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A compact finite-difference scheme for solving a one-dimensional heat transport equation at the microscale

Weizhong Dai *, Raja Nassar

Mathematics and Statistics, College of Engineering and Science, Louisiana Tech University, Ruston, LA 71272, USA

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Abstract

Heat transport at the microscale is of vital importance in microtechnology applications. The heat transport equation is different from the traditional heat diffusion equation since a second-order derivative of temperature with respect to time and a third-order mixed derivative of temperature with respect to space and time are introduced. In this study, we develop a high-order compact finite-difference scheme for the heat transport equation at the microscale. It is shown by the discrete Fourier analysis method that the scheme is unconditionally stable. Numerical results show that the solution is accurate.

MSC: 65M06; 65N12

Keywords: Compact finite difference; Stability; Heat transport equation; Discrete Fourier analysis; Microscale

1. Introduction

Heat transport through thin films is of vital importance in microtechnology applications [4,5]. For instance, thin films of metals, of dielectrics such as SiO_2, or Si semiconductors are important components of microelectronic devices. The reduction of the device size to microscale has the advantage of enhancing the switching speed of the device. On the other hand, size reduction increases the rate of heat generation which leads to a high thermal load on the microdevice. Heat transfer at the microscale is also important for the processing of materials with a pulsed laser [8,9]. Examples in metal processing are laser micro-machining, laser patterning, laser processing of diamond films from carbon ion-implanted copper substrates, and laser surface hardening. Hence, studying the thermal

* Corresponding author.
E-mail address: dai@coes.latech.edu (W. Dai).

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behavior of thin films or of microobjects is essential for predicting the performance of a microelectronic device or for obtaining the desired microstructure [4]. The heat transport equations used to describe the thermal behavior of microstructures are expressed as [7,11]

$$-\nabla \cdot \boldsymbol{q} + Q = \rho C_p \frac{\partial T}{\partial t}, \tag{1}$$

$$\boldsymbol{q}(x, y, z, t + \tau_q) = -k \nabla T(x, y, z, t + \tau_T), \tag{2}$$

where $\boldsymbol{q} = (q_1, q_2, q_3)$ is the heat flux, T is the temperature, k is the conductivity, ρ is the density, C_p is the specific heat, Q is a heat source, τ_q and τ_T are the positive constants, which are the time lags of the heat flux and temperature gradient, respectively. In the classical theory of diffusion, the heat flux vector ($\boldsymbol{q}$) and the temperature gradient (∇T) across a material volume are assumed to occur at the same instant of time. They satisfy the Fourier's law of heat conduction

$$\boldsymbol{q}(x, y, z, t) = -k \nabla T(x, y, z, t). \tag{3}$$

However, if the scale in one direction is at the microscale, i.e., the order of 0.1 μm, then the heat flux and temperature gradient in this direction will occur at different times, as shown in Eq. (2) [11]. Using Taylor series expansion, the first-order approximation of Eq. (2) gives [11]

$$\boldsymbol{q} + \tau_q \frac{\partial \boldsymbol{q}}{\partial t} = -k \left[\nabla T + \tau_T \frac{\partial}{\partial t} [\nabla T] \right]. \tag{4}$$

The divergence of Eq. (4) gives

$$\nabla \cdot \boldsymbol{q} + \tau_q \frac{\partial \nabla \cdot \boldsymbol{q}}{\partial t} = -k \left[\nabla^2 T + \tau_T \frac{\partial}{\partial t} [\nabla^2 T] \right]. \tag{5}$$

Substituting the expression of $\nabla \cdot \boldsymbol{q}$ in Eq. (1) into Eq. (5) and introducing the thermal diffusion $\alpha = k/\rho C_p$ gives [11]

$$\frac{1}{\alpha} \frac{\partial T}{\partial t} + \frac{\tau_q}{\alpha} \frac{\partial^2 T}{\partial t^2} = \nabla^2 T + \tau_T \frac{\partial}{\partial t} [\nabla^2 T] + \frac{1}{k} \left[Q + \tau_q \frac{\partial Q}{\partial t} \right]. \tag{6}$$

In the one-dimensional case, the above equation can be written as follows:

$$\frac{1}{\alpha} \frac{\partial T}{\partial t} + \frac{\tau_q}{\alpha} \frac{\partial^2 T}{\partial t^2} = \frac{\partial^2 T}{\partial x^2} + \tau_T \frac{\partial^3 T}{\partial x^2 \partial t} + g, \tag{7}$$

where $g = (1/k)[Q + \tau_q \partial Q/\partial t]$.

An analytic solution of this equation with its initial and boundary conditions may be difficult to obtain. Tzou et al. [7,11] studied the lagging behavior by solving the above heat transport Eq. (7) in a semi-infinite interval, $[0, +\infty)$. The solution was obtained by using the Laplace transform method and the Riemann-sum approximation for the inversion [2]. In this paper, we consider the interval to be finite, $0 \leqslant x, \leqslant L$, where L is of order 0.1 μm. The initial and boundary conditions are

$$T(x, 0) = T_1, \quad \frac{\partial T}{\partial t}(x, 0) = T_2, \quad 0 \leqslant x \leqslant L, \tag{8}$$

and

$$T(0, t) = T_3, \quad T(L, t) = T_4, \quad t > 0. \tag{9}$$

For simplification, we assume that $T_3 = T_4 = 0$. Also, we assume that the solution is smooth.

It is of interest to obtain a numerical solution for the above initial and boundary value problem. Recently, we have developed a finite-difference scheme of the Crank–Nicholson type by introducing an intermediate function for the heat transport equation at the microscale [3]. It is shown by the discrete energy method that the scheme is unconditionally stable. The truncation error of the scheme is $0(\Delta t^2 + \Delta x^2)$. In this paper, we will develop a compact finite-difference scheme using a compact finite difference [6] so that the truncation error could be $0(\Delta t^2 + \Delta x^4)$. The scheme is two-level in time. We will use the discrete Fourier analysis [1,10] to show that the scheme is unconditionally stable. The method is illustrated by two numerical examples.

2. Compact finite-difference scheme

To develop a compact finite-difference scheme, we first introduce

$$\theta = T + \tau_q \frac{\partial T}{\partial t} \tag{10}$$

and

$$f = \frac{\partial^2 T}{\partial x^2}. \tag{11}$$

Then, Eq. (7) can be written as follows:

$$\frac{1}{\alpha}\frac{\partial \theta}{\partial t} = f + \tau_T \frac{\partial f}{\partial t} + g. \tag{12}$$

The initial and boundary conditions in Eqs. (8) and (9) become

$$T(x,0) = T_1, \quad \theta(x,0) = T_1 + \tau_q T_2, \quad 0 \leqslant x \leqslant L, \tag{13}$$

and

$$T(0,t) = T(L,t) = 0, \quad \theta(0,t) = \theta(L,t) = 0, \quad t > 0. \tag{14}$$

We let θ_j^n denote $\theta(j\,\Delta x, n\,\Delta t)$, where Δx and Δt are the spatial and temporal mesh sizes, respectively. The finite interval, $[0,L]$, is then divided into the mesh intervals by the points $x_j = j\,\Delta x$ $(j = 0, 1, \ldots, N)$, where $N\,\Delta x = L$. We now discretize Eqs. (10) and (12) using the trapezoidal method. On the other hand, Eq. (11) is discretized using a fourth-order compact finite-difference [6]. Here, we only employ a fourth-order compact finite difference for simplification. Other higher-order compact finite differences can be seen in Ref. [6]. As such, the compact finite-difference scheme for Eqs. (10)–(12) can be written as follows:

$$\frac{1}{\alpha\,\Delta t}(\theta_j^{n+1} - \theta_j^n) = \tfrac{1}{2}(f_j^{n+1} + f_j^n) + \frac{\tau_T}{\Delta t}(f_j^{n+1} - f_j^n) + g_j^{n+(1/2)}, \tag{15}$$

$$\tfrac{1}{2}(\theta_j^{n+1} + \theta_j^n) = \tfrac{1}{2}(T_j^{n+1} + T_j^n) + \frac{\tau_q}{\Delta t}(T_j^{n+1} - T_j^n), \tag{16}$$

and

$$\tfrac{1}{10} f_{j-1}^n + f_j^n + \tfrac{1}{10} f_{j+1}^n = \frac{6}{5\Delta x^2}(T_{j-1}^n - 2T_j^n + T_{j+1}^n), \tag{17}$$

where $1 \leqslant j \leqslant N-1$. It can be seen that the truncation error at point $(j\Delta x, (n+\frac{1}{2})\Delta t)$ is $0(\Delta t^2 + \Delta x^4)$. Since there are three variables (θ, T, f) and the scheme is implicit, the computation is complicated. We now simplify the computation. From Eq. (17), we have

$$\tfrac{1}{10} f_{j-1}^{n+1} + f_j^{n+1} + \tfrac{1}{10} f_{j+1}^{n+1} = \frac{6}{5\Delta x^2}(T_{j-1}^{n+1} - 2T_j^{n+1} + T_{j+1}^{n+1}). \tag{18}$$

Adding the above equation to Eq. (17), we obtain

$$\tfrac{1}{10}(f_{j-1}^{n+1} + f_{j-1}^{n}) + (f_j^{n+1} + f_j^n) + \tfrac{1}{10}(f_{j+1}^{n+1} + f_{j+1}^{n}) = \tfrac{6}{5}\delta_x^2(T_j^{n+1} + T_j^n), \tag{19}$$

where $\delta_x^2 T_j^n = (1/\Delta x^2)(T_{j-1}^n - 2T_j^n + T_{j+1}^n)$. On the other hand, we subtract Eq. (17) from (18) to obtain

$$\tfrac{1}{10}(f_{j-1}^{n+1} - f_{j-1}^{n}) + (f_j^{n+1} - f_j^n) + \tfrac{1}{10}(f_{j+1}^{n+1} - f_{j+1}^{n}) = \tfrac{6}{5}\delta_x^2(T_j^{n+1} - T_j^n). \tag{20}$$

Multiplying Eq. (19) by $\frac{1}{2}$ and Eq. (20) by $\tau_T/\Delta t$, respectively, and adding them together, we obtain

$$\begin{aligned}
&\tfrac{1}{10}\left\{\tfrac{1}{2}(f_{j-1}^{n+1} + f_{j-1}^{n}) + \frac{\tau_T}{\Delta t}(f_{j-1}^{n+1} - f_{j-1}^{n})\right\} \\
&\quad + \left\{\tfrac{1}{2}(f_j^{n+1} + f_j^{n}) + \frac{\tau_T}{\Delta t}(f_j^{n+1} - f_j^{n})\right\} \\
&\quad + \tfrac{1}{10}\left\{\tfrac{1}{2}(f_{j+1}^{n+1} + f_{j+1}^{n}) + \frac{\tau_T}{\Delta t}(f_{j+1}^{n+1} - f_{j+1}^{n})\right\} \\
&= \tfrac{3}{5}\delta_x^2(T_j^{n+1} + T_j^n) + \tfrac{6}{5}\frac{\tau_T}{\Delta t}\delta_x^2(T_j^{n+1} - T_j^n).
\end{aligned} \tag{21}$$

By Eq. (15), we obtain from Eq. (21)

$$\begin{aligned}
&\frac{1}{10\alpha\Delta t}(\theta_{j-1}^{n+1} - \theta_{j-1}^{n}) + \frac{1}{\alpha\Delta t}(\theta_j^{n+1} - \theta_j^{n}) + \frac{1}{10\alpha\Delta t}(\theta_{j+1}^{n+1} - \theta_{j+1}^{n}) \\
&= \tfrac{3}{5}\delta_x^2(T_j^{n+1} + T_j^n) + \tfrac{6}{5}\frac{\tau_T}{\Delta t}\delta_x^2(T_j^{n+1} - T_j^n) \\
&\quad + \tfrac{1}{10}g_{j-1}^{n+(1/2)} + g_j^{n+(1/2)} + \tfrac{1}{10}g_{j+1}^{n+(1/2)}.
\end{aligned} \tag{22}$$

Solving for θ_j^{n+1} from Eq. (16) and then substituting the solution into Eq. (22), we obtain

$$\begin{aligned}
&\left[\frac{1}{10\alpha}\left(1 + \frac{2\tau_q}{\Delta t}\right) - \frac{\Delta t}{\Delta x^2}\left(\tfrac{3}{5} + \frac{6\tau_T}{5\Delta t}\right)\right] T_{j-1}^{n+1} \\
&\quad + \left[\frac{1}{\alpha}\left(1 + \frac{2\tau_q}{\Delta t}\right) + \frac{2\Delta t}{\Delta x^2}\left(\tfrac{3}{5} + \frac{6\tau_T}{5\Delta t}\right)\right] T_{j}^{n+1} \\
&\quad + \left[\frac{1}{10\alpha}\left(1 + \frac{2\tau_q}{\Delta t}\right) - \frac{\Delta t}{\Delta x^2}\left(\tfrac{3}{5} + \frac{6\tau_T}{5\Delta t}\right)\right] T_{j+1}^{n+1} \\
&= \left[\frac{1}{10\alpha}\left(-1 + \frac{2\tau_q}{\Delta t}\right) + \frac{\Delta t}{\Delta x^2}\left(\tfrac{3}{5} - \frac{6\tau_T}{5\Delta t}\right)\right] T_{j-1}^{n} \\
&\quad + \left[\frac{1}{\alpha}\left(-1 + \frac{2\tau_q}{\Delta t}\right) - \frac{2\Delta t}{\Delta x^2}\left(\tfrac{3}{5} - \frac{6\tau_T}{5\Delta t}\right)\right] T_{j}^{n} \\
&\quad + \left[\frac{1}{10\alpha}\left(-1 + \frac{2\tau_q}{\Delta t}\right) + \frac{\Delta t}{\Delta x^2}\left(\tfrac{3}{5} - \frac{6\tau_T}{5\Delta t}\right)\right] T_{j+1}^{n}
\end{aligned}$$

$$+\frac{1}{5\alpha}\theta_{j-1}^{n}+\frac{2}{\alpha}\theta_{j}^{n}+\frac{1}{5\alpha}\theta_{j+1}^{n}$$
$$+\frac{1}{\Delta t}\left(\tfrac{1}{10}g_{j-1}^{n+(1/2)}+g_{j}^{n+(1/2)}+\tfrac{1}{10}g_{j+1}^{n+(1/2)}\right). \tag{23}$$

The discretized initial and boundary conditions are

$$T_j^0=(T_1)_j, \qquad \theta_j^0=(T_1)_j+\tau_q(T_2)_j \tag{24}$$

and

$$T_0^n=T_N^n=0, \qquad \theta_0^n=\theta_N^n=0. \tag{25}$$

One may use Eq. (23) to obtain $T_j^{n+1}$and then use Eq. (16) to obtain θ_j^{n+1}.

3. Stability

A common method for studying the stability of compact finite-difference schemes is the eigenvalue analysis [6]. In the eigenvalue analysis, the compact finite-difference scheme is first written in a matrix form. The system is then reduced to an eigenvalue problem. For numerical stability, it is required that all the eigenvalues lie in the left half of the complex plane. Here, we apply another method called the discrete Fourier analysis [1,10] to study the stability.

Since $x_j=jL/N,\ j=0,1,\ldots,N$, then the discrete Fourier coefficients of a function $u(x)$ in $[0,L]$ can be written as follows:

$$\hat{u}_k=\frac{1}{N}\sum_{j=0}^{N-1}u(x_j)\mathrm{e}^{-\mathrm{i}kx_j2\pi/L}, \quad -\frac{N}{2}\leqslant k\leqslant\frac{N}{2}-1, \quad \mathrm{i}=\sqrt{-1}.$$

It can be seen that

$$u(x_j)=\frac{1}{N}\sum_{k=-N/2}^{(N/2)-1}\hat{u}_k\mathrm{e}^{\mathrm{i}kx_j2\pi/L}.$$

We further define the inner product and norm as follows:

$$(u,v)=\frac{1}{N}\sum_{j=0}^{N-1}u(x_j)\overline{v(x_j)}, \qquad \|u\|^2=(u,u).$$

Lemma 1. *$(1/N)\sum_{j=0}^{N-1}\mathrm{e}^{-\mathrm{i}px_j2\pi/L}=1,\ p=Nm,\ m=0,\pm1,\ldots$; and $(1/N)\sum_{j=0}^{N-1}\mathrm{e}^{-\mathrm{i}px_j2\pi/L}=0$, otherwise.*

Proof. It can be seen in [1].

Lemma 2 (Parseval's equations)**.**

$$\|u\|^2=\sum_{k=-N/2}^{(N/2)-1}(\hat{u}_k)^2$$

and

$$\|\nabla_x u\|_1^2 = \frac{1}{N}\sum_{j=1}^{N}\left(\frac{u(x_j)-u(x_{j-1})}{\Delta x}\right)\overline{\left(\frac{u(x_j)-u(x_{j-1})}{\Delta x}\right)}$$
$$= \frac{1}{\Delta x^2}\sum_{k=-N/2}^{(N/2)-1}(\hat{u}_k)^2 4\sin^2\frac{\omega_k}{2}.$$

where $\omega_k = 2\pi k/N$.

Proof. The first equation can be seen in [1,10]. Since

$$u(x_j)-u(x_{j-1}) = \sum_{k=-N/2}^{(N/2)-1}\hat{u}_k[\mathrm{e}^{\mathrm{i}\omega_k j}-\mathrm{e}^{\mathrm{i}\omega_k(j-1)}]$$
$$= \sum_{k=-N/2}^{(N/2)-1}\hat{u}_k 2\mathrm{i}\sin\frac{\omega_k}{2}\mathrm{e}^{\mathrm{i}\omega_k j}\mathrm{e}^{-\mathrm{i}\omega_k/2},$$

we obtain by Lemma 1

$$\|\nabla_x u\|_1^2 = \frac{1}{N}\sum_{j=1}^{N}\left(\frac{u(x_j)-u(x_{j-1})}{\Delta x}\right)\overline{\left(\frac{u(x_j)-u(x_{j-1})}{\Delta x}\right)}$$
$$= \frac{1}{N\Delta x^2}\sum_{j=1}^{N}\left(\sum_{k=-N/2}^{(N/2)-1}\hat{u}_k 2\mathrm{i}\sin\frac{\omega_k}{2}\mathrm{e}^{\mathrm{i}\omega_k j}\mathrm{e}^{-\mathrm{i}\omega_k/2}\right)\left(\sum_{m=-N/2}^{(N/2)-1}\hat{u}_m(-2\mathrm{i})\sin\frac{\omega_m}{2}\mathrm{e}^{-\mathrm{i}\omega_m j}\mathrm{e}^{\mathrm{i}\omega m/2}\right)$$
$$= \frac{1}{\Delta x^2}\sum_{k=-N/2}^{(N/2)-1}\sum_{m=-N/2}^{(N/2)-1}\left(\hat{u}_k 4\sin\frac{\omega_k}{2}\mathrm{e}^{-\mathrm{i}\omega_k/2}\hat{u}_m\sin\frac{\omega_m}{2}\mathrm{e}^{\mathrm{i}\omega m/2}\right)\left(\frac{1}{N}\sum_{j=1}^{N}\mathrm{e}^{\mathrm{i}\omega_k j}\mathrm{e}^{-\mathrm{i}\omega_m j}\right)$$
$$= \frac{1}{\Delta x^2}\sum_{k=-N/2}^{(N/2)-1}(\hat{u}_k)^2 4\sin^2\frac{\omega_k}{2}. \qquad \square$$

Theorem 1. *Suppose that* $\{T_j^n, \theta_j^n\}$ *and* $\{S_j^n, \xi_j^n\}$ *are solutions of the scheme, Eqs.* (16) *and* (23), *with the same boundary conditions* (*Eq.* (25)), *and initial values* $\{T_j^0, \theta_j^0\}$ *and* $\{S_j^0, \xi_j^0\}$, *respectively. Let* $U_j^n = T_j^n - S_j^n$, $\varepsilon_j^n = \theta_j^n - \xi_j^n$. *Then* $\{U_j^n, \varepsilon_j^n\}$ *satisfy*

$$\frac{1}{\alpha}\|\varepsilon^n\|^2 + (\tau_T+\tau_q)\|\nabla_x U^n\|_1^2 \leqslant \frac{1}{\alpha}\|\varepsilon^0\|^2 + \tfrac{3}{2}(\tau_T+\tau_q)\|\nabla_x U^0\|_1^2. \tag{26}$$

Hence, the compact finite-difference scheme is unconditionally stable with respect to the initial values.

Proof. To show stability, we consider the original equations (15)–(17) instead of Eqs. (16) and (23). Assume that solutions $\{T_j^n, \theta_j^n, f_j^n\}$ and $\{S_j^n, \xi_j^n, h_j^n\}$ are obtained using the same boundary conditions (Eq. (25)), and initial values $\{T_j^0, \theta_j^0\}$ and $\{S_j^0, \xi_j^0\}$, respectively. Let $U_j^n = T_j^n - S_j^n, \varepsilon_j^n = \theta_j^n - \xi_j^n$ and

$r_j^n = f_j^n - h_j^n$. Then $\{U_j^n, \varepsilon_j^n, r_j^n\}$ satisfy

$$\frac{1}{\alpha\,\Delta t}(\varepsilon_j^{n+1} - \varepsilon_j^n) = \tfrac{1}{2}(r_j^{n+1} + r_j^n) + \frac{\tau_T}{\Delta t}(r_j^{n+1} - r_j^n), \tag{27}$$

$$\tfrac{1}{2}(\varepsilon_j^{n+1} + \varepsilon_j^n) = \tfrac{1}{2}(U_j^{n+1} + U_j^n) + \frac{\tau_q}{\Delta t}(U_j^{n+1} - U_j^n), \tag{28}$$

and

$$\tfrac{1}{10} r_{j-1}^n + r_j^n + \tfrac{1}{10} r_{j+1}^n = \frac{6}{5\Delta x^2}(U_{j-1}^n - 2U_j^n + U_{j+1}^n). \tag{29}$$

We introduce the discrete Fourier coefficients of ε_j^n, U_j^n and r_j^n as follows:

$$\hat{\varepsilon}_k^n = \frac{1}{N}\sum_{j=0}^{N-1} \varepsilon_j^n \mathrm{e}^{-\mathrm{i}\omega_k j}, \quad \hat{U}_k^n = \frac{1}{N}\sum_{j=0}^{N-1} U_j^n \mathrm{e}^{-\mathrm{i}\omega_k j}, \quad \hat{r}_k^n = \frac{1}{N}\sum_{j=0}^{N-1} r_j^n \mathrm{e}^{-\mathrm{i}\omega_k j}.$$

Then, we have

$$\varepsilon_j^n = \sum_{k=-N/2}^{(N/2)-1} \hat{\varepsilon}_k^n \mathrm{e}^{\mathrm{i}\omega_k j}, \quad U_j^n = \sum_{k=-N/2}^{(N/2)-1} \hat{U}_k^n \mathrm{e}^{\mathrm{i}\omega_k j}, \quad r_j^n = \sum_{k=-N/2}^{(N/2)-1} \hat{r}_k^n \mathrm{e}^{\mathrm{i}\omega_k j}.$$

Substituting the above equations into Eqs. (27)–(29), we obtain

$$\frac{1}{\alpha\,\Delta t}(\hat{\varepsilon}_k^{n+1} - \hat{\varepsilon}_k^n) = \tfrac{1}{2}(\hat{r}_k^{n+1} + \hat{r}_k^n) + \frac{\tau_T}{\Delta t}(\hat{r}_k^{n+1} - \hat{r}_k^n), \tag{30}$$

$$\tfrac{1}{2}(\hat{\varepsilon}_k^{n+1} + \hat{\varepsilon}_k^n) = \tfrac{1}{2}(\hat{U}_k^{n+1} + \hat{U}_k^n) + \frac{\tau_q}{\Delta t}(\hat{U}_k^{n+1} - \hat{U}_k^n), \tag{31}$$

and

$$(1 + \tfrac{1}{5}\cos\omega_k)\hat{r}_k^n = -\frac{24}{5\Delta x^2}\sin^2\frac{\omega_k}{2}\hat{U}_k^n. \tag{32}$$

Solving for $\hat{r}_k^n$ from Eq. (32), we obtain

$$\hat{r}_k^n = -\frac{N_k}{D_k}\hat{U}_k^n, \tag{33}$$

where $N_k = (24/5\Delta x^2)\sin^2\omega_k/2$ and $D_k = 1 + \frac{1}{5}\cos\omega_k$. Substituting Eq. (33) into Eq. (30) gives

$$\frac{1}{\alpha\,\Delta t}(\hat{\varepsilon}_k^{n+1} - \hat{\varepsilon}_k^n) = -\frac{1}{2}\frac{N_k}{D_k}(\hat{U}_k^{n+1} + \hat{U}_k^n) - \frac{N_k}{D_k}\frac{\tau_T}{\Delta t}(\hat{U}_k^{n+1} - \hat{U}_k^n). \tag{34}$$

Multiplying Eq. (34) by $\hat{\varepsilon}_k^{n+1} + \hat{\varepsilon}_k^n$, we obtain

$$\frac{1}{\alpha\,\Delta t}[(\hat{\varepsilon}_k^{n+1})^2 - (\hat{\varepsilon}_k^n)^2] = -\frac{1}{2}\frac{N_k}{D_k}(\hat{U}_k^{n+1} + \hat{U}_k^n)(\hat{\varepsilon}_k^{n+1} + \hat{\varepsilon}_k^n) - \frac{N_k}{D_k}\frac{\tau_T}{\Delta t}(\hat{U}_k^{n+1} - \hat{U}_k^n)(\hat{\varepsilon}_k^{n+1} + \hat{\varepsilon}_k^n). \tag{35}$$

We then multiply Eq. (31) by $(N_k/D_k)(\hat{U}_k^{n+1} + \hat{U}_k^n)$ and $(N_k/D_k)(\hat{U}_k^{n+1} - \hat{U}_k^n)$, respectively, to obtain

$$\frac{1}{2}\frac{N_k}{D_k}(\hat{\varepsilon}_k^{n+1} + \hat{\varepsilon}_k^n)(\hat{U}_k^{n+1} + \hat{U}_k^n) = \frac{1}{2}\frac{N_k}{D_k}(\hat{U}_k^{n+1} + \hat{U}_k^n)^2 + \frac{\tau_q}{\Delta t}\frac{N_k}{D_k}[(\hat{U}_k^{n+1})^2 - (\hat{U}_k^n)^2] \tag{36}$$

and

$$\frac{1}{2}\frac{N_k}{D_k}(\hat{\varepsilon}_k^{n+1}+\hat{\varepsilon}_k^n)(\hat{U}_k^{n+1}-\hat{U}_k^n)=\frac{1}{2}\frac{N_k}{D_k}[(\hat{U}_k^{n+1})^2-(\hat{U}_k^n)^2]+\frac{\tau_q}{\Delta t}\frac{N_k}{D_k}(\hat{U}_k^{n+1}-\hat{U}_k^n)^2. \tag{37}$$

Substituting Eqs. (36) and (37) into Eq. (35), we obtain

$$\begin{aligned}&\frac{1}{\alpha\,\Delta t}[(\hat{\varepsilon}_k^{n+1})^2-(\hat{\varepsilon}_k^n)^2]+\frac{1}{2}\frac{N_k}{D_k}(\hat{U}_k^{n+1}+\hat{U}_k^n)^2+\frac{\tau_q}{\Delta t}\frac{N_k}{D_k}[(\hat{U}_k^{n+1})^2-(\hat{U}_k^n)^2]\\&\quad+\frac{\tau_T}{\Delta t}\frac{N_k}{D_k}[(\hat{U}_k^{n+1})^2-(\hat{U}_k^n)^2]+\frac{2\tau_T\tau_q}{\Delta t^2}\frac{N_k}{D_k}(\hat{U}_k^{n+1}-\hat{U}_k^n)^2\\&\quad=0.\end{aligned} \tag{38}$$

Since $N_k/D_k>0$, we may drop the second and last terms on the left-hand side of Eq. (38) and then multiply by Δt to obtain

$$\begin{aligned}\frac{1}{\alpha}(\hat{\varepsilon}_k^{n+1})^2+(\tau_T+\tau_q)\frac{N_k}{D_k}(\hat{U}_k^{n+1})^2&\leqslant\frac{1}{\alpha}(\hat{\varepsilon}_k^n)^2+(\tau_T+\tau_q)\frac{N_k}{D_k}(\hat{U}_k^n)^2\\&\leqslant\cdots\\&\leqslant\frac{1}{\alpha}(\hat{\varepsilon}_k^0)^2+(\tau_T+\tau_q)\frac{N_k}{D_k}(\hat{U}_k^0)^2.\end{aligned} \tag{39}$$

Since $(4/\Delta x^2)\sin^2\omega_k/2\leqslant N_k/D_k\leqslant\frac{3}{2}(4/\Delta x^2)\sin^2\omega_k/2$, we obtain

$$\begin{aligned}&\frac{1}{\alpha}(\hat{\varepsilon}_k^{n+1})^2+(\tau_T+\tau_q)\frac{4}{\Delta x^2}\sin^2\frac{\omega_k}{2}(\hat{U}_k^{n+1})^2\\&\quad\leqslant\frac{1}{\alpha}(\hat{\varepsilon}_k^{n+1})^2+(\tau_T+\tau_q)\frac{N_k}{D_k}(\hat{U}_k^{n+1})^2\\&\quad\leqslant\frac{1}{\alpha}(\hat{\varepsilon}_k^0)^2+(\tau_T+\tau_q)\frac{N_k}{D_k}(\hat{U}_k^0)^2\\&\quad\leqslant\frac{1}{\alpha}(\hat{\varepsilon}_k^0)^2+(\tau_T+\tau_q)\frac{3}{2}\frac{4}{\Delta x^2}\sin^2\frac{\omega_k}{2}(\hat{U}_k^0)^2.\end{aligned} \tag{40}$$

Summing k from $-N/2$ to $(N/2)-1$ gives

$$\begin{aligned}&\sum_{k=-N/2}^{(N/2)-1}\left[\frac{1}{\alpha}(\hat{\varepsilon}_k^{n+1})^2+(\tau_T+\tau_q)\frac{4}{\Delta x^2}\sin^2\frac{\omega_k}{2}(\hat{U}_k^{n+1})^2\right]\\&\quad\leqslant\sum_{k=-N/2}^{(N/2)-1}\left[\frac{1}{\alpha}(\hat{\varepsilon}_k^0)^2+(\tau_T+\tau_q)\frac{3}{2}\frac{4}{\Delta x^2}\sin^2\frac{\omega_k}{2}(\hat{U}_k^0)^2\right].\end{aligned} \tag{41}$$

Hence, we obtain Eq. (26) by Lemma 2. □

4. Numerical examples

Two examples are given to test the accuracy of the scheme, Eqs. (16) and (23), with initial and boundary conditions (24) and (25). We first consider a simple equation

$$\frac{\partial T}{\partial t}+\left(\frac{1}{\pi^2}+10^2\right)\frac{\partial^2 T}{\partial t^2}=\frac{\partial^2 T}{\partial x^2}+\left(\frac{1}{\pi^2}+10^{-6}\right)\frac{\partial^3 T}{\partial t\,\partial x^2},\quad 0\leqslant x\leqslant 10^{-4},\quad t>0, \tag{42}$$

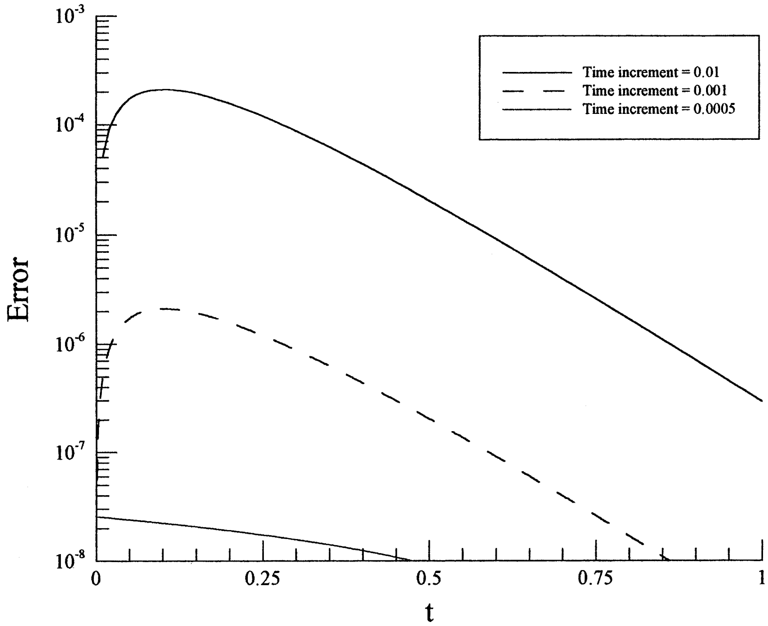

Fig. 1. Errors of the numerical solutions with different time increments and a grid size of 0.000001.

where the exact solution is

$$T(x,t) = \mathrm{e}^{-\pi^2 t}\sin(10^4\pi x), \quad 0 \leqslant x \leqslant 10^{-4}, \quad t > 0 \tag{43}$$

and test the accuracy of the solution with respect to time t.

The initial and boundary conditions are obtained based on the exact solution. To apply our scheme, we chose a grid size $\Delta x = 0.0000001$ and three time increments $\Delta t = 0.01$, 0.001 and 0.0005, respectively. To show convergence, we calculated the error of the numerical solution T for $0 \leqslant n\,\Delta t \leqslant 1$ as follows:

$$\text{Error} = \left(\frac{1}{10^{-4}} \Delta x \sum_{j=1}^{N-1} |(T_{\text{exact}})_j^n - T_j^n|^2 \right)^{1/2}.$$

Errors for three different time increments are shown in Fig. 1. From this figure, we can see that the numerical solutions are second-order accurate in time t compared with the exact solution.

We now consider another simple equation

$$\frac{1}{2}\frac{\partial T}{\partial t} + \frac{3}{2\pi^2}\frac{\partial^2 T}{\partial t^2} = \frac{\partial^2 T}{\partial x^2} + \frac{2}{\pi^2}\frac{\partial^3 T}{\partial t\,\partial x^2}, \quad 0 \leqslant x \leqslant 1, \quad t > 0, \tag{44}$$

where the exact solution is

$$T(x,t) = \mathrm{e}^{-\pi^2 t}\sin(\pi x), \quad 0 \leqslant x \leqslant 1, \quad t > 0 \tag{45}$$

and test for the accuracy of the solution with respect to space x.

The initial and boundary conditions are obtained based on the exact solution. To apply our scheme, we chose a time increment $\Delta t = 0.001$ and grid sizes $\Delta x = 0.2$, 0.1 and 0.05, respectively. To show

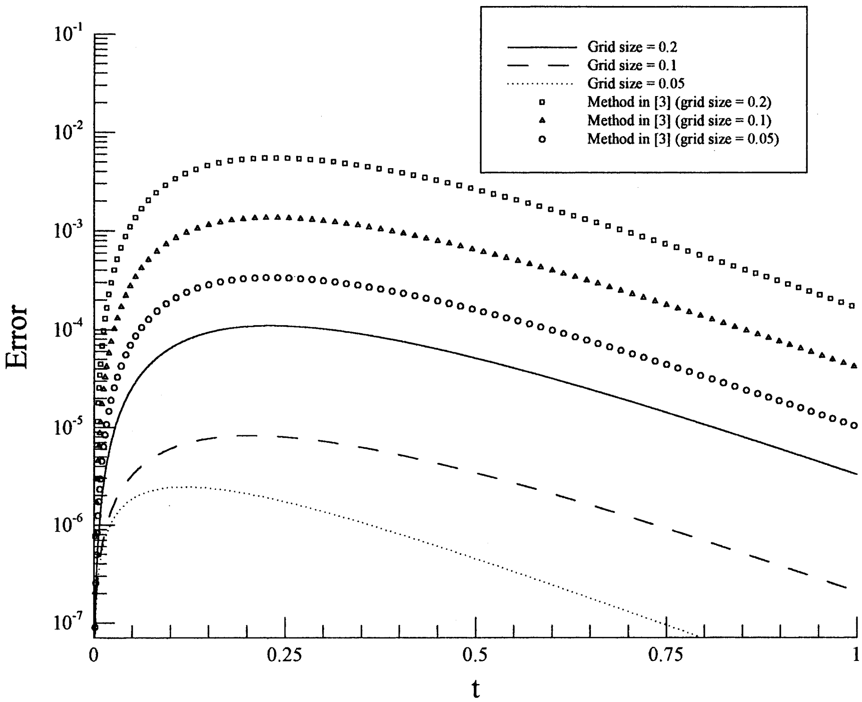

Fig. 2. Errors of the numerical solutions with different grid sizes and a time increment of 0.001.

convergence, we computed the error of the numerical solution T for $0 \leqslant n\,\Delta t \leqslant 1$ as follows:

$$\text{Error} = \left(\Delta x \sum_{j=1}^{N-1} |(T_{\text{exact}})_j^n - T_j^n|^2 \right)^{1/2}.$$

Also, we computed the errors obtained using our previous scheme in [3], that is a Crank–Nicholson type of finite-difference scheme where the truncation error is $0(\Delta t^2 + \Delta x^2)$, as follows:

$$3\,\frac{\theta_j^{n+1} - \theta_j^n}{\Delta t} = \delta_x^2[\tfrac{1}{2}T_j^n + 2\theta_j^n] + \delta_x^2[\tfrac{1}{2}T_j^{n+1} + 2\theta_j^{n+1}], \tag{46}$$

and

$$\frac{3}{\pi^2}\,\frac{T_j^{n+1} - T_j^n}{\Delta t} = -\tfrac{1}{2}(T_j^{n+1} + T_j^n) + (\theta_j^{n+1} + \theta_j^n). \tag{47}$$

Errors for three different grid sizes are shown in Fig. 2. From this figure, we can see that the numerical solutions are more accurate than those obtained by the scheme in [3].

5. Conclusion

In this study, we develop a high-order compact finite-difference scheme for a heat transport equation at the microscale. It is shown by the discrete Fourier analysis method that the scheme is unconditionally stable with respect to the initial values. Numerical results show that the solution is accurate. The method can be readily generalized to the case where a higher-order compact finite difference is employed.

References

[1] C. Canuto, M.Y. Hussaini, A. Quarteroni, T.A. Zang, Spectral Methods in Fluid Dynamics, Springer, New York, 1987.

[2] R.J. Chiffell, On the wave behavior and rate effect of thermal and thermo-mechanical waves, M.S. Thesis, University of New Mexico, Albuquerque, NM, 1994.

[3] W. Dai, R. Nassar, A finite difference method for solving the heat transport equation at the microscale, Numer. Methods Partial Differential Equations 15 (1999) 698–708.

[4] D.D. Joseph, L. Preziosi, Heat waves, Rev. Modern Phys. 61 (1989) 41–73.

[5] A.A. Joshi, A. Majumdar, Transient ballistic and diffusive phonon heat transport in thin films, J. Appl. Phys. 74 (1993) 31–39.

[6] S.K. Lele, Compact finite difference schemes with spectral-like resolution, J. Comput. Phys. 103 (1992) 16–42.

[7] M.N. Özisik, D.Y. Tzou, On the wave theory in heat conduction, ASME J. Heat Transfer 116 (1994) 526–536.

[8] T.Q. Qiu, C.L. Tien, Short-pulse laser heating on metals, Internat. J. Heat Mass Transfer 35 (1992) 719–726.

[9] T.Q. Qiu, C.L. Tien, Heat transfer mechanisms during short-pulse laser heating of metals, ASME J. Heat Transfer 115 (1993) 835–841.

[10] J.C. Strikwerda, Finite Difference Schemes and Partial Differential Equations, Chapman & Hall, New York, 1989.

[11] D.Y. Tzou, Macro To Micro Heat Transfer, Taylor & Francis, Washington DC, 1996.