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A stable and convergent three-level finite difference scheme for solving a dual-phase-lagging heat transport equation in spherical coordinates

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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 consider the heat transport equation in spherical coordinates and develop a three level finite difference scheme for solving the heat transport equation in a microsphere. It is shown that the scheme is unconditionally stable and convergent. The method is illustrated by two numerical examples.

1. Introduction

Heat transport through thin films or micro-objects is of vital importance in microtechnology applications [1,2]. 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 [3,4]. Examples in metal processing are laser micromachining, laser patterning, laser processing of diamond films from carbon ion implanted copper substrates, and laser surface hardening. Hence, studying the thermal behavior of thin films or of micro-objects is essential for predicting the performance of a microelectronic device or for obtaining the desired microstructure [2]. The heat transport equations used to describe the thermal behavior of microstructures are expressed as [5,6]:

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

$$\vec{q} + \tau_q \frac{\partial \vec{q}}{\partial t} = -k\left[\nabla T + \tau_T \frac{\partial}{\partial t}[\nabla T]\right], \tag{2}$$

where $\vec{q} = (q_1, q_2, q_3)$ is heat flux, T is temperature, k is conductivity, C_p is specific heat, ρ is density, Q is a heat source, τ_q and τ_T are positive constants, which are the time lags of the heat flux and temperature gradient, respectively. Eqs. (1) and (2) are normally termed in the literature as energy balance equation and constitutive relation of heat flux density, respectively. In the classical theory of diffusion, the heat flux vector ($\vec{q}$) 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:

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

However, if the scale in one direction is at the sub-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) [5]. The significance

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Nomenclature

A, B, C	constant coefficients	t_p	laser pulse duration
C_p	heat capacity	u_j^n	mesh function where n is the time level and j is the grid point
$E^{-1/2}$	finite difference operator	ε	difference between the exact solution and numerical solution
J	laser fluence	∇_r, $\nabla_{\bar{r}}$	first order forward, backward finite differences
k	thermal conductivity	ΔT	temperature change
L	the length of radius of the sphere	Δt, Δr	time increment, grid size
N	number of grid points	ρ	density
P_h	finite difference operator	σ	truncation error
Q	heat source	τ_q	time lag of the heat flux
R	reflectivity	τ_T	time lag of the temperature gradient
r	radius		
T, T_∞	temperature		
t, t_0	time		

of the heat transfer equations (1) and (2) as opposed to the classical heat transfer equations has been discussed in [5] (see pp. 127–128). In Fig. 5.9 (see p. 128 in [5]) the author shows that for $\tau_T = 90$ ps and $\tau_q = 8.5$ ps the predicted change in $\frac{\Delta T}{\Delta T_{\max}}$ over time gave an excellent fit to the data and was significantly different from that predicted by the classic heat transfer equations.

Analytic and numerical methods for solving the above coupled Eqs. (1) and (2) have been widely investigated [5–22]. Tzou and Özisik [5,6] considered Eqs. (1) and (2) in one dimension and eliminated the heat flux $\vec{q}$ to obtain a dimensionless heat transport equation as follows:

$$A\frac{\partial T}{\partial t} + B\frac{\partial^2 T}{\partial t^2} = \frac{\partial^2 T}{\partial x^2} + C\frac{\partial^3 T}{\partial x^2 \partial t} + G, \tag{4}$$

where $A = \frac{\rho C_p}{k}$, $B = \frac{\tau_q \rho C_p}{k}$, $C = \tau_T$, and $G = \frac{1}{k}(Q + \tau_q \frac{\partial Q}{\partial t})$. They studied the lagging behavior by solving the above heat transport equation (4) without body heating 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 [8]. Tzou and Chiu [9] also studied the temperature-dependent thermal lagging in ultrafast laser heating. Wang et al. [10–12] developed methods of measuring the phase-lags of the heat flux and the temperature gradient and obtained analytical solutions for 1D, 2D and 3D heat conduction domains under essentially arbitrary initial and boundary conditions. Solution structure theorems were also developed for both mixed and Cauchy problems of dual-phase-lagging heat conduction equations. Tang and Araki [14] derived an analytic solution in finite rigid slabs by using the Green's function method and a finite integral transform technique. Lin et al. [15] obtained an analytic solution using the Fourier series. Al-Nimr and Arpaci [16] proposed a new approach, based on the physical decoupling of the hyperbolic two-step model, to describe the thermal behavior of a thin metal film exposed to picoseconds thermal pulses. Chen and Beraun [17] employed the corrective smoothed particle method to obtain a numerical solution of ultrashort laser pulse interactions with metal films. Dai and Nassar [18] developed a two-level finite difference scheme of the Crank–Nicholson type by introducing an intermediate function for solving Eq. (4) in a finite interval. It is shown by the discrete energy method that the scheme is unconditionally stable. The scheme has been generalized to a three-dimensional rectangular thin film case where the thickness is at the sub-microscale [19]. Further, Dai and Nassar [20,21] developed high-order unconditionally stable two-level compact finite difference schemes for solving Eq. (4) in one- and three-dimensional thin films, respectively. In this article, we consider the case where the heat transport is in a microsphere. The heat transport in a microsphere is important not only in microtechnology applications (such as predicting the thermal energy around a microvoid in order to improve the efficiency of thermal processing [5]) but also in biomedical applications, such as hyperthermia cancer therapy [23]. One needs to predict the temperature distribution in a tumor in order to evaluate the thermal success of hyperthermia cancer treatments and optimize their applications. In this study, we assume that the laser irradiation is symmetric on the surface of the sphere for simplicity. As such, Eq. (4) used to describe the thermal behavior of a microsphere in spherical coordinates can be written as follows:

$$\rho C\left(\frac{\partial T}{\partial t} + \tau_q \frac{\partial^2 T}{\partial t^2}\right) = \frac{k}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial T}{\partial r}\right) + \tau_T \frac{k}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial^2 T}{\partial r \partial t}\right) + G, \quad 0 < r < L, \tag{5}$$

where L is the radius of the sphere. The initial and boundary conditions are assumed to be

$$T(r,0) = 0, \quad \frac{\partial T(r,0)}{\partial t} = 0 \tag{6}$$

and

$$\frac{\partial T(0,t)}{\partial r} = \frac{\partial T(L,t)}{\partial r} = 0. \tag{7}$$

Such boundary conditions arise from the case where the sphere is subjected to a short-pulse laser irradiation. Hence, one may assume no heat losses from the spherical surface in the short time response [5]. However, other boundary conditions can be applied without difficulty. Since the well-posedness of the dual-phase-lagging heat conduction equation, Eq. (4), and the analytic solutions of Eqs. (5)–(7) have been discussed in [10–12,22], we assume that the solution of the above initial and boundary value problem is smooth. Because the exact solution is difficult to obtain in general, our interest is in developing an unconditionally stable and convergent finite difference scheme for solving the above initial and boundary value problem. Unconditional stability and convergence are particularly important so that there are no restrictions on the mesh ratio, since the grid size in the r-direction of the solution domain is very small.

2. Finite difference scheme

We denote T_j^n as the numerical approximation of $T(j\Delta r, n\Delta t)$, where Δr and Δt are the r directional spatial and temporal mesh sizes, respectively, and $0 \leqslant j \leqslant N$ so that $N\Delta r = L$. We use the following difference operators:

$$\nabla_r T_j^n = \frac{T_{j+1}^n - T_j^n}{\Delta r}, \quad \nabla_{\bar{r}} T_j^n = \frac{T_j^n - T_{j-1}^n}{\Delta r}.$$

A three-level finite difference scheme for solving the above initial and boundary problem (Eqs. (5)–(7)) is developed as follows:

$$\begin{aligned}\rho C\left(\frac{T_j^{n+1} - T_j^{n-1}}{2\Delta t} + \tau_q \frac{T_j^{n+1} - 2T_j^n + T_j^{n-1}}{(\Delta t)^2}\right) &= \frac{k}{r_j^2} P_h\left(\frac{T_j^{n+1} + 2T_j^n + T_j^{n-1}}{4}\right) \\ &\quad + \tau_T \frac{k}{r_j^2} P_h\left(\frac{T_j^{n+1} - T_j^{n-1}}{2\Delta t}\right) + G_j^n, \quad 1 \leqslant j \leqslant N-1,\end{aligned} \tag{8}$$

where P_h is an operator such that

$$P_h(T_j) \equiv r_{j+(1/2)}^2 \frac{T_{j+1} - T_j}{(\Delta r)^2} - r_{j-(1/2)}^2 \frac{T_j - T_{j-1}}{(\Delta r)^2}. \tag{9}$$

The initial and boundary conditions are discretized as follows:

$$T_j^0 = T_j^1 = 0 \tag{10}$$

and

$$\nabla_{\bar{r}} T_1^n = 0, \quad \nabla_{\bar{r}} T_N^n = 0 \tag{11}$$

for any time level n. It should be pointed out that we use a weighted average $\frac{T_j^{n+1}+2T_j^n+T_j^{n-1}}{4}$ for stability and convergence.

The stability and convergence of the scheme (Eqs. (8)–(11)) are shown by using the discrete energy method [24,25]. Two theorems are obtained as follows:

Theorem 1. *Assume that T_j^n and S_j^n satisfy Eq. (8) and the same initial and boundary conditions, Eqs. (10) and (11), but different source terms G_1 and G_2. Let $u_j^n = T_j^n - S_j^n$. Then u_j^n satisfies, for any $0 < n\Delta t \leqslant t_0$,*

$$\begin{aligned}&4\rho C\tau_q \left\| r\left(u^{n+1} - u^n\right)\right\|^2 + k\Delta t^2 \left\| \left(E^{-1/2} r\right)\nabla_{\bar{r}}\left(u^{n+1} + u^n\right)\right\|_1^2 \\ &\quad \leqslant 2t_0\Delta t \max_{0 \leqslant m \leqslant n} \|g^m\|^2,\end{aligned} \tag{12}$$

where $g_j^n = (G_1)_j^n - (G_2)_j^n$, and $E^{-1/2}$ is a shift operator such that $E^{-1/2} r_j = r_{j-(1/2)}$. Hence, the scheme is unconditionally stable with respect to the source term.

Theorem 2. *Assume that the solution of the initial and boundary value problem, Eqs. (8)–(11), is smooth. Let $\varepsilon_j^n = T(j\Delta r, n\Delta t) - T_j^n$, where $T(j\Delta r, n\Delta t)$ and T_j^n are the exact solution and numerical solution, respectively. Then, ε_j^n satisfies, for $0 \leqslant j\Delta r \leqslant L$ and $0 \leqslant n\Delta t \leqslant t_0$,*

$$\begin{aligned}&4\rho C\tau_q \left\| r\left(\varepsilon^{n+1} - \varepsilon^n\right)\right\|^2 + k(\Delta t)^2 \left\| \left(E^{-1/2} r\right)\nabla_{\bar{r}}\left(\varepsilon^{n+1} + \varepsilon^n\right)\right\|_1^2 \\ &\quad \leqslant 4\rho C\tau_q \left\| r\left(\varepsilon^1 - \varepsilon^0\right)\right\|^2 + k(\Delta t)^2 \left\| \left(E^{-1/2} r\right)\nabla_{\bar{r}}\left(\varepsilon^1 + \varepsilon^0\right)\right\|_1^2 \\ &\qquad + 2t_0\Delta t \max_{0 \leqslant m \leqslant n}\left(\|q^m\|^2 + \|\sigma^m\|^2\right) \\ &\qquad + kt_0(C_1 + C_2)\Delta t\Delta r \max_{r,t}\left|\frac{\partial^2 T}{\partial r^2}\right|^2 \\ &\qquad + kt_0\tau_T(C_3 + C_4)\Delta t\Delta r \max_{r,t}\left|\frac{\partial^3 T}{\partial r^2 \partial t}\right|^2,\end{aligned} \tag{13}$$

where C_i, $i = 1,2,3,4$, are positive constants. Hence, the scheme is unconditionally convergent.

Here, the inner products and norms are defined as follows:

$$(u,v) = \Delta r \sum_{j=1}^{N-1} u_j \cdot v_j, \quad \|u\|^2 = (u,u)$$

and

$$\|\nabla_{\bar{r}} u\|_1^2 = (\nabla_{\bar{r}} u_j, \nabla_{\bar{r}} u_j)_1 = \Delta r \sum_{j=1}^{N} (\nabla_{\bar{r}} u_j)^2.$$

The proofs of the above two theorems are placed in Appendix A.

3. Numerical examples

To test the accuracy of our scheme, Eqs. (8) and (9), with initial and boundary conditions, Eqs. (10) and (11), we consider a simple initial and boundary value problem

$$\frac{\partial T}{\partial t}+\frac{1}{2\pi^2}\frac{\partial^2 T}{\partial t^2}=\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial T}{\partial r}\right)+\frac{1}{\pi^2 r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial^2 T}{\partial r\partial t}\right)-\frac{\pi^2}{2}e^{-\pi^2 t}\cos(\pi r), \tag{14}$$

where the exact solution is

$$T(r,t)=e^{-\pi^2 t}\cos(\pi r), \quad r\in[0,1]. \tag{15}$$

The initial and boundary conditions are chosen from the exact solution. To apply our scheme, we chose $\Delta t=0.001$ and $\Delta r=0.0025$, 0.001. Numerical results for $t=0.1$, 0.2 and 0.5 are shown in Figs. 1 and 2. In Fig. 1, the maximum errors at $t=0.1$, 0.2, and 0.5 were 4.1561×10^{-3}, 4.0482×10^{-3}, and 3.7276×10^{-3}, respectively. In Fig. 2, the maximum errors at $t=0.1$, 0.2, and 0.5 were 1.6596×10^{-3}, 1.6147×10^{-3}, and 1.4855×10^{-5}, respectively. From these two figures, we can see that the numerical solutions are convergent to the exact solution.

To demonstrate the applicability of the scheme, we investigate the temperature rise in a gold sphere. The radius (L) for the gold sphere is 0.1 μm. The properties of gold are $C_p=129$ kJ/kg/K, $k=315$ W/m/K,

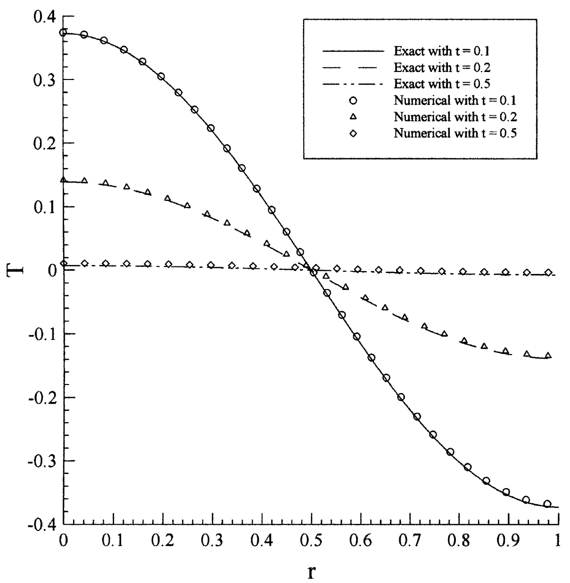

Fig. 1. Comparison of the numerical solutions with the exact solution where $\Delta r=0.0025$ and $\Delta t=0.001$.

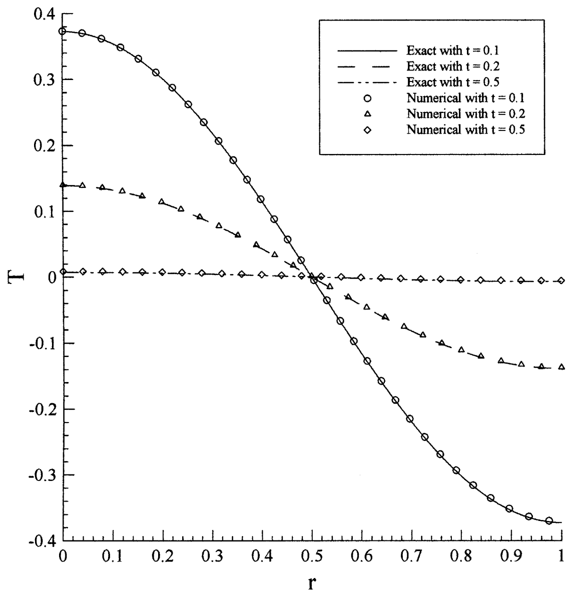

Fig. 2. Comparison of the numerical solutions with the exact solution where $\Delta r=0.001$ and $\Delta t=0.001$.

$\rho=19,300$ kg/m^3, $\tau_q=8.5$ ps (1 ps $=10^{-12}$ s) and $\tau_T=90$ ps [5].

The heat source was chosen to be [5]

$$Q(r,t)=0.94J\left[\frac{1-R}{t_p\delta}\right]e^{-\frac{L-r}{\delta}-2.77\left(\frac{t-2t_p}{t_p}\right)^2}, \tag{16}$$

where $J=13.4\frac{J}{m^2}$, $t_p=100$ fs (1 fs $=10^{-15}$ s), $\delta=15.3$ nm (1 nm $=10^{-9}$ m), and $R=0.93$.

The initial conditions were chosen as follows:

$$T(x,y,z,0)=T_\infty, \quad \frac{\partial T}{\partial t}(x,y,z,0)=0, \tag{17}$$

where $T_\infty=300$ K.

The boundary conditions were assumed to be insulated. Such boundary conditions arise from the case that the microsphere is subjected to a short-pulse laser irradiation. Hence, one may assume no heat losses from the spherical surface in the short-time response [5].

To apply our scheme, we chose three different meshes of 100, 200 and 400 grid points. The time increment was chosen to be 0.005 ps.

Fig. 3 shows the change in temperature $\left(\frac{\Delta T}{(\Delta T)\max}\right)$ on the surface of the gold sphere. The maximum temperature rise of T (i.e., $(\Delta T)\max$) on the surface of the gold sphere is about 14.60 K. It can be seen from the figure that there is a significant difference between the dual-phase-lagging behavior and diffusion (no dual-phase-lagging). Also, the maximum temperature rise of T (i.e., $(\Delta T)\max$) on the surface of the gold sphere is about 20 K for diffusion.

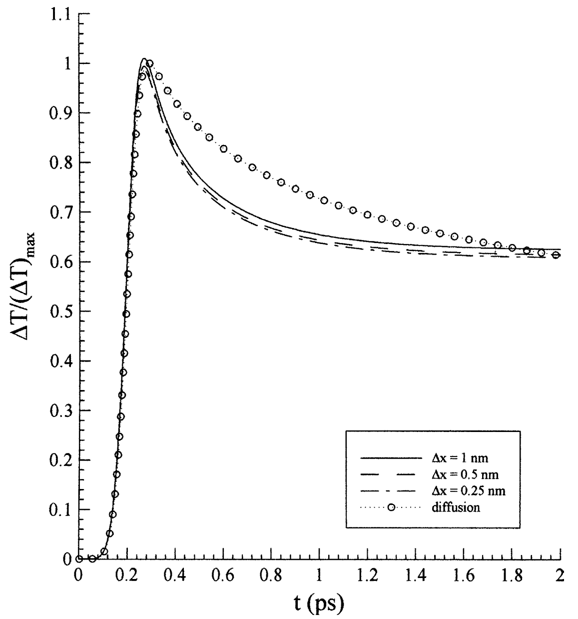

Fig. 3. Normalized temperatures at the surface of a 100-nm gold sphere irradiated with a 0.1-ps laser pulse at a fluence of 13.4 J/m^2.

Fig. 4 gives the temperature rise along the r-axis for different times ($t = 0.2$, 0.3, 0.5, 1.0 and 10.0 ps). It can be seen from Fig. 4 that the temperature rise is on the surface and heat is transferred to the center of the sphere until it approximately reaches steady state at $t = 10.0$ ps.

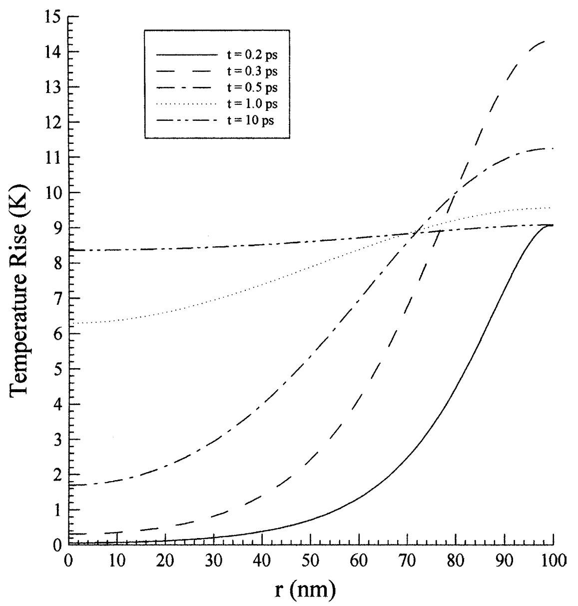

Fig. 4. Calculated temperature profiles for a 100-nm gold sphere irradiated with a 0.1-ps laser pulse at a fluence of 13.4 J/m^2.

4. Conclusion

In this study, we develop a three-level finite difference scheme for solving a dual-phase-lagging heat transport equation in spherical coordinates. It is shown by the discrete energy method that this scheme is unconditionally stable and convergent. Numerical results show that the scheme is efficient.

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Appendix A

We will employ the discrete energy method [24,25] to show the stability and convergence of the scheme, Eqs. (8)–(11). To this end, we first introduce the definitions of the inner products and norms between the mesh functions u_j and v_j. Let S_h be a set of $\{u = \{u_j\}_{j=0}^{N}\}$. For any $u,\ v \in S_h$, the inner products and norms are defined as follows:

$$(u,v) = \Delta r \sum_{j=1}^{N-1} u_j \cdot v_j, \quad \|u\|^2 = (u,u)$$

and

$$\|\nabla_{\bar{r}} u\|_1^2 = (\nabla_{\bar{r}} u_j, \nabla_{\bar{r}} u_j)_1 = \Delta r \sum_{j=1}^{N} (\nabla_{\bar{r}} u_j)^2.$$

The following Lemmas 1 and 2 can be easily obtained.

Lemma 1. *For any n,*

$$\Delta r \sum_{j=1}^{N-1} r_j^2 \left(T_j^{n+1} - 2T_j^n + T_j^{n-1}\right) \cdot \left(T_j^{n+1} - T_j^{n-1}\right)$$
$$= \Delta r \sum_{j=1}^{N-1} r_j^2 \cdot \left[\left(T_j^{n+1} - T_j^n\right)^2 - \left(T_j^n - T_j^{n-1}\right)^2\right]$$
$$= \left\|r\left(T^{n+1} - T^n\right)\right\|^2 - \left\|r\left(T^n - T^{n-1}\right)\right\|^2. \tag{A.1}$$

Lemma 2. *For any n,*

$$\Delta r \sum_{j=1}^{N} \left(E^{-1/2} r_j^2\right) \nabla_{\bar{r}} \left(T_j^{n+1} + 2T_j^n + T_j^{n-1}\right)$$
$$\cdot \nabla_{\bar{r}} \left(T_j^{n+1} - T_j^{n-1}\right)$$
$$= \Delta r \sum_{j=1}^{N} \left(E^{-1/2} r_j^2\right) \cdot \left[\left(\nabla_{\bar{r}} \left(T_j^{n+1} + T_j^n\right)\right)^2 - \left(\nabla_{\bar{r}} \left(T_j^n + T_j^{n-1}\right)\right)^2\right]$$

$$= \left\| \left(E^{-1/2}r\right)\nabla_{\bar r}\left(T^{n+1}+T^{n}\right)\right\|_1^2 - \left\| \left(E^{-1/2}r\right)\nabla_{\bar r}\left(T^{n}+T^{n-1}\right)\right\|_1^2, \quad \text{(A.2)}$$

where $E^{-1/2}$ is a shift operator such that $E^{-1/2}r_j = r_{j-(1/2)}$.

Lemma 3. *For any mesh functions T_j and S_j,*

$$\Delta r\sum_{j=1}^{N-1}P_h(T_j)\cdot S_j = -\Delta r\sum_{j=1}^{N}r_{j-(1/2)}^2\nabla_{\bar r}T_j\cdot\nabla_{\bar r}S_j - r_{(1/2)}^2\nabla_{\bar r}T_1\cdot S_0 + r_{N-(1/2)}^2\nabla_{\bar r}T_N\cdot S_N. \quad \text{(A.3)}$$

Proof. One may obtain from Eq. (9) that

$$\begin{aligned}
\Delta r\sum_{j=1}^{N-1}P_h(T_j)\cdot S_j
&= \Delta r\sum_{j=1}^{N-1}r_{j+(1/2)}^2\frac{T_{j+1}-T_j}{(\Delta r)^2}S_j - \Delta r\sum_{j=1}^{N-1}r_{j-(1/2)}^2\frac{T_j-T_{j-1}}{(\Delta r)^2}S_j\\
&= \Delta r\sum_{j=2}^{N}r_{j-(1/2)}^2\frac{T_j-T_{j-1}}{(\Delta r)^2}S_{j-1} - \Delta r\sum_{j=1}^{N-1}r_{j-(1/2)}^2\frac{T_j-T_{j-1}}{(\Delta r)^2}S_j\\
&= \Delta r\sum_{j=1}^{N}r_{j-(1/2)}^2\frac{T_j-T_{j-1}}{(\Delta r)^2}S_{j-1} - \Delta r\sum_{j=1}^{N}r_{j-(1/2)}^2\frac{T_j-T_{j-1}}{(\Delta r)^2}S_j\\
&\quad - r_{(1/2)}^2\frac{T_1-T_0}{\Delta r}S_0 + r_{N-(1/2)}^2\frac{T_N-T_{N-1}}{\Delta r}S_N\\
&= -\Delta r\sum_{j=1}^{N}r_{j-(1/2)}^2\nabla_{\bar r}T_j\cdot\nabla_{\bar r}S_j - r_{(1/2)}^2\frac{T_1-T_0}{\Delta r}S_0\\
&\quad + r_{N-(1/2)}^2\frac{T_N-T_{N-1}}{\Delta r}S_N\\
&= -\Delta r\sum_{j=1}^{N}r_{j-(1/2)}^2\nabla_{\bar r}T_j\cdot\nabla_{\bar r}S_j - r_{(1/2)}^2\nabla_{\bar r}T_1\cdot S_0\\
&\quad + r_{N-(1/2)}^2\nabla_{\bar r}T_N\cdot S_N. \qquad \square
\end{aligned} \quad \text{(A.4)}$$

Proof of Theorem 1. It can be seen that u_j^n satisfies

$$\rho C\left(\frac{u_j^{n+1}-u_j^{n-1}}{2\Delta t} + \tau_q\frac{u_j^{n+1}-2u_j^n+u_j^{n-1}}{(\Delta t)^2}\right) = \frac{k}{r_j^2}P_h\left(\frac{u_j^{n+1}+2u_j^n+u_j^{n-1}}{4}\right) + \tau_T\frac{k}{r_j^2}P_h\left(\frac{u_j^{n+1}-u_j^{n-1}}{2\Delta t}\right) + g_j^n, \quad 1\leqslant j\leqslant N-1 \quad \text{(A.5)}$$

and the initial condition

$$u_j^0 = u_j^1 = 0, \quad 1\leqslant j\leqslant N-1 \quad \text{(A.6)}$$

and boundary condition

$$\nabla_{\bar r}u_1^n = 0, \quad \nabla_{\bar r}u_N^n = 0, \qquad n\geqslant 0. \quad \text{(A.7)}$$

Multiplying Eq. (A.5) by $4(\Delta t)^2\Delta r\cdot r_j^2(u_j^{n+1}-u_j^{n-1})$ and summing j from 1 to $N-1$, we obtain by Lemmas 1–3 and Eq. (A.7)

$$\begin{aligned}
&2\rho C\Delta t\|r(u^{n+1}-u^{n-1})\|^2 + 4\rho C\tau_q\Big[\|r(u^{n+1}-u^n)\|^2 - \|r(u^n-u^{n-1})\|^2\Big]\\
&= -k(\Delta t)^2\Big[\left\|\left(E^{-1/2}r\right)\nabla_{\bar r}(u^{n+1}+u^n)\right\|_1^2 - \left\|\left(E^{-1/2}r\right)\nabla_{\bar r}(u^n+u^{n-1})\right\|_1^2\Big]\\
&\quad - 2k\Delta t\tau_T\left\|\left(E^{-1/2}r\right)\nabla_{\bar r}(u^{n+1}-u^{n-1})\right\|_1^2 + \Big(g^n, 4(\Delta t)^2r^2(u^{n+1}-u^{n-1})\Big).
\end{aligned} \quad \text{(A.8)}$$

By Cauchy–Schwarz's inequality, we obtain

$$\begin{aligned}
4(\Delta t)^2\big(g^n, r^2(u^{n+1}-u^{n-1})\big)
&\leqslant 2(\Delta t)^2\Big[\|g^n\|^2 + \|r^2(u^{n+1}-u^{n-1})\|^2\Big]\\
&\leqslant 2(\Delta t)^2\Big[\|g^n\|^2 + L^2\|r(u^{n+1}-u^{n-1})\|^2\Big].
\end{aligned} \quad \text{(A.9)}$$

Hence, Eq. (A.8) becomes

$$\begin{aligned}
&\Delta t(2\rho C - 2\Delta tL^2)\left\|r(u^{n+1}-u^{n-1})\right\|^2 + 4\rho C\tau_q\Big[\left\|r(u^{n+1}-u^n)\right\|^2 - \left\|r(u^n-u^{n-1})\right\|^2\Big]\\
&\quad + k(\Delta t)^2\Big[\left\|\left(E^{-1/2}r\right)\nabla_{\bar r}(u^{n+1}+u^n)\right\|_1^2 - \left\|\left(E^{-1/2}r\right)\nabla_{\bar r}(u^n+u^{n-1})\right\|_1^2\Big]\\
&\quad + 2k\Delta t\tau_T\left\|\left(E^{-1/2}r\right)\nabla_{\bar r}(u^{n+1}-u^{n-1})\right\|_1^2\\
&\leqslant 2\Delta t^2\|g^n\|^2.
\end{aligned} \quad \text{(A.10)}$$

Choosing Δt so that $2\rho C - 2\Delta tL^2 \geqslant 0$, dropping out the first and fourth terms on the left-hand-side of Eq. (A.10), and then using Eq. (A.6), we obtain

$$\begin{aligned}
&4\rho C\tau_q\left\|r(u^{n+1}-u^n)\right\|^2 + k(\Delta t)^2\left\|\left(E^{-1/2}r\right)\nabla_{\bar r}(u^{n+1}+u^n)\right\|_1^2\\
&\leqslant 4\rho C\tau_q\left\|r(u^n-u^{n-1})\right\|^2 + k(\Delta t)^2\left\|\left(E^{-1/2}r\right)\nabla_{\bar r}(u^n+u^{n-1})\right\|_1^2 + 2(\Delta t)^2\|g^n\|^2\\
&\leqslant \cdots \leqslant 4\rho C\tau_q\left\|r(u^1-u^0)\right\|^2 + k\Delta t^2\left\|\left(E^{-1/2}r\right)\nabla_{\bar r}(u^1+u^0)\right\|_1^2 + 2n\Delta t^2\max_{0\leqslant m\leqslant n}\|g^m\|^2\\
&\leqslant 2t_0\Delta t\max_{0\leqslant m\leqslant n}\|g^m\|^2,
\end{aligned} \quad \text{(A.11)}$$

which completes the proof. $\square$

Proof of Theorem 2. It can be seen that ε_j^n satisfies

$$\rho C\left(\frac{\varepsilon_j^{n+1}-\varepsilon_j^{n-1}}{2\Delta t} + \tau_q\frac{\varepsilon_j^{n+1}-2\varepsilon_j^n+\varepsilon_j^{n-1}}{(\Delta t)^2}\right) = \frac{k}{r_j^2}P_h\left(\frac{\varepsilon_j^{n+1}+2\varepsilon_j^n+\varepsilon_j^{n-1}}{4}\right) + \tau_T\frac{k}{r_j^2}P_h\left(\frac{\varepsilon_j^{n+1}-\varepsilon_j^{n-1}}{2\Delta t}\right) + q_j^n + \sigma_j^n \quad \text{(A.12)}$$

and initial and boundary conditions

$$\varepsilon_j^0 = f_j^0, \quad \varepsilon_j^1 = f_j^1 \quad \text{(A.13)}$$

and

$$\frac{\varepsilon_1^n-\varepsilon_0^n}{\Delta r}=g_1^n,\quad \frac{\varepsilon_N^n-\varepsilon_{N-1}^n}{\Delta r}=g_2^n \tag{A.14}$$

for any level n. Here, $g_1^n=\frac{1}{2}\Delta r\frac{\partial^2 T(\theta\Delta r,n\Delta t)}{\partial r^2}$, $g_2^n=\frac{1}{2}\Delta r\frac{\partial^2 T((N-1+\zeta)\Delta r,n\Delta t)}{\partial r^2}$, where $0\leqslant\theta,\ \zeta\leqslant 1$. Furthermore, q_j^n represents the error between $G(j\Delta r,n\Delta t)$ and G_j^n, and σ_j^n represents the truncation error of the scheme. It can be seen that $\sigma_j^n=O(\Delta t^2+\Delta r^2)$.

Multiplying Eq. (A.12) by $4(\Delta t)^2\Delta r\cdot r_j^2(\varepsilon_j^{n+1}-\varepsilon_j^{n-1})$, summing j from 1 to $N-1$, and using Lemmas 1–3, one obtains

$$\begin{aligned}
&2\rho C\Delta t\|r(\varepsilon^{n+1}-\varepsilon^{n-1})\|^2+4\rho C\tau_q\Big[\|r(\varepsilon^{n+1}-\varepsilon^{n})\|^2\\
&\quad-\|r(\varepsilon^{n}-\varepsilon^{n-1})\|^2\Big]+k(\Delta t)^2\Big[\|(E^{-1/2}r)\nabla_{\bar r}(\varepsilon^{n+1}+\varepsilon^{n})\|_1^2\\
&\quad-\|(E^{-1/2}r)\nabla_{\bar r}(\varepsilon^{n}+\varepsilon^{n-1})\|_1^2\Big]\\
&\quad+2k\tau_T\Delta t\|(E^{-1/2}r)\nabla_{\bar r}(\varepsilon^{n+1}-\varepsilon^{n-1})\|_1^2\\
&\quad=k(\Delta t)^2r_{N-(1/2)}^2\nabla_{\bar r}(\varepsilon_N^{n+1}+2\varepsilon_N^n+\varepsilon_N^{n-1})\cdot(\varepsilon_N^{n+1}-\varepsilon_N^{n-1})\\
&\quad-k(\Delta t)^2r_{(1/2)}^2\nabla_{\bar r}(\varepsilon_1^{n+1}+2\varepsilon_1^n+\varepsilon_1^{n-1})\cdot(\varepsilon_0^{n+1}-\varepsilon_0^{n-1})\\
&\quad+2\Delta tk\tau_Tr_{N-(1/2)}^2\nabla_{\bar r}(\varepsilon_N^{n+1}-\varepsilon_N^{n-1})\cdot(\varepsilon_N^{n+1}-\varepsilon_N^{n-1})\\
&\quad-2\Delta tk\tau_Tr_{(1/2)}^2\nabla_{\bar r}(\varepsilon_1^{n+1}-\varepsilon_1^{n-1})\cdot(\varepsilon_0^{n+1}-\varepsilon_0^{n-1})\\
&\quad+4(\Delta t)^2(q^n,r^2(\varepsilon^{n+1}-\varepsilon^{n-1}))\\
&\quad+4(\Delta t)^2(\sigma^n,r^2(\varepsilon^{n+1}-\varepsilon^{n-1})).
\end{aligned}\tag{A.15}$$

We now estimate each term of the right-hand-side of Eq. (A.15). Using the generalized Cauchy–Schwarz's inequality and Eq. (A.14), we estimate the first term as follows:

$$\begin{aligned}
&\left|k(\Delta t)^2r_{N-(1/2)}^2\nabla_{\bar r}(\varepsilon_N^{n+1}+2\varepsilon_N^n+\varepsilon_N^{n-1})\cdot(\varepsilon_N^{n+1}-\varepsilon_N^{n-1})\right|\\
&\quad=\Big|k(\Delta t)^2r_{N-(1/2)}^2(g_2^{n+1}+2g_2^n+g_2^{n-1})\cdot(\varepsilon_{N-1}^{n+1}-\varepsilon_{N-1}^{n-1}\\
&\qquad+\Delta r(g_2^{n+1}-g_2^{n-1}))\Big|\\
&\quad\leqslant k(\Delta t)^2\Big[\Delta r\cdot r_{N-(1/2)}^4(\varepsilon_{N-1}^{n+1}-\varepsilon_{N-1}^{n-1})^2\\
&\qquad+\frac{C_1}{\Delta r}\left(|g_2^{n+1}|^2+|g_2^n|^2+|g_2^{n-1}t|^2\right)\Big]\\
&\quad\leqslant k(\Delta t)^2L^2\|r(\varepsilon^{n+1}-\varepsilon^{n-1})\|^2\\
&\qquad+\frac{kC_1(\Delta t)^2}{\Delta r}\left(|g_2^{n+1}|^2+|g_2^n|^2+|g_2^{n-1}|^2\right)\\
&\quad\leqslant k(\Delta t)^2L^2\|r(\varepsilon^{n+1}-\varepsilon^{n-1})\|^2\\
&\qquad+kC_1(\Delta t)^2\Delta r\max_{r,t}\left|\frac{\partial^2T}{\partial r^2}\right|^2,
\end{aligned}\tag{A.16}$$

where C_1 is a positive constant. Using a similar argument, we estimate the second, third and fourth terms as follows

$$\begin{aligned}
&\left|k(\Delta t)^2r_{(1/2)}^2\nabla_{\bar r}(\varepsilon_1^{n+1}+2\varepsilon_1^n+\varepsilon_1^{n-1})\cdot(\varepsilon_0^{n+1}-\varepsilon_0^{n-1})\right|\\
&\quad=\Big|k(\Delta t)^2r_{(1/2)}^2(g_1^{n+1}+2g_1^n+g_1^{n-1})\\
&\qquad\cdot(\varepsilon_1^{n+1}-\varepsilon_1^{n-1}-\Delta r(g_1^{n+1}-g_1^{n-1}))\Big|\\
&\quad\leqslant k(\Delta t)^2\Big[\Delta r\cdot r_{(1/2)}^4(\varepsilon_1^{n+1}-\varepsilon_1^{n-1})^2\\
&\qquad+\frac{C_2}{\Delta r}\left(|g_1^{n+1}|^2+|g_1^n|^2+|g_1^{n-1}|^2\right)\Big]\\
&\quad\leqslant k(\Delta t)^2L^2\|r(\varepsilon^{n+1}-\varepsilon^{n-1})\|^2\\
&\qquad+\frac{kC_2(\Delta t)^2}{\Delta r}\left(|g_1^{n+1}|^2+|g_1^n|^2+|g_1^{n-1}|^2\right)\\
&\quad\leqslant k(\Delta t)^2L^2\|r(\varepsilon^{n+1}-\varepsilon^{n-1})\|^2\\
&\qquad+kC_2(\Delta t)^2\Delta r\max_{r,t}\left|\frac{\partial^2T}{\partial r^2}\right|^2,
\end{aligned}\tag{A.17}$$

$$\begin{aligned}
&\left|2\Delta tk\tau_Tr_{N-(1/2)}^2\nabla_{\bar r}(\varepsilon_N^{n+1}-\varepsilon_N^{n-1})\cdot(\varepsilon_N^{n+1}-\varepsilon_N^{n-1})\right|\\
&\quad=\Big|2\Delta tk\tau_Tr_{N-(1/2)}^2(g_2^{n+1}-g_2^{n-1})\cdot(\varepsilon_{N-1}^{n+1}-\varepsilon_{N-1}^{n-1}\\
&\qquad+\Delta r(g_2^{n+1}-g_2^{n-1}))\Big|\\
&\quad\leqslant k\tau_T\Big[(\Delta t)^2\Delta r\cdot r_{N-(1/2)}^4(\varepsilon_{N-1}^{n+1}-\varepsilon_{N-1}^{n-1})^2\\
&\qquad+\frac{C_3}{\Delta r}|g_2^{n+1}-g_2^{n-1}|^2\Big]\\
&\quad\leqslant k\tau_T(\Delta t)^2L^2\|r(\varepsilon^{n+1}-\varepsilon^{n-1})\|^2\\
&\qquad+k\tau_TC_3(\Delta t)^2\Delta r\max_{r,t}\left|\frac{\partial^3T}{\partial r^2\partial t}\right|^2
\end{aligned}\tag{A.18}$$

and

$$\begin{aligned}
&\left|2\Delta tk\tau_Tr_{(1/2)}^2\nabla_{\bar r}(\varepsilon_1^{n+1}-\varepsilon_1^{n-1})\cdot(\varepsilon_0^{n+1}-\varepsilon_0^{n-1})\right|\\
&\quad=\Big|2\Delta tk\tau_Tr_{(1/2)}^2(g_1^{n+1}-g_1^{n-1})\\
&\qquad\cdot(\varepsilon_1^{n+1}-\varepsilon_1^{n-1}-\Delta r(g_1^{n+1}-g_1^{n-1}))\Big|\\
&\quad\leqslant k\tau_T\left[(\Delta t)^2\Delta r\cdot r_{(1/2)}^4(\varepsilon_1^{n+1}-\varepsilon_1^{n-1})^2+\frac{C_4}{\Delta r}|g_1^{n+1}-g_1^{n-1}|^2\right]\\
&\quad\leqslant k\tau_T(\Delta t)^2L^2\|r(\varepsilon^{n+1}-\varepsilon^{n-1})\|^2\\
&\qquad+k\tau_TC_4(\Delta t)^2\Delta r\max_{r,t}\left|\frac{\partial^3T}{\partial r^2\partial t}\right|^2,
\end{aligned}\tag{A.19}$$

where C_2, C_3 and C_4 are positive constants. Using Cauchy–Schwarz's inequality, we estimate the fifth and sixth terms as follows

$$\begin{aligned}
&|4\Delta t^2(q^n,r^2(\varepsilon^{n+1}-\varepsilon^{n-1}))|\\
&\quad\leqslant 2\Delta t^2\left[\|q^n\|^2+L^2\|r(\varepsilon^{n+1}-\varepsilon^{n-1})\|^2\right]
\end{aligned}\tag{A.20}$$

and

$$\left|4\Delta t^2\left(\sigma^n, r^2\left(\varepsilon^{n+1}-\varepsilon^{n-1}\right)\right)\right| \leqslant 2\Delta t^2\left[\|\sigma^n\|^2 + L^2\left\|r\left(\varepsilon^{n+1}-\varepsilon^{n-1}\right)\right\|^2\right]. \tag{A.21}$$

Substituting Eqs. (A.17)–(A.21) into Eq. (A.16), we obtain

$$\begin{aligned}
&\Delta t\left(2\rho C - 4L^2\Delta t - 2kL^2\Delta t - 2kL^2\tau_T\Delta t\right)\left\|r\left(\varepsilon^{n+1}-\varepsilon^{n-1}\right)\right\|^2 \\
&\quad + 4\rho C\tau_q\left[\left\|r\left(\varepsilon^{n+1}-\varepsilon^{n}\right)\right\|^2 - \left\|r\left(\varepsilon^{n}-\varepsilon^{n-1}\right)\right\|^2\right] \\
&\quad + k\Delta t^2\left[\left\|\left(E^{-1/2}r\right)\nabla_{\bar r}\left(\varepsilon^{n+1}+\varepsilon^{n}\right)\right\|_1^2 \right.\\
&\quad \left. - \left\|\left(E^{-1/2}r\right)\nabla_{\bar r}\left(\varepsilon^{n}+\varepsilon^{n-1}\right)\right\|_1^2\right] \\
&\quad + 2k\Delta t\tau_T\left\|\left(E^{-1/2}r\right)\nabla_{\bar r}\left(\varepsilon^{n+1}-\varepsilon^{n-1}\right)\right\|_1^2 \\
&\quad \leqslant 2\Delta t^2\left(\|q^n\|^2 + \|\sigma^n\|^2\right) \\
&\qquad + k(C_1+C_2)(\Delta t)^2\Delta r\max_{r,t}\left|\frac{\partial^2 T}{\partial r^2}\right|^2 \\
&\qquad + k\tau_T(C_3+C_4)(\Delta t)^2\Delta r\max_{r,t}\left|\frac{\partial^3 T}{\partial r^2\partial t}\right|^2.
\end{aligned} \tag{A.22}$$

Choosing Δt so that $2\rho C - 4L^2\Delta t - 2kL^2\Delta t - 2kL^2\tau_T\Delta t \geqslant 0$, and dropping out the first and fourth terms on the left-hand-side of Eq. (A.22), we obtain

$$\begin{aligned}
&4\rho C\tau_q\left\|r\left(\varepsilon^{n+1}-\varepsilon^{n}\right)\right\|^2 + k(\Delta t)^2\left\|\left(E^{-1/2}r\right)\nabla_{\bar r}\left(\varepsilon^{n+1}+\varepsilon^{n}\right)\right\|_1^2 \\
&\quad \leqslant 4\rho C\tau_q\left\|r\left(\varepsilon^{n}-\varepsilon^{n-1}\right)\right\|^2 \\
&\qquad + k(\Delta t)^2\left\|\left(E^{-1/2}r\right)\nabla_{\bar r}\left(\varepsilon^{n}+\varepsilon^{n-1}\right)\right\|_1^2 \\
&\qquad + 2(\Delta t)^2\left(\|q^n\|^2 + \|\sigma^n\|^2\right) \\
&\qquad + k(C_1+C_2)(\Delta t)^2\Delta r\max_{r,t}\left|\frac{\partial^2 T}{\partial r^2}\right|^2 \\
&\qquad + k\tau_T(C_3+C_4)(\Delta t)^2\Delta r\max_{r,t}\left|\frac{\partial^3 T}{\partial r^2\partial t}\right|^2 \\
&\quad \leqslant \cdots \leqslant 4\rho C\tau_q\left\|r\left(\varepsilon^{1}-\varepsilon^{0}\right)\right\|^2 \\
&\qquad + k(\Delta t)^2\left\|\left(E^{-1/2}r\right)\nabla_{\bar r}\left(\varepsilon^{1}+\varepsilon^{0}\right)\right\|_1^2 \\
&\qquad + 2t_0\Delta t\max_{0\leqslant m\leqslant n}\left(\|q^m\|^2 + \|\sigma^m\|^2\right) \\
&\qquad + kt_0(C_1+C_2)\Delta t\Delta r\max_{r,t}\left|\frac{\partial^2 T}{\partial r^2}\right|^2 \\
&\qquad + kt_0\tau_T(C_3+C_4)\Delta t\Delta r\max_{r,t}\left|\frac{\partial^3 T}{\partial r^2\partial t}\right|^2,
\end{aligned} \tag{A.23}$$

which completes the proof. □

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