An Efficient Simultaneous Estimation of Temperature-Dependent Thermophysical Properties

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Abstract: In this paper we derive the first-order and second-order one-step GPS applied to the estimation of thermophysical properties. Solving the resultant algebraic equations, which usually converges within ten iterations, it is not difficult to estimate the unknown temperature-dependent thermal conductivity and heat capacity simultaneously, if some supplemented data of measured temperature at a time T is provided. When the measured temperature in the conducting slab is contaminated by noise, our estimated results are also good. The new method does not require any prior information on the functional forms of thermal conductivity and heat capacity. Numerical examples are examined to show that the new approaches, namely the one-step estimation method (OSEM), have high accuracy and efficiency even there are only few measured data.

keyword: One-step Group preserving scheme, Inverse heat conduction problem, Estimation of thermophysical properties.

1 Introduction

Inverse problems and their stable and efficient computations are presently becoming more and more important in many fields of engineering and science. They typically result in mathematical models that are not well-posed in the sense of Hadamard, which means that one or more of the following well-posed properties are lost: for all admissible data the solution exists; for all admissible data the solution is unique; the solution depends continuously on the data. The problems that fail to meet these prerequisites are said to be ill-posed.

Over the last several decades, much interest has been directed towards the employment of inverse techniques to solving the engineering problems that cannot be depicted by direct methods. This situation transpires when all the required data to solve a direct problem or to procure a trustworthy direct solution is not available immediately. Inverse problems are much more difficult to solve than the direct ones. The reason for this is that they are usually ill-posed and very sensitive to the measurement errors of data.

For heat conduction problems, a practical engineering interest is that of which the thermophysical properties depend 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 has been used to integrate the resulting quasilinear parabolic equations when the thermophysical properties are dependent on temperature, some applicable to any type of temperature-dependent thermophysical properties, and others restricted to particular types. In some 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 problem is 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 problem, which involves the determination of initial condition, the surface temperature or heat flux conditions, energy generation or thermophysical properties from the temperature measurements undertaken at a finite number of points within the body, is still an open subject required more study to clarify its behaviors and properties no matter from analytical or numerical aspect. For example, Ling and Atluri (2006) have proposed matrix algebraic method to study the solution stability of inverse heat conduction problems, and of which, Chang, Liu and Chang (2005) have proposed a group preserving scheme to calculate the unknown boundary temperature.

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The determination of temperature-dependent thermophysical properties from a measured temperature profile is one of the inverse heat conduction problem. It is more difficult than that of the determination of the thermophysical properties of temporal-dependent type and spatial-dependent type. In order to calculate this inverse problem, there appears certain progress of the methodology in this issue, including the Laplace transformation method [Chen and Lin (1998)], the conjugate gradient method [Alifanov and Mikhailov (1978), Huang, Yan and Chen (1995), Huang and Yan (1995)], the least-square method [Huang and Ozisik (1991)], the linear inverse method [Yang (1998, 1999, 2000)], the Davidon-Fletcher-Powell method [Tervola (1989)], the Kirchhoff and other transformation methods [Lesnic, Elliott and Ingham (1995), Lesnic (2002), Kim, Kim and Kim (2003)], and the boundary element method [Lesnic, Elliott and Ingham (1996)].

Since the development of group preserving scheme (GPS) by Liu (2001), there have appeared several advances in this direction. First, the GPS is proved to be very effective to deal with ordinary differential equations (ODEs) with special structures as shown by Liu (2005) for stiff equations and by Liu (2006a) for ODEs with multiple constraints. Then, Liu (2006b) has developed a one-step GPS method, which is named the Lie-group shooting method (LGSM), to calculate the multiple solutions of second order ODEs. About the partial differential equations (PDEs), Liu (2006c) has developed the numerical line method together with the GPS to calculate the solutions of Burgers equation. The same strategy is also used by Liu and Ku (2005) to solve the Landau-Lifshitz equation, where an effective combination of GPS and Runge-Kutta method is employed to enhance the stability and accuracy of numerical solutions. 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 (BGPS) have been successfully developed by the author, such that the new numerical methods can be used to solve the backward in time Burgers equation by Liu (2006d), and the backward in time heat conduction equation by Liu, Chang and Chang (2006).

All that made the development of the so-called one-step estimation method (OSEM) based on the Lie-group possible. Liu (2006e) has used this concept to develop the numerical estimation method for the unknown temperature-dependent heat conductivity of one-dimensional heat conduction equation. This new method is rather promising to provide better results than other numerical methods. In this paper we would develop the one-step first and second orders group preserving schemes and derive quasilinear algebraic equations for the inverse problem of estimating the temperature-dependent thermophysical properties. The new method is fully different from the other numerical methods cited above. It is an extension of the work of Liu (2004, 2006e).

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. The major contributions of this paper are applying the group preserving property of the resultant system in the numerical scheme and giving a conviction that the proposed scheme with only one-step forward is workable to the inverse heat conduction problem. Specifically, the proposed schemes are easy to implement and the computational time is saving. Through this study, we may have an easily-implemented one-step estimation method (OSEM) used in the estimation of temperature-dependent thermophysical properties, the accuracy and efficiency of which are much better than before.

2 Group-preserving scheme for ODEs

2.1 A Lie algebra formulation for ODEs

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 not only with the evolution of state variables but also the evolution of the magnitude of state variables vector. That is, for an n ordinary differential equations system:

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

we can embed it to the following $n+1$-dimensional augemented dynamical system:

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

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 equation (1), but the inclusion of the second row in Eq. (2) gives us a Minkowskian structure of the augmented state variables of $\mathbf{X} := (\mathbf{u}^\mathbf{t}, \|\mathbf{u}\|)^\mathbf{t}$ satisfying the cone condition:

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

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

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

where the dot between two n-dimensional vectors denotes their Euclidean inner product. The cone condition is thus a natural constraint on the dynamical system (2).

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

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

with a constraint (3), where

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

satisfying

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

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

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

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

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

where G_0^0 is the 00th component of $\mathbf{G}$, which is a proper orthochronous Lorentz group denoted by $SO_o(n,1)$. The

term orthochronous used in the special relativity theory is referred to the preservation of time orientation. However, it should be understood here as the preservation of the sign of $\|\mathbf{u}\| > 0$.

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

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

where $\mathbb{D}$ is a domain of $\mathbb{R}^n \times \mathbb{R}$, and $\mathcal{L}$ is known as a Lipschitz constant, the new system has the advantage of devising group-preserving numerical scheme as follows [Liu (2001)]:

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

where $\mathbf{X}_\ell$ denotes the numerical value of $\mathbf{X}$ at the discrete time t_ℓ, and $\mathbf{G}(\ell) \in SO_o(n,1)$ 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 a closed-form representation:

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

where

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

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

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

From $\mathbf{f}_\ell\cdot\mathbf{u}_\ell \geq -\|\mathbf{f}_\ell\|\|\mathbf{u}_\ell\|$ we can prove that

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

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 yields a coupled system of ODEs, which are then numerically integrated. For the one-dimensional heat conduction equation we adopt the numerical method of line to discretize the partial derivatives of u with respect to the spatial coordinate x by

$$\frac{\partial u(x,t)}{\partial x}\bigg|_{x=i\Delta x} = \frac{u_{i+1}(t) - u_i(t)}{\Delta x}, \tag{18}$$

$$\frac{\partial^2 u(x,t)}{\partial x^2}\bigg|_{x=i\Delta x} = \frac{u_{i+1}(t) - 2u_i(t) + u_{i-1}(t)}{(\Delta x)^2}, \tag{19}$$

where Δx is a uniform discretization spacing length, and $u_i(t) = u(i\Delta x, t)$, such that we have

$$\frac{\partial}{\partial x}\left[k(u)\frac{\partial u}{\partial x}\right]\bigg|_{x=i\Delta x} = \frac{k(u_{i+1}) - k(u_i)}{u_{i+1} - u_i}\left[\frac{u_{i+1} - u_i}{\Delta x}\right]^2$$
$$+ \frac{k(u_i)}{(\Delta x)^2}[u_{i+1} - 2u_i + u_{i-1}]. \tag{20}$$

Then, the one-dimensional heat conduction equation with temperature-dependent thermal conductivity and heat capacity:

$$c(u)\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left[k(u)\frac{\partial u}{\partial x}\right] \tag{21}$$

becomes n coupled nonlinear ODEs:

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

where $c_i = c(u_i)$ and $k_i = k(u_i)$.

For a direct heat conduction problem, the next step is to advance the solution from the given boundary conditions and initial condition to the desired time T. Really, Eq. (22) has totally n-coupled nonlinear differential equations for the n variables $u_i(t), i = 1, 2, \ldots, n$, which can be numerically integrated to obtain the solutions for direct problems.

3.2 One-step GPS

Applying scheme (16) to the n ODEs in Eq. (22) we can compute the heat conduction equation by GPS. Assuming that the total time T is divided by K steps, that is, the time stepsize we use in the GPS is $\Delta t = T/K$, and 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 applying Eq. (13) step-by-step we can obtain

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

where $\mathbf{X}_K$ 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 $SO_o(n, 1)$, 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 $\mathbf{G}$. Hence, we have

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

This is a one-step transformation from $\mathbf{X}(0)$ to $\mathbf{X}(T)$.

The most simple method to calculate $\mathbf{G}(T)$ is given by

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

where

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

That is, we use the initial values of $\mathbf{u}(0)$ to calculate $\mathbf{G}(T)$. Then from Eq. (24) we obtain a one-step GPS:

$$\mathbf{u}_K = \mathbf{u}_0 + \eta\mathbf{f}_0 = \mathbf{u}_0 + \frac{b\|\mathbf{u}_0\|\|\mathbf{f}_0\| + (a-1)\mathbf{f}_0 \cdot \mathbf{u}_0}{\|\mathbf{f}_0\|^2}\mathbf{f}_0. \tag{27}$$

The above one-step GPS method is an adventure in the computational technique; however, the accuracy and efficiency are demonstrated by numerical examples given below.

4 Identifying the temperature-dependent thermo-physical properties

Let us consider a heat conducting slab composed of temperature-dependent material with heat conduction

functions $c(u) > 0$ and $k(u) > 0$ in Eq. (21) to be estimated. In order to identify the heat conduction functions of $c(u)$ and $k(u)$, let us impose the following conditions:

$$u(0,t) = u_0, \quad u(1,t) = 0, \tag{28}$$

$$u(x,0) = u^0(x) = u_0(1-x), \quad u(x,T) = u^T(x), \tag{29}$$

where u_0 is a fixed temperature, and $u^0(x)$ and $u^T(x)$ are two temperature distributions in the slab measured at two different times $t = 0$ and $t = T$.

Let us write

$$\frac{\partial}{\partial x}\left[k(u)\frac{\partial u}{\partial x}\right] = k'(u)\left[\frac{\partial u}{\partial x}\right]^2 + k(u)\frac{\partial^2 u}{\partial x^2}, \tag{30}$$

and Eq. (21) becomes a quasilinear heat conduction equation:

$$c(u)\frac{\partial u}{\partial t} = k'(u)\left[\frac{\partial u}{\partial x}\right]^2 + k(u)\frac{\partial^2 u}{\partial x^2}. \tag{31}$$

Given $u(x,t)$, the above equation can be viewed as a first order differential equation for $k(u)$ with u as independent variable. To be an independent variable in the estimation of $k(u)$ we suppose that u is a monotonic function of x, which can be achieved by specifying a suitable u_0 and a small t, since u is a monotonically decreasing function of x at $t = 0$. On the other hand, we suppose that $c(0)$ and $k(0)$ are known through the measurement. At the same time the coefficients $c_i = c(u_i)$, $k_i = k(u_i)$, $i = 1, \dots, n$ in Eq. (31) are unknown to be estimated below.

4.1 Estimation of thermal diffusivity

Let $y_i := k_i/c_i$ be the thermal diffusivity at the i-th grid point, and suppose that the number of grid points is large enough or $c(u)$ is a slowly changing function, such that we can further approximate Eq. (22) by

$$\dot{u}_i(t) = \frac{1}{(\Delta x)^2}\{y_{i+1}[u_{i+1}(t) - u_i(t)] - y_i[u_i(t) - u_{i-1}(t)]\}. \tag{32}$$

When applying the one-step GPS to Eq. (32) from time $t = 0$ to time $t = T$ we obtain a quasilinear algebraic equation to calculate y_i:

$$u_i^T = u_i^0 + \frac{\eta_a}{(\Delta x)^2}[y_{i+1}(u_{i+1}^0 - u_i^0) - y_i(u_i^0 - u_{i-1}^0)], \tag{33}$$

where u_i^T and u_i^0 are two measured temperatures at the i-th grid point. However, η_a in the above is not a constant but a nonlinear function of y_i as defined by Eq. (27) with

$$\mathbf{u}_0 := [u_1^0, \dots, u_n^0]^\mathsf{t}, \tag{34}$$

$$\mathbf{f}_0 := \frac{1}{(\Delta x)^2}[y_2(u_2^0 - u_1^0) - y_1(u_1^0 - u_0^0),$$
$$\dots, y_{n+1}(u_{n+1}^0 - u_n^0) - y_n(u_n^0 - u_{n-1}^0)]^\mathsf{t}. \tag{35}$$

It is not difficult to rewrite Eq. (33) as

$$y_i = \frac{1}{u_i^0 - u_{i-1}^0}\left[y_{i+1}(u_{i+1}^0 - u_i^0) - \frac{(\Delta x)^2}{\eta_a}(u_i^T - u_i^0)\right]. \tag{36}$$

In order to use the above equation to solve y_i, let us guess an initial y_i, and η_a can be determined before the use of Eq. (36).

Therefore, if we start from a given $y_{n+1} = k(0)/c(0)$ we can proceed to find $y_n, \dots, y_1$ sequentially by the above equation. Substituting the new y_i into η_a again we can use Eq. (36) to generate another y_i again until the values of y_i converge with a specified stopping criterion:

$$\sum_{i=1}^{n} |y_i^{j+1} - y_i^j|^2 \le \varepsilon, \tag{37}$$

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

In the following we consider two methods to proceed the estimations of thermophysical properties.

4.2 Estimation of thermal conductivity and heat capacity

4.2.1 The first method

In the above process we can estimate $y(u) = k(u)/c(u)$ but not $c(u)$ or $k(u)$ alone. However, if we can estimate $y(u)$ accurately (see examples below), then we can rewrite Eq. (22) as

$$\dot{u}_i(t) = \frac{y_i}{(\Delta x)^2}\{\frac{k_{i+1}}{k_i}[u_{i+1}(t) - u_i(t)] - [u_i(t) - u_{i-1}(t)]\}, \tag{38}$$

and use the above equation to estimate k_i very effectively. When applying the one-step GPS to Eq. (38) from time $t = 0$ to time $t = T$ we obtain a quasilinear algebraic equation to solve k_i:

$$u_i^T = u_i^0 + \frac{\eta_b y_i}{(\Delta x)^2}\left[\frac{k_{i+1}}{k_i}(u_{i+1}^0 - u_i^0) - (u_i^0 - u_{i-1}^0)\right], \quad (39)$$

where y_i, $i = 1,\ldots,n$, were already known from the previous estimation provided in Section 4.1. η_b in the above is a nonlinear function of k_{i+1}/k_i as defined by Eq. (27) with

$$\mathbf{u}_0 := [u_1^0, \ldots, u_n^0]^{\mathrm{t}}, \quad (40)$$

$$\mathbf{f}_0 := \frac{1}{(\Delta x)^2}\left[\frac{y_1 k_2}{k_1}(u_2^0 - u_1^0) - (u_1^0 - u_0^0),\right.$$
$$\left.\ldots, \frac{y_n k_{n+1}}{k_n}(u_{n+1}^0 - u_n^0) - (u_n^0 - u_{n-1}^0)\right]^{\mathrm{t}}. \quad (41)$$

It is not difficult to rewrite Eq. (39) as

$$k_i = k_{i+1}\left[\frac{u_i^0 - u_{i-1}^0}{u_{i+1}^0 - u_i^0} + \frac{(\Delta x)^2(u_i^T - u_i^0)}{\eta_b y_i(u_{i+1}^0 - u_i^0)}\right]^{-1}. \quad (42)$$

In order to use the above equation to solve k_i, let us guess an initial k_i, and η_b can be determined before the use of Eq. (42).

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_b again we can use Eq. (42) to generate another k_i again until the values of k_i converge with a specified stopping criterion:

$$\sum_{i=1}^{n}|k_i^{j+1} - k_i^j|^2 \le \varepsilon. \quad (43)$$

When both y and k are estimated we can calculate the heat capacity by $c = k/y$.

4.2.2   The second method

Let us consider the following variable transformation:

$$U = \int_0^u y(\xi)d\xi = \int_0^u \frac{k(\xi)}{c(\xi)}d\xi, \quad (44)$$

where U is a monotonic function of u because of $y(u) = k(u)/c(u) > 0$. With this transformation in mind, it immediately follows that

$$\frac{\partial U}{\partial t} = \frac{k}{c}\frac{\partial u}{\partial t}, \quad (45)$$

$$\frac{\partial U}{\partial x} = \frac{k}{c}\frac{\partial u}{\partial x}, \quad (46)$$

$$\frac{\partial^2 U}{\partial x^2} = \frac{\partial}{\partial x}\left[\frac{k}{c}\frac{\partial u}{\partial x}\right] = \frac{1}{c}\frac{\partial}{\partial x}\left[k\frac{\partial u}{\partial x}\right] + k\frac{\partial}{\partial x}\left[\frac{1}{c}\frac{\partial u}{\partial x}\right]. \quad (47)$$

From Eqs. (21), (45) and (47) we obtain

$$\frac{\partial U}{\partial t} = \frac{k}{c}\left(\frac{\partial^2 U}{\partial x^2} - k\frac{\partial}{\partial x}\left[\frac{1}{c}\frac{\partial u}{\partial x}\right]\right). \quad (48)$$

However, the partial derivative of u can be replaced by the partial derivative of U through Eq. (46):

$$\frac{\partial U}{\partial t} = \frac{k}{c}\left(\frac{\partial^2 U}{\partial x^2} - k\frac{\partial}{\partial x}\left[\frac{1}{k}\frac{\partial U}{\partial x}\right]\right) = \frac{k}{c}\frac{1}{k}\frac{\partial k}{\partial U}\left(\frac{\partial U}{\partial x}\right)^2, \quad (49)$$

where k is supposed to be a function of U.

In terms of y we thus obtain a first order nonlinear partial differential equation for U:

$$\frac{\partial U}{\partial t} = \frac{y}{k}\frac{\partial k}{\partial U}\left(\frac{\partial U}{\partial x}\right)^2. \quad (50)$$

Consider the following forward difference:

$$\frac{y}{k}\frac{\partial k}{\partial U}\left(\frac{\partial U}{\partial x}\right)^2\bigg|_{x=i\Delta x} = \frac{y_i}{k(U_i)}\frac{k(U_{i+1}) - k(U_i)}{U_{i+1} - U_i}\left[\frac{U_{i+1} - U_i}{\Delta x}\right]^2 \quad (51)$$

and then Eq. (50) becomes n-coupled nonlinear ODEs:

$$\dot{U}_i(t) = \frac{y_i}{(\Delta x)^2}\left(\frac{k_{i+1}}{k_i} - 1\right)[U_{i+1}(t) - U_i(t)] \quad (52)$$

with unknown coefficients $k_i = k(U_i)$, $i = 1,\ldots,n$. Notice that y_i, $i = 1,\ldots,n$, were already calculated previously.

When apply the one-step GPS to Eq. (52) from time $t = 0$ to time $t = T$, we obtain a quasilinear equation for k_i:

$$U_i^T = U_i^0 + \frac{y_i \eta_c}{(\Delta x)^2}\left(\frac{k_{i+1}}{k_i} - 1\right)[U_{i+1}^0 - U_i^0], \quad (53)$$

where U_i^T and U_i^0 are two transformed temperatures at the i-th grid point calculated by Eq. (44). Here η_c is still defined by Eq. (27) but with

$$\mathbf{u}_0 := [U_1^0, \ldots, U_n^0]^t, \tag{54}$$

$$\mathbf{f}_0 := \frac{1}{(\Delta x)^2} \left[y_1 \left(\frac{k_2}{k_1} - 1 \right) (U_2^0 - U_1^0), \right.$$
$$\left. \ldots, y_n \left(\frac{k_{n+1}}{k_n} - 1 \right) (U_{n+1}^0 - U_n^0) \right]^t. \tag{55}$$

It is not difficult to rewrite Eq. (53) as

$$k_i = k_{i+1} \left[1 + \frac{(\Delta x)^2 (U_i^T - U_i^0)}{\eta_c y_i (U_{i+1}^0 - U_i^0)} \right]^{-1}. \tag{56}$$

From Eq. (44) we have

$$U_i^T - U_i^0 = \int_{u_i^0}^{u_i^T} \frac{k(\xi)}{c(\xi)} d\xi,$$

$$U_{i+1}^0 - U_i^0 = \int_{u_i^0}^{u_{i+1}^0} \frac{k(\xi)}{c(\xi)} d\xi.$$

If we let the grid length be small enough, then

$$\frac{U_i^T - U_i^0}{U_{i+1}^0 - U_i^0} = \frac{u_i^T - u_i^0}{u_{i+1}^0 - u_i^0}$$

is a good approximation, and Eq. (56) changes to

$$k_i = k_{i+1} \left[1 + \frac{(\Delta x)^2 (u_i^T - u_i^0)}{\eta_c y_i (u_{i+1}^0 - u_i^0)} \right]^{-1}. \tag{57}$$
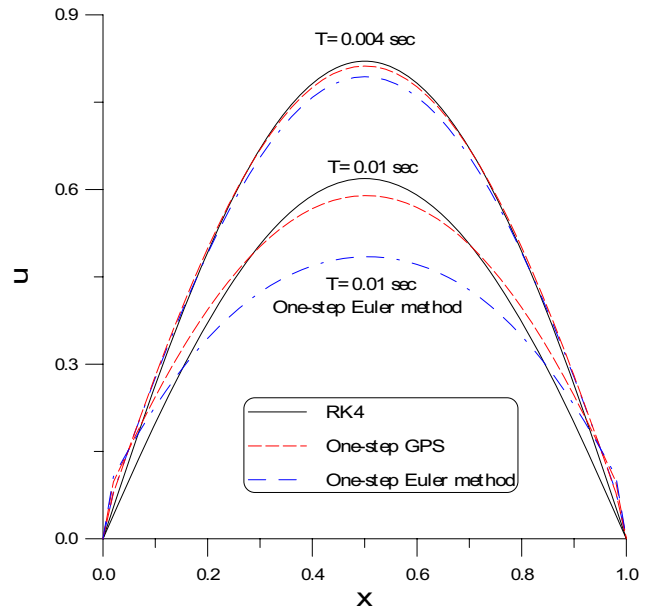
The other procedures to estimate k_i are similar to the ones in Section 4.2.1.

4.3 Example 1

Let us consider Eq. (21) with the following thermophysical properties [Huang and Yan (1995) and Yang (2000)]:

$$k(u) = a_1 + a_2 \exp \left(\frac{u}{a_3} \right) + a_4 \sin \left(\frac{u}{a_5} \right), \tag{58}$$

$$c(u) = b_1 + b_2 u + b_3 u^2. \tag{59}$$

Figure 1 : Comparing numerical solutions of one-step GPS and Euler method for Example 1 with "exact" solutions calculated by RK4.

In the following calculations we will fix $a_1 = 1$, $a_2 = 4.5$, $a_3 = 80$, $a_4 = 2.5$ and $a_5 = 3$, and $b_1 = 1.2$, $b_2 = 0.02$ and $b_3 = 0.00001$.

Before embarking the calculation of inverse problem, let us apply the one-step GPS on this quasilinear heat conduction problem with the above $c(u)$ and $k(u)$, and with the initial condition $u^0(x) = \sin \pi x$ and boundary conditions $u(0,t) = u(1,t) = 0$. In Fig. 1 the numerical results at times $T = 0.004$ sec and $T = 0.01$ sec calculated respectively by the fourth-order Runge-Kutta method (RK4) and one-step GPS were compared. We have fixed $\Delta x = 1/50$ and $\Delta t = 0.00001$ sec for RK4 and $\Delta t = 0.004$ sec and $\Delta t = 0.01$ sec for one-step GPS. It can be seen that for this nonlinear heat conducting problem the one-step GPS is effective. In the same figure we also plotted the numerical results obtained by the one-step Euler method. Unlike to the one-step GPS, the one-step Euler method gives large errors of solutions. The major reason for its failure of the Euler method, and also other numerical methods, in the calculations with one-step is that they are not of the group preserving schemes, such that the transitivity and closureness of Lie group are not applicable in these numerical methods.

We have the idea and method to apply the one-step GPS

method to estimate the temperature-dependent thermal conductivity and heat capacity. The above numerical results can support this idea, because the one-step GPS can provide rather accurate numerical solutions if the time step employed is within a reasonable size. The estimation is divided into two parts: the first part estimates the thermal diffusivity $y(u)$ and the second part estimates the thermal conductivity $k(u)$ and then the heat capacity $c(u) = k(u)/y(u)$.

In order to assess the validity of the new estimation method let us consider the following errors:

$$\max_{i \in \{1,\dots,n\}} \frac{|y(u_i) - \hat{y}(u_i)|}{\hat{y}(u_i)} \times 100\%,$$

$$\max_{i \in \{1,\dots,n\}} \frac{|k(u_i) - \hat{k}(u_i)|}{\hat{k}(u_i)} \times 100\%,$$

$$\max_{i \in \{1,\dots,n\}} \frac{|c(u_i) - \hat{c}(u_i)|}{\hat{c}(u_i)} \times 100\%,$$

$$\frac{1}{n} \sum_{i=1}^{n} \frac{|y(u_i) - \hat{y}(u_i)|}{\hat{y}(u_i)} \times 100\%,$$

$$\frac{1}{n} \sum_{i=1}^{n} \frac{|k(u_i) - \hat{k}(u_i)|}{\hat{k}(u_i)} \times 100\%,$$

$$\frac{1}{n} \sum_{i=1}^{n} \frac{|c(u_i) - \hat{c}(u_i)|}{\hat{c}(u_i)} \times 100\%,$$

where $y(u)$ and $\hat{y}(u)$ denote the exact and estimated values of thermal diffusivity, $k(u)$ and $\hat{k}(u)$ denote the exact and estimated values of thermal conductivity, and $c(u)$ and $\hat{c}(u)$ denote the exact and estimated values of heat capacity. The first three errors are called normalized maximum errors (NME), and the last three are called average relative errors (ARE).

In this identification of $y(u)$, $k(u)$ and $c(u)$ we have fixed $u_0 = 15$, $\Delta x = 1/20$ and $T = 0.00001$ sec. Let us suppose an initial guess $y_i = 1$, $i = 1,\dots,n$. Applying Eq. (36) to solve y_i, after three iterations the solutions of y_i converge to the exact values according to the criterion (37) with $\varepsilon = 10^{-15}$ as shown in Fig. 2(a), and the result as shown in Fig. 2(b) is very good with a normalized maximum error of NME(y)=0.0002027. When y is available we then apply Eq. (42) to solve k with an initial guess $k_i = 0.5$, $i = 1,\dots,n$. After two iterations the solutions of k_i converge to the exact values according to the criterion (43) with $\varepsilon = 10^{-15}$ as shown in Fig. 2(a), and the result as shown in Fig. 2(b) is very good with NME(k)=0.0002288. From y and k, c is calculated by
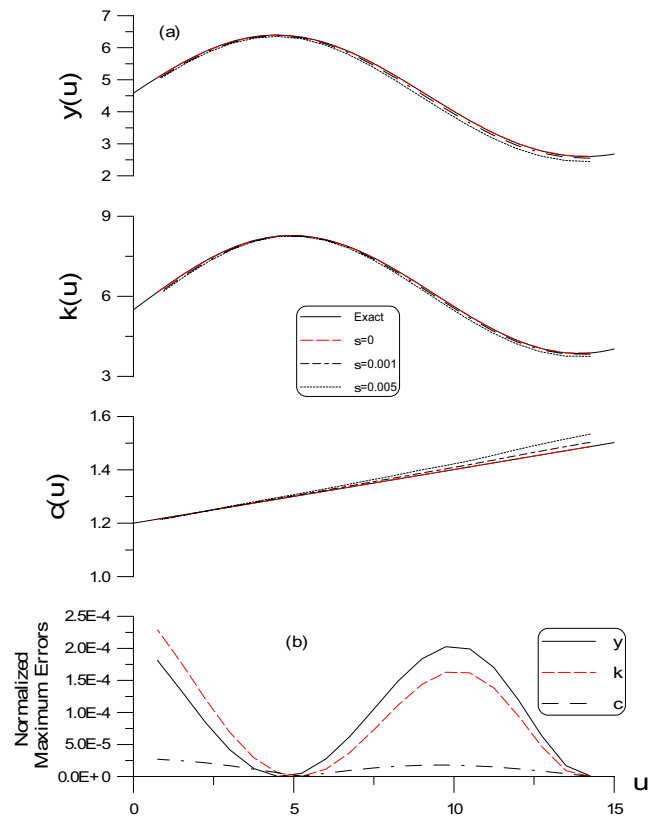
Figure 2 : Estimating $y(u)$, $k(u)$ and $c(u)$ for Example 1: (a) comparing exact solutions and numerical solutions calculated by one-step GPS, (b) normalized maximum errors with $s = 0$.

$c = k/y$. The result as shown in Fig. 2(b) is very good with NME(c)=0.0000269. In this estimation by the one-step GPS, it requires totally five iterations, which shows that the speed of convergence is very fast.

In Table 1 we further compare our results of this case with others. When the average relative errors of thermal conductivity and heat capacity are, respectively, ARE(k)=0.00771% and ARE(c)=0.00116% in the present approach, the results of Yang (2000) are ARE(k)=0.012% and ARE(c)=0.012% and the results of Huang and Yan (1995) are ARE(k)=0.510% and ARE(c)=0.69%. The accuracy in these estimations are respectively in the fifth order of our method, the fourth order of Yang (2000) and the third order of Huang and Yan (1995). Through this comparison one might highly appreciate the accuracy of the new estimation method.

In the case when the measured data are contaminated by random noise, we are concerned with the stability

Table 1 : The comparison of present method with other methods for Example 1

$s = 0$	Stopping criterion	NI	ARE(y) (%)	ARE(k) (%)	ARE(c) (%)
Huang and Yan (1995)	1×10^{-8}	148	–	0.510	0.69
Yang (2000)	2.3×10^{-10}	7	–	0.012	0.012
One-step GPS	1×10^{-15}	5	0.00837	0.00771	0.00116
$s = 0.001$					
Huang and Yan (1995)	1.32×10^{-5}	57	–	1.502	0.706
Yang (2000)	2.0×10^{-8}	7	–	0.026	0.035
One-step GPS	1×10^{-15}	7	1.102	0.702	0.404
$s = 0.005$					
Huang and Yan (1995)	3.2×10^{-4}	26	–	4.101	1.026
Yang (2000)	5.0×10^{-7}	6	–	0.137	0.168
One-step GPS	1×10^{-15}	8	2.653	1.578	1.108
$s = 0.01$					
Yang (2000)	2.0×10^{-6}	6	–	0.280	0.666
Second-order one-step GPS	1×10^{-15}	9	1.287	1.171	0.259
$s = 0.025$					
Yang (2000)	1.25×10^{-5}	6	–	0.705	0.831
Second-order one-step GPS	1×10^{-15}	9	1.546	1.381	0.190

of the new estimation method OSEM, which is investigated by adding the different levels of random noise on the measured data at time T. We use the function RANDOM_NUMBER given in Fortran to generate the noisy data $R(i)$, where $R(i)$ are random numbers taken values in $[-1, 1]$. The numerical results contaminated by noise were compared with the numerical result without considering random noise in Fig. 2(a). The noise is obtained by multiplying $R(i)$ by a factor s. It can be seen that the noise levels with $s = 0.001, 0.005$ disturb the numerical solutions to deviate from the exact solutions small, where we use $T = 0.0005$ sec and $T = 0.0009$ sec for each case. It appears that large measurement error makes the estimated result away from the exact solution. For the case of $s = 0.001$ we have NME(y)=0.02228, NME(k)=0.01335 and NME(c)=0.01092, and for the case of $s = 0.005$ we have NME(y)=0.0612, NME(k)=0.0319 and NME(c)=0.0313. For the noised estimations we also compared our results with that calculated by Huang and Yan (1995) and Yang (2000) in Table 1. When the noise is added, the accuracy of our estimations are lost about

two orders, which shows that the present approach can be improved. The improvement will be made in Section 5 by considering a higher order numerical method.

The robustness of the results obtained by Yang (2000) can be seen. However, the method by Yang (2000) required to suppose some suitable thermophysical functions a priori and the number of measured data was up to 120 used to estimate the unknown coefficients. More precisely, the method by Yang (2000) is a method of coefficients estimation, but is not a method of the functions estimation. The numbers of iteration (NI) used in the converged solutions were also compared in Table 1. Even we use a rather stringent convergent criterion, the new estimation method is very effective and converges more fast than that of Huang and Yan (1995). A typical computation of our method spends the CPU time about one second in our PC-586 with pentium-100.

For saving sensors the number of grid points cannot be too large, at which the data are measured. In order to get another data in addition those at the grid points which are measured through the mounted sensors, we can apply the Lagrange interpolation technique [e.g., Rivlin (1969)] to
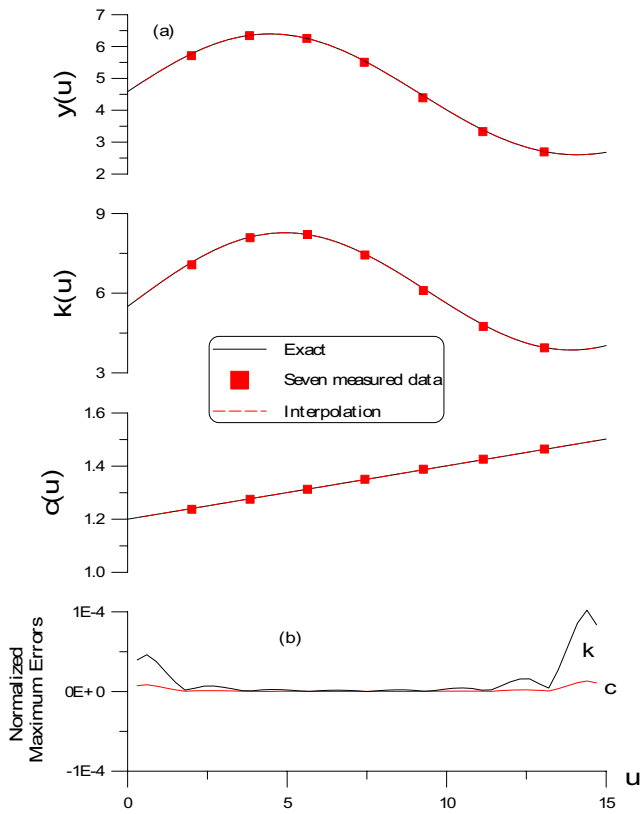
Figure 3 : Estimating thermophysical properties for Example 1 using only seven measured data: (a) comparing exact solutions and numerical solutions calculated by one-step GPS, (b) normalized maximum errors.

construct a smooth polynomial function $F(x)$ to pass the n distinct points as shown in Appendix. In Fig. 3 we use only seven measured data at the interior of the slab. The results in the estimation of thermophysical properties are rather good as can be seen from Fig. 3(a). Through the interpolation it is hardly distinct these curves from the exact ones. Fig. 3(b) displays the NME(k) and NME(c), which are very small in the order of 10^{-4}.

In Fig. 4 we plot the variation of average relative errors in the estimation of thermophysical properties with respect to different final times of T taken in the OSEM in the range of $[0.00001, 0.001]$, but fixed the grid length to be $\Delta x = 1/20$. There 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. However, even up to $T = 0.001$ sec the average relative error is also small in the order of 10^{-3}.
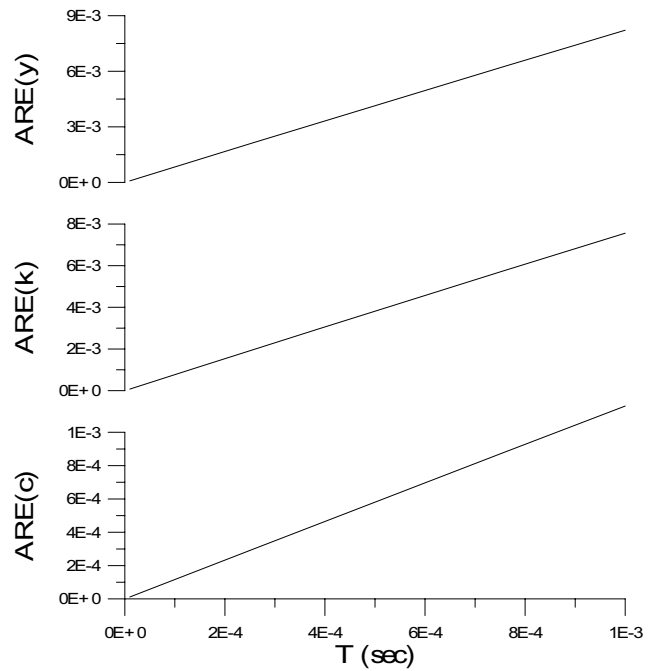
Figure 4 : In the estimation of thermophysical properties for Example 1 we plot the average relative errors with different T.

Next, we investigate the influence of grid numbers on the average relative error. In Fig. 5 we plot the variation of average relative errors in the estimation of thermophysical properties with respect to different grid numbers taken in the one-step GPS method in the range of $[5, 200]$, but fixed the final time $T = 0.0005$ sec. The average relative error tends to a saturated value when the grid number increases. It is interesting that when the grid numbers are smaller than twenty the average relative errors decrease fast. This favors to use a small number of measured data to estimate the thermophysical properties.

4.4 Example 2

Let us consider Eq. (21) with the following thermal conductivity and heat capacity [Lesnic, Elliott and Ingham (1996)]:

$$k(u) = c(u) = 1 + 2u. \tag{60}$$

In the identification of $k(u)$ and $c(u)$ we have fixed $u_0 = 5$, $\Delta x = 1/10$ and $T = 0.001$ sec. We first applying Eq. (36) to solve y, after two iterations the solutions
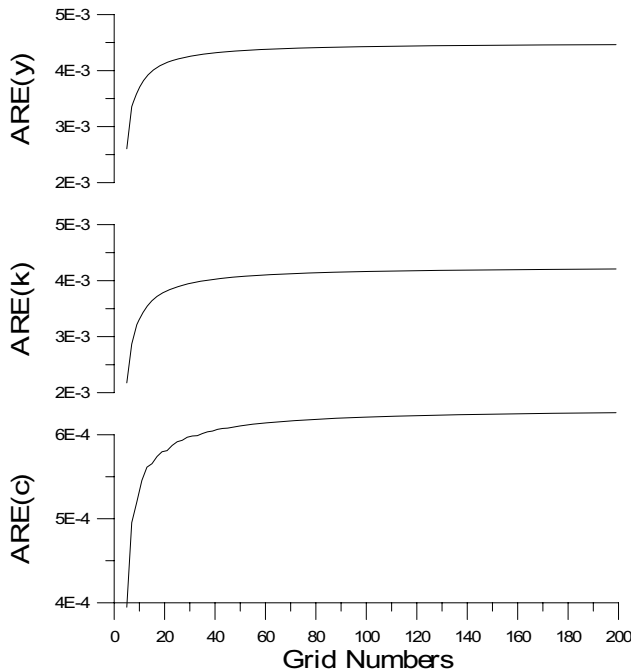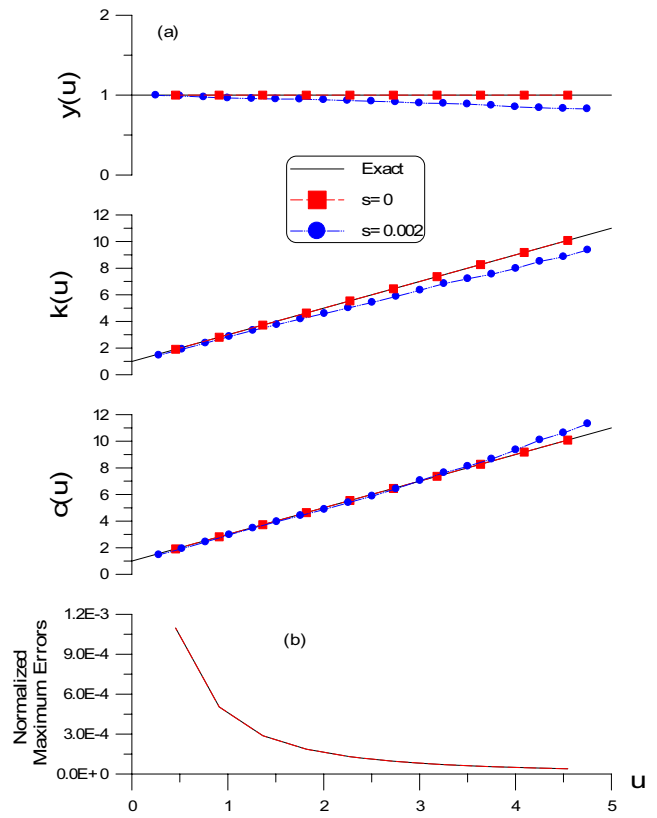
Figure 5 : In the estimation of thermophysical properties for Example 1 we plot the average relative errors with different grid numbers.

Figure 6 : Estimating $y(u)$, $k(u)$ and $c(u)$ for Example 2: (a) comparing exact solutions and numerical solutions calculated by one-step GPS with $s = 0, 0.002$, (b) normalized maximum errors with $s = 0$.

of y_i converge to the exact values according to the criterion (37) with $\varepsilon = 10^{-15}$ as shown in Fig. 6(a). Then we applying Eq. (57) to solve k, after three iterations, the solutions of k_i converge to the exact values according to the criterion (43) with $\varepsilon = 10^{-15}$ as shown in Fig. 6(a). The results as shown in Fig. 6(b) are very good with small normalized maximum errors.

Even adding the noise level with $s = 0.002$, it only slightly disturbs the numerical solutions deviating from the exact solutions as shown in Fig. 6(a). For this example we use the second method in Section 4.2.2 to calculate k and c.

5   Second order estimation technique

In Section 3.2 we have used a first-order scheme to calculate $\mathbf{G}(T)$; however, in order to increase the accuracy and robustness of our estimation method, we can employ a second-order technique to calculate $\mathbf{G}(T)$, which is evaluated at the mid-point by

$$\mathbf{G}(T) = \begin{bmatrix} \mathbf{I}_n + \frac{(\hat{a}-1)}{\|\hat{\mathbf{f}}_0\|^2}\hat{\mathbf{f}}_0\hat{\mathbf{f}}_0^{\mathsf{t}} & \frac{\hat{b}\hat{\mathbf{f}}_0}{\|\hat{\mathbf{f}}_0\|} \\ \frac{\hat{b}\hat{\mathbf{f}}_0^{\mathsf{t}}}{\|\hat{\mathbf{f}}_0\|} & \hat{a} \end{bmatrix}, \tag{61}$$
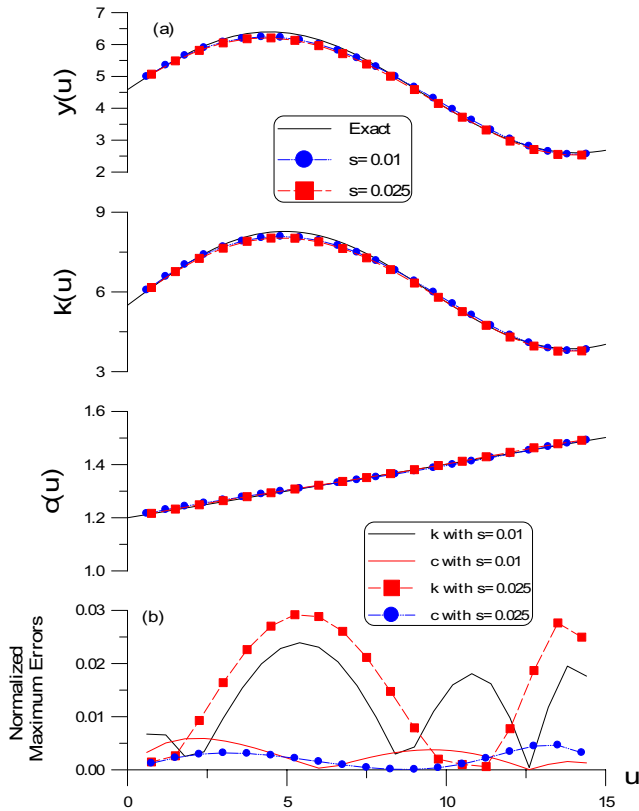
where

$$\hat{a} := \cosh\left(\frac{T\|\hat{\mathbf{f}}_0\|}{\|\hat{\mathbf{u}}_0\|}\right), \quad \hat{b} := \sinh\left(\frac{T\|\hat{\mathbf{f}}_0\|}{\|\hat{\mathbf{u}}_0\|}\right). \tag{62}$$

That is, we use the average of initial values of $\mathbf{u}(0)$ and final vaules of $\mathbf{u}(T)$ to calculate $\mathbf{G}(T)$, where

$$\hat{\mathbf{u}}_0 = \frac{1}{2}[\mathbf{u}_0 + \mathbf{u}_T],$$

$$\hat{\mathbf{f}}_0 = \mathbf{f}\left(\frac{1}{2}[\mathbf{u}_0 + \mathbf{u}_T]\right)$$

Figure 7 : Estimating thermophysical properties for Example 1: (a) comparing exact solutions and numerical solutions calculated by the second-order one-step GPS, (b) normalized maximum errors with $s = 0.01, 0.025$.

are taking the values of the state variable and vector field at the mid-point. Then from Eq. (24) we obtain a second-order one-step GPS:

$$\mathbf{u}_T = \mathbf{u}_0 + \hat{\eta}\hat{\mathbf{f}}_0 = \mathbf{u}_0 + \frac{\hat{b}\|\mathbf{u}_0\|\|\hat{\mathbf{f}}_0\| + (\hat{a}-1)\hat{\mathbf{f}}_0 \cdot \mathbf{u}_0}{\|\hat{\mathbf{f}}_0\|^2}\hat{\mathbf{f}}_0. \quad (63)$$

When applying the second-order one-step GPS to Eq. (32) we obtain

$$u_i^T = u_i^0 + \frac{\hat{\eta}_a}{(\Delta x)^2}[y_{i+1}(\hat{u}_{i+1}^0 - \hat{u}_i^0) - y_i(\hat{u}_i^0 - \hat{u}_{i-1}^0)], \quad (64)$$

where $\hat{u}_i^0 = (u_i^T + u_i^0)/2$. The above $\hat{\eta}_a$ is defined by Eq. (63) with

$$\hat{\mathbf{u}}_0 := [\hat{u}_1^0, \ldots, \hat{u}_n^0]^t, \quad (65)$$

$$\hat{\mathbf{f}}_0 := \frac{1}{(\Delta x)^2}[y_2(\hat{u}_2^0 - \hat{u}_1^0) - y_1(\hat{u}_1^0 - \hat{u}_0^0),$$
$$\ldots, y_{n+1}(\hat{u}_{n+1}^0 - \hat{u}_n^0) - y_n(\hat{u}_n^0 - \hat{u}_{n-1}^0)]^t. \quad (66)$$

It is not difficult to rewrite Eq. (64) as

$$y_i = \frac{1}{\hat{u}_i^0 - \hat{u}_{i-1}^0}\left[y_{i+1}(\hat{u}_{i+1}^0 - \hat{u}_i^0) - \frac{(\Delta x)^2}{\hat{\eta}_a}(u_i^T - u_i^0)\right]. \quad (67)$$

The procedure to obtain a converged y_i is the same as that given in Section 4.1.

Similarly, applying the second-order one-step GPS to Eq. (38) we obtain

$$u_i^T = u_i^0 + \frac{\hat{\eta}_b y_i}{(\Delta x)^2}\left[\frac{k_{i+1}}{k_i}(\hat{u}_{i+1}^0 - \hat{u}_i^0) - (\hat{u}_i^0 - \hat{u}_{i-1}^0)\right], \quad (68)$$

where $\hat{\eta}_b$ is defined by Eq. (63) with

$$\hat{\mathbf{u}}_0 := [\hat{u}_1^0, \ldots, \hat{u}_n^0]^t, \quad (69)$$

$$\hat{\mathbf{f}}_0 := \frac{1}{(\Delta x)^2}\left[\frac{y_1 k_2}{k_1}(\hat{u}_2^0 - \hat{u}_1^0) - (\hat{u}_1^0 - \hat{u}_0^0),\right.$$
$$\left. \ldots, \frac{y_n k_{n+1}}{k_n}(\hat{u}_{n+1}^0 - \hat{u}_n^0) - (\hat{u}_n^0 - \hat{u}_{n-1}^0)\right]^t. \quad (70)$$

Similarly, we can rewrite Eq. (68) as

$$k_i = k_{i+1}\left[\frac{\hat{u}_i^0 - \hat{u}_{i-1}^0}{\hat{u}_{i+1}^0 - \hat{u}_i^0} + \frac{(\Delta x)^2(u_i^T - u_i^0)}{\hat{\eta}_b y_i(\hat{u}_{i+1}^0 - \hat{u}_i^0)}\right]^{-1}. \quad (71)$$

The procedure to obtain a converged k_i is the same as that given in Section 4.2.1.

Through this modification we estimate the thermophysical properties of Example 1 again under the large noises with $s = 0.01$ and $s = 0.025$. In these calculations we have used $\Delta x = 1/5$, that is, there are only four measured data required at time $T = 0.005$ sec. For this highly noised estimations we also compared our results with that calculated by Yang (2000) in Table 1. For the case of $s = 0.01$ we have NME(y)=0.0256, NME(k)=0.0234 and NME(c)=0.0059, and for the case of $s = 0.025$ we have NME(y)=0.0321, NME(k)=0.0292 and NME(c)=0.0046. Through this modification the accuracy of this estimations are better than that used the first-order one-step GPS in Section 4, where we have considered only small noises cases with $s = 0.001$ and $s = 0.005$. In Fig. 7 we also compared the estimated y, k and c with the exact ones, which can be seen are rather good with the normalized maximum errors smaller than

0.03. From these estimations it can be seen that the second-order one-step GPS is better than the first-order one-step GPS; however, the second-order one-step GPS is slightly complicated than the first-order one-step GPS.

6 Conclusions

In this paper we were concerned with the numerical solution of an inverse problem for estimating the temperature-dependent thermal conductivity and heat capacity of a one-dimensional quasilinear heat conduction equation. The key point was the construction of a one-step group preserving scheme. By employing the one-step GPS we have derived quasilinear algebraic equations required to determine the temperature-dependent thermal conductivity and heat capacity under a given initial temperature and a measured temperature at time T. Two numerical examples of the inverse problems were worked out, which show that our estimation method OSEM is applicable even for the thermal functions in a large temperature range. Under the noisy measured final temperature the one-step GPS was also robust enough to estimate the unknown thermal conductivity and heat capacity with a minimum measured data. Especially, when the measured data was highly noised, we may employ the second-order one-step GPS to estimate thermal conductivity and heat capacity. Through this study, it can conclude that the new estimation methods are accurate and effective.

Appendix A:

In this appendix we give a brief sketch of the Lagrange interpolation technique [e.g., Rivlin (1969)]. Let (x_i, u_i), where x_i locates at the i-th grid point and u_i is the numerical result at that point, and then the Lagrange interpolation function is given by

$$F(x) = \sum_{i=1}^{n} u_i L_i(x), \tag{A.1}$$

where

$$L_i(x) = \frac{\prod_{j=1, \ j \neq i}^{n} (x - x_j)}{\prod_{j=1, \ j \neq i}^{n} (x_i - x_j)}. \tag{A.2}$$

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