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High-order finite difference methods for a second order dual-phase-lagging models of microscale heat transfer

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ABSTRACT

In this paper, a compact alternating direction implicit (ADI) method, which combines the fourth-order compact difference for the approximations of the second spatial derivatives and the approximation factorizations of difference operators, is firstly presented for solving two-dimensional (2D) second order dual-phase-lagging models of microscale heat transfer. By the discrete energy method, it is shown that it is second-order accurate in time and fourth-order accurate in space with respect to L^2-norms. Additionally, the compact ADI method is successfully generalized to solve corresponding three-dimensional (3D) problem. Also, the convergence result of the solver for 3D case is given rigorously. Finally, numerical examples are carried out to testify the computational efficiency of the algorithms and exhibit the correctness of theoretical results.

1. Introduction

Over the years, microtechnologies (cf. [1–7,9–12]), which often are closely relevant to heat transport through thin films and the high-rate heating on thin film structures, have been widely applied in industry, and have been tremendously developed because of the great advancement of short-pulse laser technologies and their applications to micromanufacturing processes. Taking metal processing for example, there exist many important applications, such as, laser surface hardening, laser micro-machining, laser processing of diamond films from carbon ion-implanted copper substrates and laser patterning. As we know, microelectronic devices are often composed of the thin films of metals, of dielectrics such as SiO_2, or Si semiconductors. Generally speaking, the smaller the device size is, the quicker switching speed it has. However, the device size reduction makes the heat-generation rate rapidly increase, thus yielding a higher thermal load on the microdevice. Thereby, it is very essential to research the thermal behavior of thin films for predicting the performance of a microelectronic device or devising the preferable microstructure.

Traditional heat conduction equation (i.e. diffusion equation) is derived using the combination of the conservation of energy principle and Fourier law, which are defined as follow

$$-\nabla \cdot \mathbf{q} + Q = \rho C_p \frac{\partial T}{\partial t} \tag{1.1a}$$

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$$\mathbf{q}(\mathbf{x},t) = -\kappa \nabla T(\mathbf{x},t), \tag{1.1b}$$

respectively. Here $\mathbf{q}$, T, κ, ρ, C_p and Q are the heat flux, the temperature, the conductivity, the density, the specific heat and heat source, respectively. From (1.1a)–(1.1b), we can observe that the heat flux and the temperature gradient across a material volume are supposed to arise at the same instant of time, that is $\mathbf{q}(\mathbf{x},t) = -\kappa\nabla T(\mathbf{x},t)$. However, in the process of the heat transfers at a microscale direction, the heat flux and temperature gradient in this direction will occur at different times. In this case, Fourier law (1.1a), which is invalid, is replaced by (cf. [4–7,9–12])

$$\mathbf{q}(\mathbf{x},t+\tau_q) = -\kappa \nabla T(\mathbf{x},t+\tau_T), \tag{1.2}$$

where τ_q and τ_T are two corresponding phase lags. In the both sides of (1.2), applying the Taylor series formula to expand (1.2) at ($\mathbf{x}$, t), then a first-order approximation of (1.2) is derived as

$$\mathbf{q} + \tau_q \frac{\partial \mathbf{q}}{\partial t} = -k\left[\nabla T + \tau_T \frac{\partial}{\partial t}(\nabla T)\right], \tag{1.3}$$

which is used along with (1.1a) to gives that

$$\frac{1}{\tilde{\alpha}}\frac{\partial T}{\partial t} + \frac{\tau_q}{\tilde{\alpha}}\frac{\partial^2 T}{\partial t^2} = \Delta T + \tau_T \Delta \frac{\partial T}{\partial t} + \frac{1}{\kappa}\left(Q + \tau_q \frac{\partial Q}{\partial t}\right), \tag{1.4}$$

which $\tilde{\alpha} = k/\rho C_p$.

In recent years, a great deal of effort has been devoted to developing high-order numerical solvers for problems (1.4). For example, a second-order finite difference method (FDM), compact FDM and approximate analytic method have been created for one-dimensional (1D) Eq. (1.4) in [4–6], respectively. Also, second-order FDM and compact FDM for two-dimensional (2D) and three-dimensional (3D) Eq. (1.4) have been developed in [12] and [7,8], respectively. Besides, other high-performance solvers including ADI FDM [13–15], compact ADI method [16,17], finite element method (FEM) [18,20], finite volume element method (FVEM) [19], Pseudospectral collocation method [21,22], Douglas-Gunn time-splitting method [23] and Runge–Kutta method [24,25], etc., have been established and examined, entirely.

Comparably, utilizing the Taylor series formula to expand Eq. (1.2) at ($\mathbf{x}$, t) and providing a second-order approximations with respect to τ_q and τ_T, and then combining this second-order approximation with Eq. (1.1a), we can also deduce another second-order dual-phase-lag (DPL) model as follows

$$\frac{1}{\tilde{\alpha}}\frac{\partial T}{\partial t} + \frac{\tau_q}{\tilde{\alpha}}\frac{\partial^2 T}{\partial t^2} + \frac{\tau_q^2}{2\tilde{\alpha}}\frac{\partial^3 T}{\partial t^3} = \Delta T + \tau_T \Delta \frac{\partial T}{\partial t} + \frac{\tau_T^2}{2}\Delta \frac{\partial^2 T}{\partial t^2} + \frac{1}{\kappa}\left(Q + \tau_q \frac{\partial Q}{\partial t} + \frac{\tau_q^2}{2}\frac{\partial^2 Q}{\partial t^2}\right). \tag{1.5}$$

From the derivation of Eq. (1.5), we can observe that higher order approximations are used in (1.2). Hence, model (1.5) may be more accurate than model (1.4) as they are applied to describe microscale heat transfer. As a result, from the physical point of view, it is meaningful to develop excellent numerical method for solving Eq. (1.5).

Exact solutions to 1D Eq. (1.5) can firstly be given in the form of infinite double series of sine functions of the spatial variables by using the method of separation of variables in [10]. Then approximation solutions can be obtained by truncating these exact infinite series solutions. Moreover, the second-order FDM and fourth-order compact FDM are suggested for the numerical solutions of 1D Eq. (1.5) in [9] and [11], respectively. However, very little attention has been paid to the solution of high-dimensional Eq. (1.5).

It is well-known that a large block tridiagonal system, which needs to be solved at each time step for high-dimensional problems, gives rise to highly computational burden. It is well-known that ADI methods can equivalently transfer the solution of a multi-dimensional problems into the solutions of series of independent 1D problems, thus tremendously saving time cost. Hence, for efficiently solving these complex problems, compact ADI methods, which preserve the high-order spatial accuracy of compact difference schemes and the high efficiency of ADI methods, are a preferable choice.

In this paper, we discuss the application of the compact ADI methods to solve the following nonlinear initial boundary value problems (IBVP)

$$A\frac{\partial T}{\partial t} + B\frac{\partial^2 T}{\partial t^2} + C\frac{\partial^3 T}{\partial t^3} = \alpha \Delta T + D\Delta \frac{\partial T}{\partial t} + E\Delta \frac{\partial^2 T}{\partial t^2} + f(\mathbf{x},t), \quad (\mathbf{x},t) \in \Omega \times [0,\hat{T}], \tag{1.6a}$$

$$T(\mathbf{x},t) = \psi(\mathbf{x},t), \qquad (\mathbf{x},t) \in \partial\Omega \times [0,\hat{T}], \tag{1.6b}$$

$$T(\mathbf{x},0) = \phi(\mathbf{x}), \qquad T_t(\mathbf{x},0) = \varphi(\mathbf{x}), \qquad T_{tt}(\mathbf{x},0) = \nu(\mathbf{x}) \qquad \mathbf{x} \in \bar{\Omega}, \tag{1.6c}$$

in which $\mathbf{x} = (x,y) \in \Omega := (a_1,b_1) \times (a_2,b_2)$ for two-dimensional case, or, in the case of three-dimensional (3D) case, $\mathbf{x} = (x,y,z) \in \Omega := (a_1,b_1) \times (a_2,b_2) \times (a_3,b_3)$, and $\partial\Omega$ is the boundary of Ω, $\bar{\Omega} = \Omega \cup \partial\Omega$, A, B, C, D, E and α are positive constants. Moreover, let functions $f(\mathbf{x}, t)$, $\psi(\mathbf{x}, t)$, $\phi(\mathbf{x})$, $\varphi(\mathbf{x}, t)$ and $\nu(\mathbf{x})$ be smooth sufficiently so that our methods can attain the convergence rate and consistency claimed.

2. Denotations and lemmas

For temporal discretization, $\exists N \in \mathbb{Z}^+$, such that $\tau = \hat{T}/N$. Write $t_n = n\tau$, $0 \le n \le N$. $\forall\, v^n \in S_{\Delta t} = \{v^n | 0 \le n \le N\}$, introduce $\delta_t v^{n+1/2} = (v^{n+1} - v^n)/\tau$ and $v^{n+\frac{1}{2}} = (v^{n+1} + v^n)/2$.