilinear algebraic equation to determine the unknown thermal conductivity under a given initial temperature and a measured temperature perturbed by noise at time T. The new method does not require any prior information on the functional form of thermal conductivity. Several examples are examined to show that the new approach has high accuracy and efficiency, and the number of iterations spent in solving the quasilinear algebraic equation is smaller than five even in a large temperature range.

Keywords: One-step group-preserving scheme; Thermal conductivity; Inverse heat conduction problem; Semi-discretization

1. Introduction

For heat conduction problems, a case of practical engineering interest is that in which the thermal conductivity property depends on the temperature itself. Many theoretical and experimental methods were developed to measure the thermophysical properties of materials. On the other hand, a number of numerical methods have been used to integrate the resulting quasilinear parabolic equations when thermal conductivity is dependent on temperature, some applicable to any type of temperature-dependent thermal conductivity, and others restricted to particular types, e.g., exponential or linear dependence. In other cases, algebraic solutions have been expressed in terms of a single integral, for example, the Boltzmann transformation and the Kirchhoff transformation.

Roughly speaking, the direct heat conduction problems are already a mature subject, which is concerned with the determination of temperature at the interior points of a body when initial and boundary conditions, thermophysical properties and heat generation are specified. Conversely, the inverse heat conduction problems, which involve the determination of initial condition, the surface temperature or heat flux conditions, energy generation or thermophysical properties from the temperature measurements taken at a finite number of points within the body, are still in a silent progress required more study to clarify the behaviors and properties of inverse problems no matter from analytical or numerical aspect.

The determination of temperature-dependent thermal conductivity from a measured temperature profile is one of the inverse heat conduction problems. It is more difficult than that of the determination of the thermal conductivity of temporal-dependent type or spatial-dependent type. In order to calculate this inverse problem, there appears much advance in this issue, including boundary element method [1], finite element method [2], the Laplace transformation method [3], the conjugate gradient method [4–6], the least-square method [7], the linear inverse method [8–10], the Davidon–Fletcher–Powell method [11], the Kirchhoff and other transformation methods [12–14].

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Nomenclature

$\mathbf{A}$	augmented matrix
a, b	coefficients defined in Eq. (26)
a_ℓ, b_ℓ	coefficients defined in Eq. (15)
a_i, $i = 1,\ldots,5$	coefficients used in Eq. (29)
a_i, $i = 1,\ldots,8$	coefficients used in Eq. (43)
$\mathbb{D}$	a domain in $\mathbb{R}^n \times \mathbb{R}$
$\mathbb{E}^n$	n-dimensional Euclidean space
$\mathbf{f}$	n-dimensional vector field
$\mathbf{f}_\ell$	numerical value of $\mathbf{f}$ at the ℓth time step
$\mathbf{g}$	$n+1$-dimensional Minkowski metric
$\mathbf{G}$	an element of Lorentz group
$\mathbf{G}_i$, $i = 1,\ldots,K$	elements of Lorentz group
G_0^0	the 00th component of $\mathbf{G}$
$\mathbf{I}_n$	n-dimensional unit matrix
$k(u)$	temperature-dependent thermal conductivity
$\hat{k}(u)$	an estimation of $k(u)$
k_i	$:=k(u_i)$
$\mathscr{L}$	Lipschitz constant
$\Vert\bullet\Vert$	Euclidean norm
$\mathbb{M}^{n+1}$	$n+1$-dimensional Minkowski space
n	number of interior grid points
$\mathbb{R}$	the set of real numbers
$\mathbb{R}^n$	n-dimensional real space
$R(i)$	random numbers
s	noise level
$SO_0(n,1)$	$n+1$-dimensional Lorentz group
$so(n,1)$	the Lie algebra of $SO_0(n,1)$
t	time
t_ℓ	discretized time of ℓth step
Δt	time increment
T	total time
u	temperature distribution
u_R	a temperature interval
u_i	numerical value of u at the ith grid point
u_0	fixed temperature at left boundary
$u^0(x)$	initial temperature distribution
$u^T(x)$	temperature distribution at time T
u_i^0	the value of $u^0(x)$ at the ith grid point
u_i^T	the value of $u^T(x)$ at the ith grid point
$\mathbf{u}$	n-dimensional vector
$\mathbf{u}_\ell$	numerical value of $\mathbf{u}$ at the ℓth time step
v	$:=u(x,t) - x$
x	space variable
Δx	lattice spacing length of x
$\mathbf{X}$	$n+1$-dimensional augmented vector
$\mathbf{X}_\ell$	numerical value of $\mathbf{X}$ at the ℓth time step
$\mathbf{X}_0$	the value of $\mathbf{X}$ at the initial time
$\mathbf{X}_T$	the numerical value of $\mathbf{X}$ at time T

Greek symbols

ε	stopping criterion
η	adaptive factor used in one-step GPS
η_ℓ	adaptive factor at the ℓth time step
σ	boundary noise level

Subscripts and superscripts

i, j	indices
K	index
t	transpose

In this paper we would develop a one-step group-preserving scheme and a quasilinear algebraic equation for the inverse problem of estimating the temperature-dependent thermal conductivity. The new method is very different from the above methods. It is an extension of the work by Liu [15,16].

Our proposed scheme is based on the numerical method of line which is a well-developed numerical method that transforms partial differential equations into a system of ordinary differential equations (ODEs). The major contributions of this paper are applying the group-preserving property of the resultant system in the development of a one-step numerical scheme and giving a conviction that the proposed scheme is workable to the inverse problems. Specifically, the proposed scheme is efficient and time saving. Through this study, we may have an easy-implementation and explicit one-step group-preserving scheme (GPS) used in the estimation of temperature-dependent thermal conductivity, the accuracy and efficiency of which are rather better.

2. Group-preserving scheme

2.1. A Lie algebra formulation

Group-preserving scheme (GPS) can preserve the internal symmetry group of the considered system. Although we do not know previously the symmetry group of non-linear differential equations systems, Liu [15] has embedded them into the augmented dynamical systems, which deal with the evolution not only of state variables but also the magnitude of the state variables vector. That is, for an n ordinary differential equations system:

$$\dot{\mathbf{u}} = \mathbf{f}(\mathbf{u}, t), \quad \mathbf{u} \in \mathbb{R}^n, \ t \in \mathbb{R}, \tag{1}$$

we can embed it into the following $n+1$-dimensional augmented dynamical system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{bmatrix} \mathbf{u} \\ \Vert\mathbf{u}\Vert \end{bmatrix} = \begin{bmatrix} \mathbf{0}_{n\times n} & \frac{\mathbf{f}(\mathbf{u},t)}{\Vert\mathbf{u}\Vert} \\ \frac{\mathbf{f}^{\mathrm{t}}(\mathbf{u},t)}{\Vert\mathbf{u}\Vert} & 0 \end{bmatrix}\begin{bmatrix} \mathbf{u} \\ \Vert\mathbf{u}\Vert \end{bmatrix}. \tag{2}$$

Here we assume $\|\mathbf{u}\| > 0$ and hence the above system is well-defined.

It is obvious that the first row in Eq. (2) is the same as the original Eq. (1), but the inclusion of the second row in Eq. (2) gives us a Minkowskian structure of the augmented state variables of $\mathbf{X} := (\mathbf{u}^{\mathrm{t}}, \|\mathbf{u}\|)^{\mathrm{t}}$ satisfying the cone condition:

$$\mathbf{X}^{\mathrm{t}}\mathbf{g}\mathbf{X} = 0, \tag{3}$$

where

$$\mathbf{g} = \begin{bmatrix} \mathbf{I}_n & \mathbf{0}_{n\times 1} \\ \mathbf{0}_{1\times n} & -1 \end{bmatrix} \tag{4}$$

is a Minkowski metric, $\mathbf{I}_n$ is the identity matrix of order n, and the superscript t stands for the transpose. In terms of $(\mathbf{u}, \|\mathbf{u}\|)$, Eq. (3) becomes

$$\mathbf{X}^{\mathrm{t}}\mathbf{g}\mathbf{X} = \mathbf{u}\cdot\mathbf{u} - \|\mathbf{u}\|^2 = \|\mathbf{u}\|^2 - \|\mathbf{u}\|^2 = 0, \tag{5}$$

where the dot between two n-dimensional vectors denotes their scalar product. The cone condition is thus a natural constraint that we can impose on the dynamical system (2).

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

$$\dot{\mathbf{X}} = \mathbf{A}\mathbf{X} \tag{6}$$

with a constraint (3), where

$$\mathbf{A} := \begin{bmatrix} \mathbf{0}_{n\times n} & \frac{\mathbf{f}(\mathbf{u},t)}{\|\mathbf{u}\|} \\ \frac{\mathbf{f}^{\mathrm{t}}(\mathbf{u},t)}{\|\mathbf{u}\|} & 0 \end{bmatrix}, \tag{7}$$

satisfying

$$\mathbf{A}^{\mathrm{t}}\mathbf{g} + \mathbf{g}\mathbf{A} = \mathbf{0} \tag{8}$$

is a Lie algebra $so(n,1)$ of the proper orthochronous Lorentz group $SO_0(n,1)$. This fact prompts us to devise the so-called group-preserving scheme, whose discretized mapping $\mathbf{G}$ exactly preserves the following properties:

$$\mathbf{G}^{\mathrm{t}}\mathbf{g}\mathbf{G} = \mathbf{g}, \tag{9}$$

$$\det \mathbf{G} = 1, \tag{10}$$

$$G_0^0 > 0, \tag{11}$$

where G_0^0 is the 00th component of $\mathbf{G}$. It is a proper orthochronous Lorentz group denoted by $SO_0\ (n,1)$. The term orthochronous used in the special relativity theory is referred to the preservation of time orientation. Here it should be understood as the preservation of the sign of $\|\mathbf{u}\|$.

Remarkably, the original n-dimensional dynamical system (1) in $\mathbb{E}^n$ can be embedded naturally into an augmented $n+1$-dimensional dynamical system (6) in $\mathbb{M}^{n+1}$. That two systems are mathematically equivalent. Although the dimension of the new system is raising one more, it has been shown that under the Lipschitz condition of

$$\|\mathbf{f}(\mathbf{u},t) - \mathbf{f}(\mathbf{y},t)\| \leqslant \mathscr{L}\|\mathbf{u}-\mathbf{y}\| \quad \forall(\mathbf{u},t),(\mathbf{y},t)\in\mathbb{D}, \tag{12}$$

where $\mathbb{D}$ is a domain of $\mathbb{R}^n\times\mathbb{R}$ and $\mathscr{L}$ is known as a Lipschitz constant, the new system has the advantage of allowing us to develop the group-preserving numerical scheme [15]:

$$\mathbf{X}_{\ell+1} = \mathbf{G}(\ell)\mathbf{X}_\ell, \tag{13}$$

where $\mathbf{X}_\ell$ denotes the numerical value of $\mathbf{X}$ at the discrete time t_ℓ, and $\mathbf{G}(\ell)\in SO_0(n,1)$ is the group value at time t_ℓ.

2.2. GPS for differential equations system

The Lie group generated from $\mathbf{A}\in so(n,1)$ is known as a proper orthochronous Lorentz group. An exponential mapping of $\mathbf{A}(\ell)$ admits the closed-form representation:

$$\exp[\Delta t\mathbf{A}(\ell)] = \begin{bmatrix} \mathbf{I}_n + \frac{(a_\ell-1)}{\|\mathbf{f}_\ell\|^2}\mathbf{f}_\ell\mathbf{f}_\ell^{\mathrm{t}} & \frac{b_\ell\mathbf{f}_\ell}{\|\mathbf{f}_\ell\|} \\ \frac{b_\ell\mathbf{f}_\ell^{\mathrm{t}}}{\|\mathbf{f}_\ell\|} & a_\ell \end{bmatrix}, \tag{14}$$

where

$$a_\ell := \cosh\left(\frac{\Delta t\|\mathbf{f}_\ell\|}{\|\mathbf{u}_\ell\|}\right), \quad b_\ell := \sinh\left(\frac{\Delta t\|\mathbf{f}_\ell\|}{\|\mathbf{u}_\ell\|}\right). \tag{15}$$

Substituting the above $\exp[\Delta t\mathbf{A}(\ell)]$ for $\mathbf{G}(\ell)$ into Eq. (13) and taking its first row, we obtain

$$\mathbf{u}_{\ell+1} = \mathbf{u}_\ell + \eta_\ell\mathbf{f}_\ell = \mathbf{u}_\ell + \frac{(a_\ell-1)\mathbf{f}_\ell\cdot\mathbf{u}_\ell + b_\ell\|\mathbf{u}_\ell\|\|\mathbf{f}_\ell\|}{\|\mathbf{f}_\ell\|^2}\mathbf{f}_\ell. \tag{16}$$

From $\mathbf{f}_\ell\cdot\mathbf{u}_\ell \geqslant -\|\mathbf{f}_\ell\|\,\|\mathbf{u}_\ell\|$ we can prove that the adaptive factor η_ℓ satisfying

$$\eta_\ell \geqslant \frac{\|\mathbf{u}_\ell\|}{\|\mathbf{f}_\ell\|}\left[1 - \exp\left(-\frac{\Delta t\|\mathbf{f}_\ell\|}{\|\mathbf{u}_\ell\|}\right)\right] > 0 \quad \forall\Delta t > 0. \tag{17}$$

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

The theory of Lie-group and Lie-algebra has been developed for a long time. However, the Lie-group methods to be employed on the numerical methods are only developed very recently as shown by Liu [15]. The GPS method is very effective to deal with ODEs with special structures as shown by Liu [17] for stiff equations and by Liu [18] for ODEs with constraints.

3. Solving the heat conduction problems by one-step GPS

3.1. Semi-discretization

The numerical method of line is simple in concept that for a given system of partial differential equations discretizes all but one of the independent variables. The semi-discrete procedure yields a coupled system of ordinary differential equations which are then numerically integrated.

Let us consider a heat conducting slab composed of temperature-dependent material with a thermal conductivity function $k(u)$:

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left[k(u)\frac{\partial u}{\partial x}\right], \tag{18}$$

and write

$$\frac{\partial}{\partial x}\left[k(u)\frac{\partial u}{\partial x}\right] = k'(u)\left[\frac{\partial u}{\partial x}\right]^2 + k(u)\frac{\partial^2 u}{\partial x^2}. \tag{19}$$

Then, Eq. (18) becomes a quasilinear heat conduction equation:

$$\frac{\partial u}{\partial t} = k'(u)\left[\frac{\partial u}{\partial x}\right]^2 + k(u)\frac{\partial^2 u}{\partial x^2}. \tag{20}$$

We adopt the numerical method of line to discretize the spatial coordinate x by considering the following finite difference:

$$\frac{\partial}{\partial x}\left[k(u)\frac{\partial u}{\partial x}\right]\Bigg|_{x=i\Delta x} = \frac{k(u_{i+1}) - k(u_i)}{u_{i+1} - u_i}\left[\frac{u_{i+1} - u_i}{\Delta x}\right]^2 + \frac{k(u_i)}{(\Delta x)^2}[u_{i+1} - 2u_i + u_{i-1}], \tag{21}$$

and then Eq. (20) becomes n-coupled non-linear ODEs:

$$\dot{u}_i(t) = \frac{1}{(\Delta x)^2}\{k_{i+1}[u_{i+1}(t) - u_i(t)] - k_i[u_i(t) - u_{i-1}(t)]\} \tag{22}$$

with coefficients $k_i = k(u_i)$, $i = 1, \ldots, n$. Here, Δx is a uniform discretization spacing length, and $u_i(t) = u(i\Delta x, t)$.

The next step is to advance the solution from the initial condition to the desired time T. Really, Eq. (22) has totally n coupled non-linear differential equations for the n variables $u_i(t)$, $i = 1, 2, \ldots, n$, which can be numerically integrated to obtain the solutions.

3.2. One-step GPS

Applying scheme (16) to Eq. (22) we can compute the heat conduction equation by GPS. Assume that the total time T is divided into 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 the desired time $t = T$. By Eq. (13) we can obtain

$$\mathbf{X}_T = \mathbf{G}_K(\Delta t)\cdots\mathbf{G}_1(\Delta t)\mathbf{X}_0, \tag{23}$$

where $\mathbf{X}_T$ approximates the real $\mathbf{X}(T)$ within a certain accuracy depending on Δt. However, let us recall that each $\mathbf{G}_i$, $i = 1, \ldots, K$, is an element of the Lie group $SO_0(n, 1)$, and by the closure property of 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

$$\mathbf{X}_T = \mathbf{G}(K\Delta t)\mathbf{X}_0 = \mathbf{G}(T)\mathbf{X}_0. \tag{24}$$

This is a one-step transformation from $\mathbf{X}_0$ to $\mathbf{X}_T$.

One feasible method to calculate $\mathbf{G}(T)$ is given by

$$\mathbf{G}(T) = \exp[T\mathbf{A}(0)] = \begin{bmatrix} \mathbf{I}_n + \frac{(a-1)}{\|\mathbf{f}_0\|^2}\mathbf{f}_0\mathbf{f}_0^{\rm t} & \frac{b\mathbf{f}_0}{\|\mathbf{f}_0\|} \\ \frac{b\mathbf{f}_0^{\rm t}}{\|\mathbf{f}_0\|} & a \end{bmatrix}, \tag{25}$$

where

$$a := \cosh\left(\frac{T\|\mathbf{f}_0\|}{\|\mathbf{u}_0\|}\right), \quad b := \sinh\left(\frac{T\|\mathbf{f}_0\|}{\|\mathbf{u}_0\|}\right). \tag{26}$$

Then from Eq. (16) we obtain a one-step GPS:

$$\mathbf{u}_T = \mathbf{u}_0 + \eta\mathbf{f}_0, \tag{27}$$

$$\eta = \frac{(a-1)\mathbf{f}_0\cdot\mathbf{u}_0 + b\|\mathbf{u}_0\|\|\mathbf{f}_0\|}{\|\mathbf{f}_0\|^2}. \tag{28}$$

The accuracy and efficiency are demonstrated by numerical examples given below.

3.3. Test the accuracy of one-step GPS

In this section we are going to test the accuracy of one-step GPS through two numerical examples. The first example with $k(u) = 1$ has a closed-form solution, and for the second example with [6,9]

$$k(u) = a_1 + a_2\exp\left(\frac{u}{a_3}\right) + a_4\sin\left(\frac{u}{a_5}\right), \tag{29}$$

there has no closed-form solution available.

3.3.1. Example 1

In order to test our numerical results by the one-step GPS, let us consider the one-dimensional heat conduction equation

$$u_t = u_{xx}, \quad 0 < x < 1, \ \ 0 < t < T \tag{30}$$

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

$$u(x,t) = \mathrm{e}^{-\pi^2 t}\sin\pi x + x. \tag{31}$$

The numerical solution by GPS was summarized in Table 1 to show the numerical values at point $x = 0.5$ for different times, where $n = 20$ and $\Delta t = 0.001$ s were used in our calculation. In the same table the Galerkin solutions

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

Time (s)	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

given by Fletcher [19] with $N = 2, 3$ orders are also included to compare with exact solution (31) as well as with 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, let us by a variable transformation $v(x,t) = u(x,t) - x$ write Eq. (30) to

$$v_t = v_{xx}, \quad 0 < x < 1, \ 0 < t < T \tag{32}$$

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 $v(x,t)$, and then $u(x,t) = v(x,t) + x$. 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 fix $\Delta x = 1/200$ 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 $T = 0.4$ s, we compare three computations in Fig. 1(a) by the one-step Euler method, the one-step fourth-order Runge–Kutta method (RK4) and one-step GPS, where $\Delta x = 1/100$ and $\Delta t = 0.4$ s were fixed. It can be seen that while the one-step GPS results in 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 by the one-step GPS, the RK4 method requires 40 000 steps, i.e., $\Delta t = 0.00001$ s as shown in Fig. 1(b) for the comparison of numerical errors.

3.3.2. Example 2: direct problem

Let us consider Eq. (18) with the thermal conductivity given by Eq. (29), and with the following initial and boundary conditions:

$$u(x,0) = \sin \pi x, \quad u(0,t) = u(1,t) = 0. \tag{33}$$

In the calculations we will fix $a_1 = 1$, $a_2 = 4.5$, $a_3 = 80$, $a_4 = 2.5$ and $a_5 = 5$.

Before embarking the calculation of inverse problem, let us apply the one-step GPS on this quasilinear heat conduction problem. Since for this example we are lack of a closed-form solution we use a very fine time stepsize of the RK4 to calculate the "exact" solution. In Fig. 2 the numerical results at times $T = 0.004$ s and $T = 0.01$ s calculated respectively by the RK4 and one-step GPS were compared. We have fixed $\Delta x = 1/50$ and $\Delta t = 0.00001$ s for RK4 and $\Delta t = T = 0.004$ s and $\Delta t = T = 0.01$ s for one-step GPS. It can be seen that for this non-linear heat conducting problem the one-step GPS is effective. In the same figure we are also plotted the numerical results obtained by the one-step Euler method. Unlike the one-step GPS, the one-step Euler method gave solutions with large errors. Furthermore, we find that the one-step RK4 cannot be applied to this calculation.

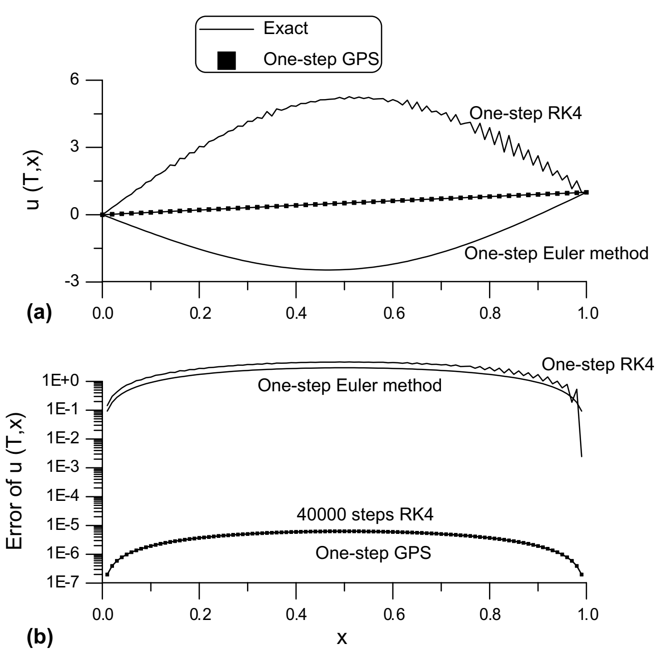

Fig. 1. Comparing numerical solutions of one-step GPS, RK4 and Euler methods for Example 1 in (a), and the numerical errors were compared in (b).

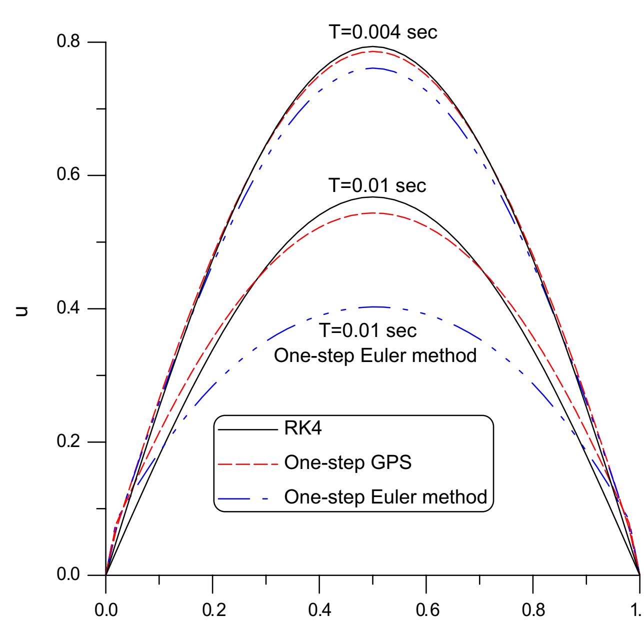

Fig. 2. Comparing numerical solutions of one-step GPS and Euler methods for Example 2 with "exact" solutions calculated by RK4.

4. Identifying the temperature-dependent thermal conductivity

4.1. u is an independent variable in the estimation of k(u)

In order to identify the thermal conductivity function $k(u)$ in Eq. (18), let us impose the following conditions:

$$u(0,t) = u_0, \quad u(1,t) = 0, \tag{34}$$

$$u(x,0) = u^0(x) = u_0(1-x), \quad u(x,T) = u^{\mathrm{T}}(x), \tag{35}$$

where u_0 is a fixed temperature at the left-end of the slab, and $u^0(x)$ and $u^{\mathrm{T}}(x)$ are two temperature distributions of the slab measured at two different times $t = 0$ and $t = T$.

Given $u(x,t)$, Eq. (20) can be viewed as the first-order differential equation for $k(u)$ with u as an independent variable. For u plays a role of the independent variable in the estimation of $k(u)$ we suppose that it is a monotonic function of x, which can be achieved by specifying a suitable u_0 and a small t, since $u(x,0)$ is a monotonically decreasing function of x in the interval of $x \in [0,1]$ as shown in Eq. (35). On the other hand, we suppose that the initial condition of $k(u)$ denoted by $k(0)$ can be known through a precise measurement at the right end of the slab where $u = 0$ is fixed. However, we will consider a possible noise disturbance on the measurement of $k(0)$, which will be called the boundary noise below.

4.2. One-step GPS quasilinear equation

When apply the one-step GPS as shown by Eq. (27) to integrate Eq. (22) from time $t = 0$ to time $t = T$ we obtain a quasilinear equation for k_i:

$$u_i^{\mathrm{T}} = u_i^0 + \frac{\eta}{(\Delta x)^2}\{k_{i+1}[u_{i+1}^0 - u_i^0] - k_i[u_i^0 - u_{i-1}^0]\}, \tag{36}$$

where u_i^T and u_i^0 are two measured temperatures at the ith grid point when $t = T$ and $t = 0$. However, η in the above is not a constant but a non-linear function of k_i as defined by Eq. (28) with

$$\mathbf{u}_0 := [u_1^0, \ldots, u_n^0]^{\mathrm{t}}, \tag{37}$$

$$\mathbf{f}_0 := \frac{1}{(\Delta x)^2}[k_2(u_2^0 - u_1^0) - k_1(u_1^0 - u_0^0), \ldots, k_{n+1}(u_{n+1}^0 - u_n^0) - k_n(u_n^0 - u_{n-1}^0)]^{\mathrm{t}}. \tag{38}$$

It is not difficult to rewrite Eq. (36) as

$$k_i = \frac{u_{i+1}^0 - u_i^0}{u_i^0 - u_{i-1}^0} k_{i+1} - \frac{(\Delta x)^2(u_i^T - u_i^0)}{\eta(u_i^0 - u_{i-1}^0)}. \tag{39}$$

In order to utilize the above equation to solve k_i, let us guess an initial k_i, and η can be determined before the use of Eq. (39).

Therefore, if we start from a given $k_{n+1} = k(0)$ we can proceed to find $k_n, \ldots, k_1$ sequentially by the above equation. Substituting the new k_i into η again we can use Eq. (39) to generate another k_i until the values of k_i converge according to a specified stopping criterion:

$$\sum_{i=1}^{n} |k_i^{j+1} - k_i^j|^2 \leqslant \epsilon, \tag{40}$$

which means that the L^2-norm of the difference between the $j+1$th and the jth iterations of k_i is smaller than the given criterion ϵ.

4.3. Example 2: inverse problem

In Section 3.3.2 we have calculated the Example 2 with different numerical methods by viewing it as a direct problem. Let us return to this example again, and apply the above estimation method to this example by viewing it as an inverse problem.

Through the above discussion we have the idea to apply the one-step GPS method to estimate the temperature-dependent thermal conductivity. For this example the exact $k(u)$ is given by Eq. (29).

In the identification of $k(u)$ we have fixed the initial and boundary conditions to be

$$u(x,0) = u^0(x) = u_0(1-x) = 30(1-x),$$

$$u(0,t) = u_0 = 30, \quad u(1,t) = 0. \tag{41}$$

The data $u(x_i, T)$ is thus calculated by the one-step GPS under the above conditions, where $\Delta x = 1/200$ and $T = 0.0001$ s were used.

The data required in the estimation of k_i, $i = 1, \ldots, n$, by Eq. (39) are now available through $u_i^0 = 30(1 - x_i)$ and $u_i^T = u(x_i, T)$, where $x_i = i\Delta x$ is the coordinate of the ith grid point.

Let us suppose an initial $k_i = 0$, $i = 1, \ldots, n$. Applying Eq. (39) after three iterations, the numerical solutions of k_i converge to the exact values according to the criterion (40) with $\epsilon = 10^{-15}$ as shown in Fig. 3(a), and the results are better with a maximum error of 0.0167606 as shown in Fig. 3(b) with the curve marked by $s = 0$.

In the case when the final measured data are contaminated by random noise, we are concerned with the stability of the one-step GPS estimation method, which is investigated by adding different levels of random noise on the final data, i.e., $u_i^{\mathrm{T}} + sR(i)$, where $R(i)$ are random numbers in $[-1, 1]$ generated from the function RANDOM_NUMBER given in Fortran. The numerical results with noise were compared with the numerical result without considering random noise in Fig. 3, where $T = 0.0005$ s was used for both noisy cases. It can be seen that the noise levels with $s = 0.001$ and 0.002 perturb the numerical solutions deviating from the exact solution small. It appears that large measurement error makes the estimated result away from the exact solution.

In Fig. 4 we plot the variation of maximum errors in the estimation of $k(u)$ with respect to different final times of T taken in the one-step GPS method in the range of $[0.00001, 0.003]$, but fixed the grid length $\Delta x = 1/200$. There

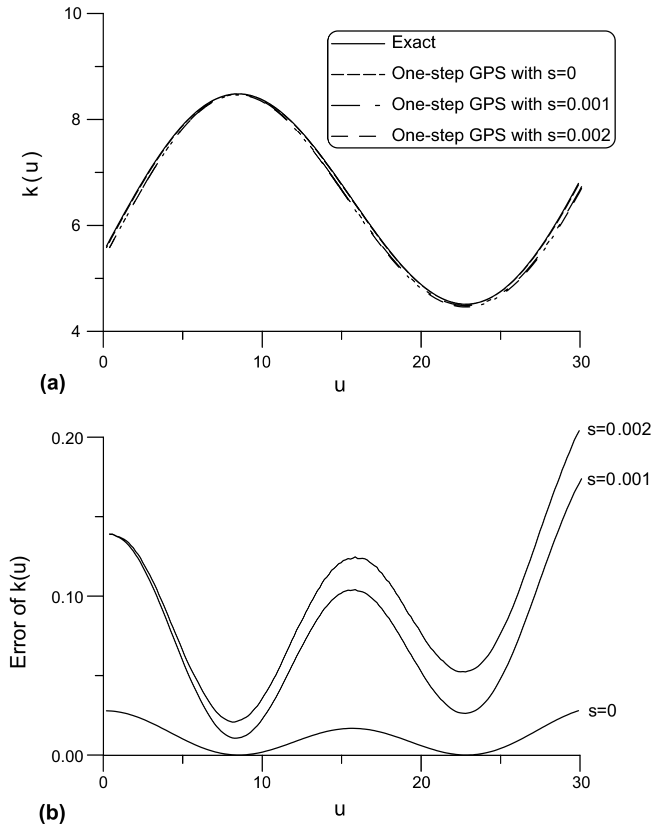

Fig. 3. Estimating $k(u)$ for Example 2 with different noise levels: (a) comparing exact solution and numerical solutions calculated by one-step GPS and (b) numerical errors.

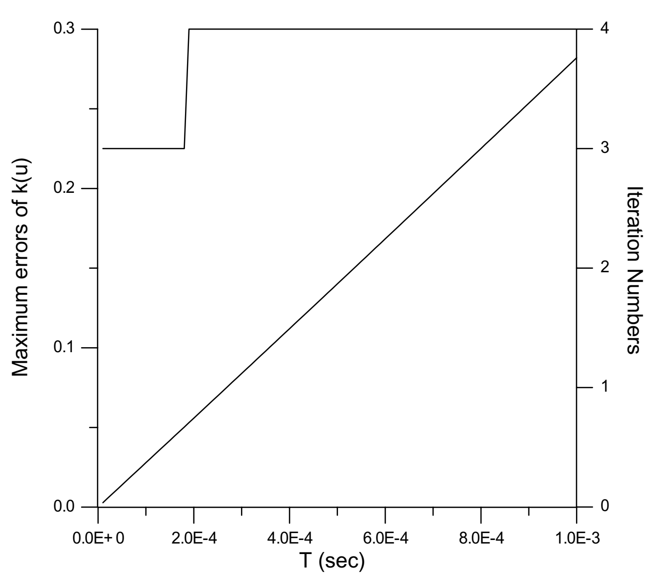

Fig. 4. In the estimation of $k(u)$ for Example 2 we plot the maximum errors and iteration numbers with different T.

appears a linear curve, which indicates that the maximum error is increasing when T increases. This is due to the fact that when T is larger the one-step GPS is less accurate.

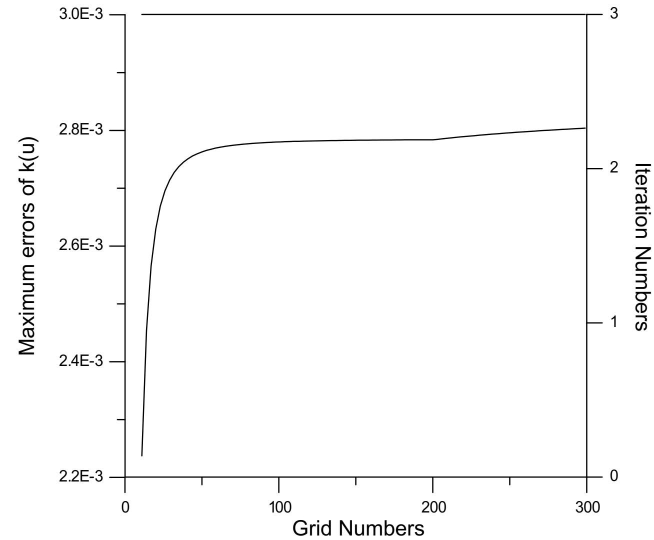

Fig. 5. In the estimation of $k(u)$ for Example 2 we plot the maximum errors and iteration numbers with different grid numbers.

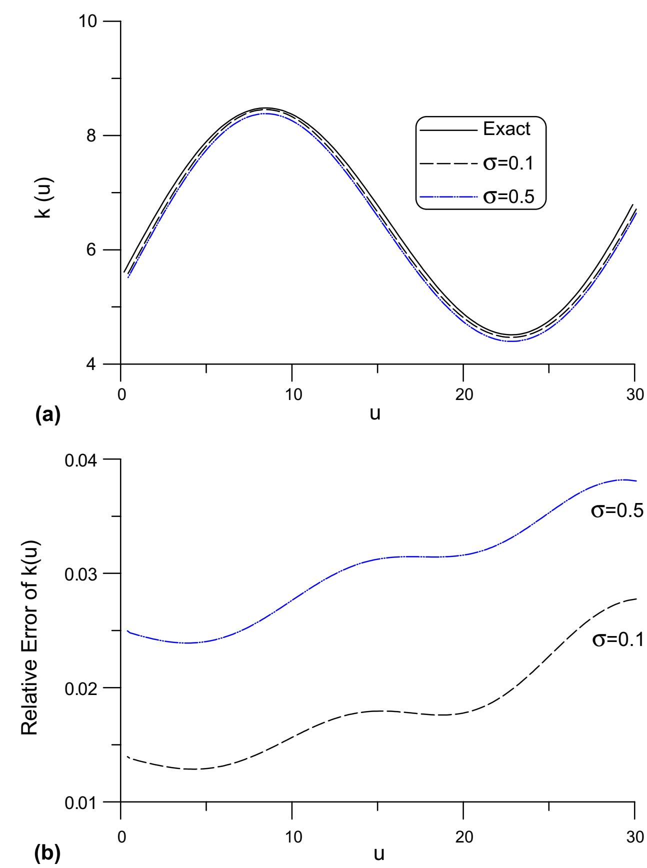

Fig. 6. Estimating $k(u)$ for Example 2 with boundary noise: (a) comparing exact solution and numerical solutions calculated by one-step GPS and (b) numerical errors.

However, even up to $T = 0.003$ s the maximum error is also small in the order of 0.282073.

In terms of the relative error:

$$\frac{\int_{u_R} |k(u) - \hat{k}(u)| \mathrm{d}u}{\int_{u_R} k(u) \mathrm{d}u} \times 100\% \qquad (42)$$

as defined by Yang [9], where $k(u)$ and $\hat{k}(u)$ denote the exact and estimated values of thermal conductivity, and $u_R = [0, 30]$ is the temperature interval, our estimation has a maximum relative error in the order of 0.0533. When $T \leqslant 2 \times 10^{-4}$ the one-step GPS requires three interactions and in the other range it requires four iterations. They show that the speed of convergence is very fast.

Next, we investigate the influence of grid numbers on the maximum error. In Fig. 5 we plot the variation of maximum errors in the estimation of $k(u)$ with respect to different grid numbers taken in the one-step GPS method in the range of [20, 300], but fixed the final time $T = 0.00001$ s. The maximum error increases when the grid number increases. Since $T = 0.00001$ s is very small, in all calculations they require only three iterations, and the maximum errors are smaller than 0.002804.

In the above we are assumed that the initial value $k(0)$ is exactly known. However, since it is a quantity obtained through the measurement carried out at the right boundary of the slab, the inherent measurement error and noise may be exhibited.

In the case when the data $k(0)$ is contaminated by a random boundary noise, we investigate the stability of our estimation method by adding a random noise into $k(0)$. We use $k(0) + \sigma R(i)$ to replace $k(0)$ as an initial value on the calculation of $k(u)$. Therefore, if we start from $k_{n+1} = k(0) + \sigma R(i)$ we can proceed to find $k_n, \ldots, k_1$ sequentially by Eq. (39) until they converge according to the criterion (40).

The numerical results with a fixed noise $s = 0.001$ on the final data and the boundary noises $\sigma = 0.1$ and 0.5 were compared with the exact solution in Fig. 6. The other parameters used are the same as that used in Fig. 3. It can be seen that the noise levels with $\sigma = 0.1$ and 0.5 disturb the numerical solutions deviating from the exact solution small as shown in Fig. 6(a). By using the relative error defined by Eq. (42), we also plot the numerical errors in Fig. 6(b), which appears that the relative errors can be controlled smaller than 3.8% even the boundary disturbance is large up to 9.11%.

4.4. Example 3

Then, let us consider Eq. (18) with the following thermal conductivity [9]:

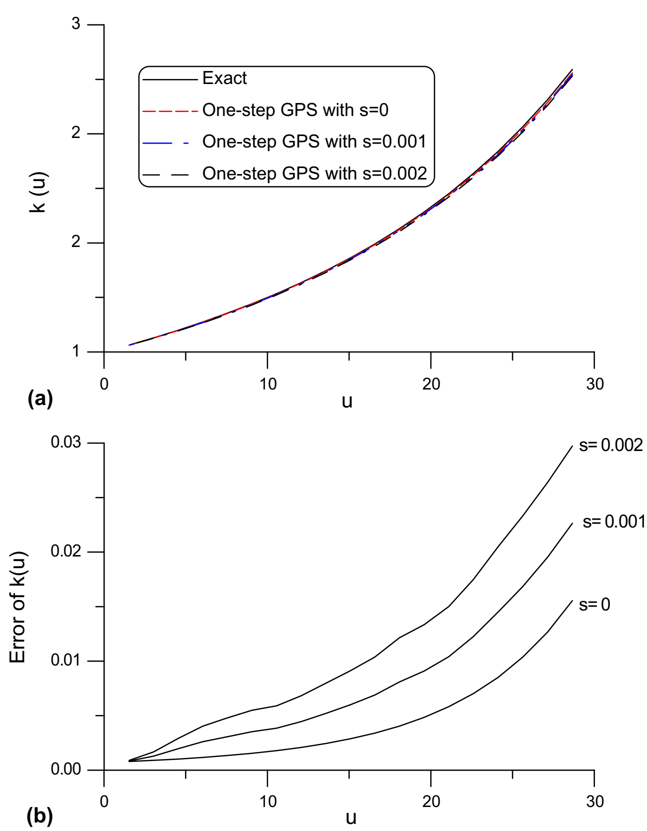

Fig. 7. Estimating $k(u)$ for Example 3 with different noise levels: (a) comparing exact solution and numerical solutions calculated by one-step GPS and (b) numerical errors.

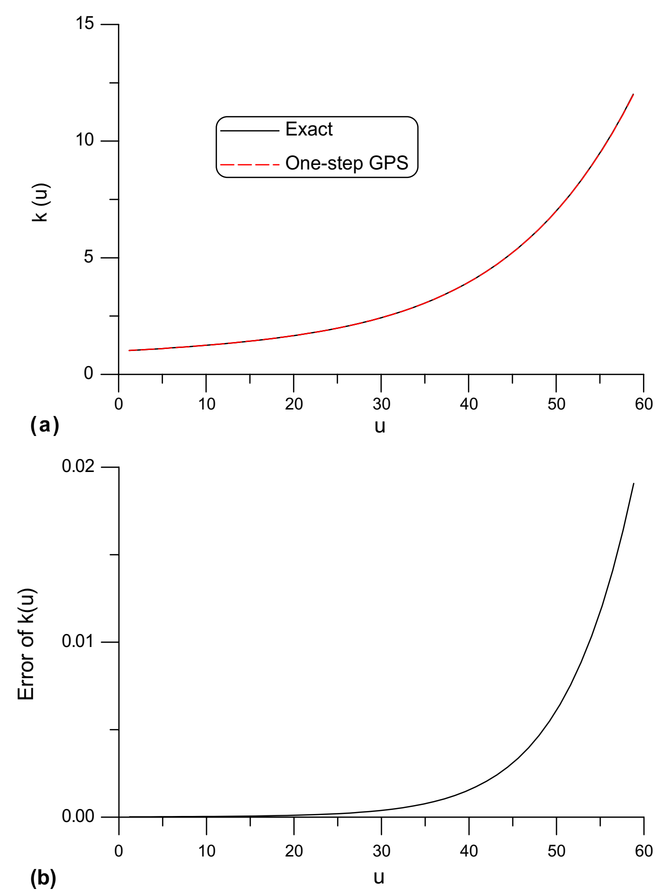

Fig. 8. Estimating $k(u)$ for Example 3 with a large temperature range: (a) comparing exact solution and numerical solution calculated by one-step GPS and (b) numerical error.

$$k(u) = a_1 + a_2\left(\frac{u}{a_8}\right) + a_3\left(\frac{u}{a_8}\right)^2 + a_4\left(\frac{u}{a_8}\right)^3 + a_5\left(\frac{u}{a_8}\right)^4 + a_6\left(\frac{u}{a_8}\right)^5 + a_7\left(\frac{u}{a_8}\right)^6 \quad (43)$$

with $a_1 = a_2 = a_3 = a_4 = a_5 = a_6 = a_7 = 1$ and $a_8 = 50$.

In this identification of $k(u)$ we have fixed the initial and boundary conditions

$$u(x,0) = u_0(1-x) = 30(1-x), \quad u(0,t) = u_0 = 30, \quad u(1,t) = 0, \quad (44)$$

and $\Delta x = 1/20$ and $T = 0.002$ s.

Applying Eq. (39) after four iterations, the numerical solutions of k_i converge to the exact values according to the criterion (40) with $\epsilon = 10^{-15}$ as shown in Fig. 7(a), and the results are very good with a maximum error of 0.015533 and the relative error of 0.003066 as shown in Fig. 7(b).

Even adding the noise levels with $s = 0.001$ and 0.002, they disturb the numerical solutions deviating from the exact solution very small, with a maximum error of 0.022634 and the relative error of 0.005322 for $s = 0.001$, and with a maximum error of 0.029735 and the relative error of 0.007577 for $s = 0.002$.

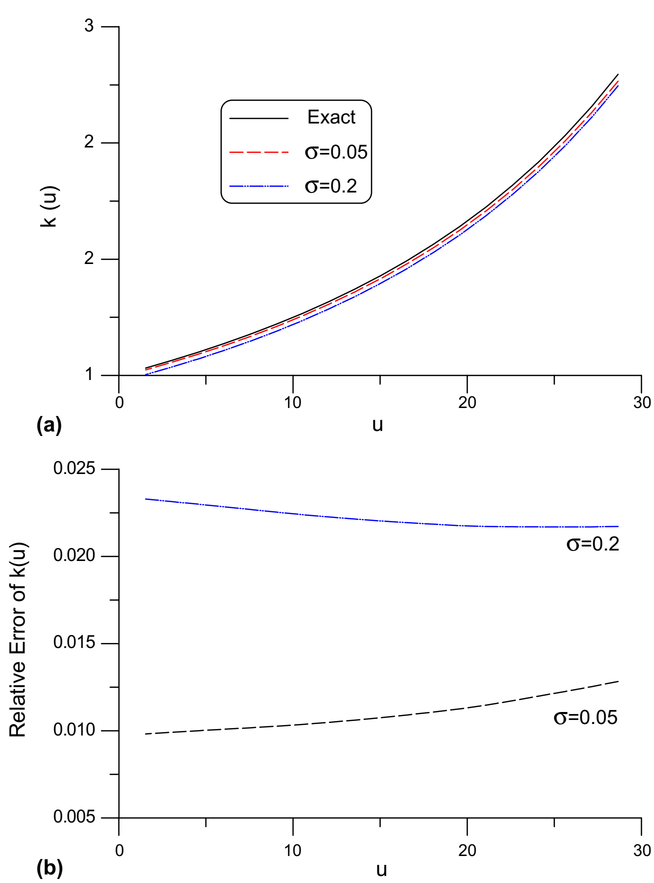

Fig. 9. Estimating $k(u)$ for Example 3 with boundary noise: (a) comparing exact solution and numerical solutions calculated by one-step GPS and (b) numerical errors.

Then, we extend the temperature range to a maximum temperature of 60, that is, we use $u_0 = 60$ to be the left boundary temperature. Thus, the initial and boundary conditions used in this estimation are

$$u(x,0) = 60(1-x), \quad u(0,t) = 60, \quad u(1,t) = 0. \quad (45)$$

Even for this case our estimation of the temperature-dependent thermal conductivity is also good as shown in Fig. 8, where we have fixed $\Delta x = 1/50$ and $T = 0.00001$ s. The numerical solution deviating from the exact solution very small with a maximum error of 0.019076 and a relative error of 0.00072135.

Finally, the numerical results with a fixed noise $s = 0.001$ on the final data and the boundary noises $\sigma = 0.05$ and 0.2 were also compared with the exact solution in Fig. 9(a). The other parameters used are the same as that used in Fig. 7. It can be seen that the relative error can be controlled smaller than 2.5% as shown in Fig. 9(b), even the boundary disturbance is about 6.7% of the exact value.

5. Conclusions

In this paper we were concerned with the numerical solution of an inverse problem for estimating the temperature-dependent thermal conductivity of a one-dimensional quasilinear heat conduction equation. The key point was the construction of a future cone and a one-step group-preserving scheme. It is the first time that we could construct a geometry (future cone), algebra (Lie algebra) and group (Lie group) description of the inverse problems governed by differential equations.

By employing the one-step GPS we have derived a quasilinear algebraic equation to determine the temperature-dependent thermal conductivity under a given initial temperature and a measured temperature at time T. Two numerical examples of the inverse problems were work out, which show that our estimation method is applicable even for a large temperature range. Under the noisy measured final temperature and the boundary measurement noise the one-step GPS was also robust enough to estimate the unknown thermal conductivity. This new technique is accurate and effective, deserving an extension to the estimation of other thermophysical properties in the non-linear heat conduction problems. Recently, the GPS methods are employed to solving the backward heat conduction problem [20] and the sideways heat conduction problem [21].

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