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A stable finite difference scheme for solving a hyperbolic two-step model in a 3D micro sphere exposed to ultrashort-pulsed lasers

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Abstract

Purpose – To develop a numerical method for solving hyperbolic two-step micro heat transport equations, which have attracted attention in thermal analysis of thin metal films exposed to ultrashort-pulsed lasers.

Design/methodology/approach – An energy estimation for the hyperbolic two-step model in a three-dimensional (3D) micro sphere irradiated by ultrashort-pulsed lasers is first derived, and then a finite difference scheme for solving the hyperbolic two-step model based on the energy estimation is developed. The scheme is shown to be unconditionally stable and satisfies a discrete analogue of the energy estimation. The method is illustrated by investigating the heat transfer in a micro gold sphere exposed to ultrashort-pulsed lasers.

Findings – Provides information on normalized electron temperature change with time on the surface of the sphere, and shows the changes in electron and lattice temperatures.

Research limitations/implications – The hyperbolic two-step model is considered under the assumption of constant thermal properties.

Practical implications – A useful tool to investigate the temperature change in a micro sphere irradiated by ultrashort-pulsed lasers.

Originality/value – Provides a new unconditionally stable finite difference scheme for solving the hyperbolic two-step model in a 3D micro sphere irradiated by ultrashort-pulsed lasers.

Keywords Finite difference methods, Stability (control theory), Heat transfer, Numerical analysis

Paper type Research paper

Nomenclature

C_e, C_l	= heat capacity	$\vec{q}_e = \langle q_e^r, q_e^\phi, q_e^\theta \rangle$	= heat flux associated with electrons
G	= electron-lattice coupling factor	$\vec{q}_l = \langle q_l^r, q_l^\phi, q_l^\theta \rangle$	= heat flux associated with the lattice
J	= laser fluence		
k_e, k_l	= thermal conductivity	R	= radius of the sphere
N_r, N_ϕ, N_θ	= numbers of grid points	R_l	= reflectivity
Q	= heart source	r, ϕ, θ	= spherical coordinates

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r_i, ϕ_j, θ_k	$= (i-\frac{1}{2})\Delta r, (j-\frac{1}{2})\Delta\phi, (k-\frac{1}{2})\Delta\theta$, respectively	δ	= laser penetration depth
T_e, T_l	= electron temperature and lattice temperature	∇_r, ∇_ϕ, ∇_θ	= first-order forward finite differences
$\bar{T}^n$	$= \frac{1}{4}(T^{n+1} + 2T^n + 2T^{n-1})$	$\nabla_{\bar{r}}$, $\nabla_{\bar{\phi}}$, $\nabla_{\bar{\theta}}$	= first-order backward finite differences
t, t_0	= time	∇t, ∇r, $\nabla\phi$, $\nabla\theta$	= time increment, grid sizes
t_p	= laser pulse duration	τ_e, τ_l	= electron and lattice relaxation times, respectively
u_{ijk}^n	= mesh function where n is the time level and ijk is the grid point		

1. Introduction

Ultrashort-pulsed lasers with pulse durations of the order of sub-picosecond to femtosecond domain possess exclusive capabilities in limiting the undesirable spread of the thermal process zone in the heated sample (Tzou *et al.*, 2002). They have been widely applied in structural monitoring of thin metal films (Opsal, 1991), laser micromachining (Knapp *et al.*, 1990) and patterning (Elliot and Piwczyk, 1989), structural tailoring of microfilms (Grigoropoulos, 1994), and laser synthesis and processing in thin-film deposition (Narayan *et al.*, 1991).

For an ultrashort-pulsed laser, the heating involves high-rate heat flow from electrons to lattices in the picosecond domains. Depending on the temperature, electrons have a heat capacity two to three orders of magnitude smaller than that of lattices. When heated by photons (lasers), the laser energy is primarily absorbed by the free electrons that are confined within skin depth during the excitation. Electrons first shoot up to several hundreds or thousands of degrees within a few picoseconds without disturbing the metal lattices. A major portion of the thermal electron energy is then transferred to the lattices. Meanwhile another part of the energy diffuses to the electrons in the deeper region of the target. Because the pulse duration is so short, the laser is turned off before thermal equilibrium between the electrons and lattices is reached. In this time interval, the heat flux is essentially limited to the region within the electron thermal diffusion length. This stage is termed non-equilibrium heating due to the large differences of temperatures in electrons and lattices (Chen and Beraun, 2001). The lattice temperature then increases as a result of lattice-electron coupling, resulting in a new thermal property termed lattice-electron coupling factor. The energy equations describing the continuous energy flow from hot electrons to lattices during non-equilibrium heating can be written as (Anisimov *et al.*, 1974; Chen and Beraun, 2001; Chen *et al.*, 2003; Dai *et al.*, 2004; Naji *et al.*, 2003; Qiu and Tien, 1992, 1993, 1994; Tzou, 1995, 1996; Tzou *et al.*, 2002):

$$C_e \frac{\partial T_e}{\partial t} = \nabla[k_e \nabla T_e] - G(T_e - T_l) + Q, \tag{1}$$

$$C_l \frac{\partial T_l}{\partial t} = G(T_e - T_l), \tag{2}$$

Where T_e is electron temperature, T_l – lattice temperature, k_e – thermal conductivity in thermal equilibrium, C_e and C_l – volumetric heat capacity, G – electron-lattice coupling factor, Q – ultrashort-pulsed laser heating source, and ∇ – the gradient operator.

The above coupled equations (1) and (2) are often referred to as parabolic two-step micro heat transport equations. However, when the laser pulse duration is much shorter than the electron-lattice thermal relaxation time that is the characteristic time for the activation of ballistic behavior in the electron gas, the parabolic two-step model may lose accuracy (Qiu and Tien, 1993; Tzou, 1995). As Qiu and Tien (1994) pointed out, the relaxation time increases dramatically as the temperature decreases from 0.04 ps at room temperature to about 10 ps at 10 K. They (Qiu and Tien, 1993) developed the hyperbolic two-step heat transport equations based on the macroscopic averages of the electric and heat currents carried by electrons in the momentum space. The hyperbolic two-step model in a general form can be written as follows (Al-Nimr *et al.*, 1999; Al-Nimr and Arpaci, 2000; Al-Nimr and Alkam, 2003; Al-Odat *et al.*, 2002; Chen and Bearun, 2001; Chen *et al.*, 2003; Qiu and Tien, 1994):

$$C_e \frac{\partial T_e}{\partial t} = -\nabla \cdot \vec{q}_e - G(T_e - T_l) + Q, \tag{3}$$

$$\tau_e \frac{\partial \vec{q}_e}{\partial t} + \vec{q}_e = -k_e \nabla T_e, \tag{4}$$

$$C_l \frac{\partial T_l}{\partial t} = -\nabla \cdot \vec{q}_l + G(T_e - T_l), \tag{5}$$

$$\tau_l \frac{\partial \vec{q}_l}{\partial t} + \vec{q}_l = -k_l \nabla T_l, \tag{6}$$

Where $\bar{q}_e$ and $\bar{q}_l$ are the heat fluxes associated with electrons and the lattice, respectively. Here, τ_e is the electron relaxation and τ_l is the lattice relaxation time. It can be seen that if τ_e and τ_l are zero, the hyperbolic two-step model will reduce to the parabolic two-step model.

Recently, we have developed a stable three-level finite difference scheme for solving the parabolic two-step model in a three-dimensional (3D) micro sphere heated by ultrashort-pulsed lasers (Kaba and Dai, 2005). In this paper, we extend our investigation to the hyperbolic two-step model in a micro sphere exposed to ultrashort-pulsed lasers and develop a stable three-level finite difference scheme for solving the hyperbolic two-step model in a 3D micro sphere heated by ultrashort-pulsed lasers.

2. Governing equations

Based on equations (3)-(6) and the gradient operator ∇ in spherical coordinates (Ozisik, 1993), the hyperbolic two-step model in a metal micro sphere can be expressed as follows:

$$C_e \frac{\partial T_e}{\partial t} = -\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 q_e^r\right) - \frac{1}{r\sin\phi}\frac{\partial}{\partial\phi}\left(\sin\phi\, q_e^\phi\right) - \frac{1}{r\sin\phi}\left(\frac{\partial q_e^\theta}{\partial\theta}\right) - G(T_e - T_l) + Q, \tag{7}$$

$$\tau_e \frac{\partial q_e^r}{\partial t} + q_e^r = -k_e \frac{\partial T_e}{\partial t}, \tag{8a}$$

$$\tau_e \frac{\partial q_e^\phi}{\partial t} + q_e^\phi = -\frac{k_e}{r}\frac{\partial T_e}{\partial \phi}, \tag{8b}$$

$$\tau_e \frac{\partial q_e^\theta}{\partial t} + q_e^\theta = -\frac{k_e}{r\sin\phi}\frac{\partial T_e}{\partial \theta}, \tag{8c}$$

and:

$$C_l \frac{\partial T_l}{\partial t} = -\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 q_l^r\right) - \frac{1}{r\sin\phi}\frac{\partial}{\partial \phi}\left(\sin\phi q_l^\phi\right) - \frac{1}{r\sin\phi}\left(\frac{\partial q_l^\phi}{\partial \theta}\right) + G(T_e - T_l), \tag{9}$$

$$\tau_l \frac{\partial q_l^r}{\partial t} + q_l^r = -k_l \frac{\partial T_l}{\partial r}, \tag{10a}$$

$$\tau_l \frac{\partial q_l^\phi}{\partial t} + q_l^\phi = -\frac{k_l}{r}\frac{\partial T_l}{\partial \phi}, \tag{10b}$$

$$\tau_l \frac{\partial q_l^\theta}{\partial t} + q_l^\theta = -\frac{k_l}{r\sin\phi}\frac{\partial T_l}{\partial \theta}, \tag{10c}$$

Where r, ϕ, and θ are spherical coordinates with $0 \le r \le R$, $0 \le \theta \le 2\pi$, $0 \le \phi \le \pi$, and q_e^r, q_e^ϕ, and q_e^θ are the components of $\vec{q}_e$ corresponding to r, ϕ, and θ coordinates, respectively. Similarly, q_l^r, q_l^ϕ, and q_l^θ are the components of $\vec{q}_l$.

The initial and boundary conditions are assumed to be:

$$\vec{q}_e = \vec{q}_l = \vec{0}, \quad T_e = T_l = T_0, \quad \text{at} \quad t = 0, \tag{11}$$

and:

$$\vec{q}_e = \left\langle q_e^r, q_e^\phi, q_e^\theta \right\rangle = \vec{0}, \quad \vec{q}_l = \left\langle q_l^r, q_l^\phi, q_l^\theta \right\rangle = \vec{0}, \quad \text{at} \quad r = R, t > 0, \tag{12}$$

where T_0 is an initial temperature. The boundary condition arises from the fact that there are no heat losses from the surface of the sphere in the short time response (Tzou, 1996).

It can be seen that:

$$T_e(r,\phi,\theta,t) = T_e(r,\phi,\theta \pm 2\pi,t), \quad T_l(r,\phi,\theta,t) = T_l(r,\phi,\theta \pm 2\pi,t), \tag{13a}$$

$$\vec{q}_e(r,\phi,\theta,t) = \vec{q}_e(r,\phi,\theta \pm 2\pi,t), \quad \vec{q}_l(r,\theta,\phi,t) = \vec{q}_l(r,\theta \pm 2\pi,\phi,t). \tag{13b}$$

The above problem satisfies an energy estimation as follows:

Theorem 1. Assume that coefficients C_e, C_l, k_e, G, τ_e and τ_l are positive constants, and that the solutions T_e, T_l, $\vec{q}_e$ and $\vec{q}_l$ of the above initial and boundary value problem are smooth. A stronger estimate holds as follows:

For any t in the time interval $[0, t_0]$,

$$F(t) \le e^{t_0}\left[F(0) + \int_0^{t_0} \Phi(s)\,ds\right], \tag{14}$$

Where:

$$
\begin{aligned}
F(t) = & \int_0^R \int_0^{2\pi} \int_0^{\pi} \left[C_e T_e^2 + C_l T_l^2 \right] r^2 \sin\phi \, dr \, d\theta \, d\phi \\
& + \frac{\tau_e}{k_e} \int_0^R \int_0^{2\pi} \int_0^{\pi} \left[\left(q_e^r\right)^2 + \left(q_e^\phi\right)^2 + \left(q_e^\theta\right)^2 \right] r^2 \sin\phi \, dr \, d\theta \, d\phi \\
& + \frac{\tau_l}{k_l} \int_0^R \int_0^{2\pi} \int_0^{\pi} \left[\left(q_l^r\right)^2 + \left(q_l^\phi\right)^2 + \left(q_l^\theta\right)^2 \right] r^2 \sin\phi \, dr \, d\theta \, d\phi,
\end{aligned} \tag{15}
$$

$$
\Phi(t) = \frac{1}{C_e} \int_0^R \int_0^{2\pi} \int_0^{\pi} r^2 Q^2 \sin\phi \, dr \, \mathrm{d}\theta \, d\phi, \tag{16}
$$

and t_0 is a constant.

The proof of theorem 1 can be seen in the Appendix section. It should be pointed out that obtaining an energy estimation is important for determining if the problem is well-posed, which is related to the existence and uniqueness of the solution of the problem. The above obtained energy estimation implies that the problem, equations (7)-(13), is well-posed in the sense of the definition described in Strikwerads (1989)'s book. The energy estimation is also helpful for developing a numerical scheme. It is desirable that the developed numerical scheme should present a discrete analogue of the energy estimation. This implies that the numerical scheme is stable.

3. Finite difference scheme

To develop such a finite difference scheme, we first design a staggered grid where, T_e, T_l, $\vec{q}_e$, and $\vec{q}_l$ are located as shown in Figure 1. Here, we denote, $r_i = (i - 1/2)\Delta r$, $\phi_j = (j - 1/2)\Delta\phi$, $\theta_k = (k - 1/2)\Delta\theta$, where $i = 1, \ldots, N_r$; $j = 1, \ldots, N_\phi$; $k = 1, \ldots, N_\theta$; so that $N_r \Delta_r = R$, $N_\phi \Delta\phi = \pi$, and $N_\theta \Delta\theta = 2\pi$. Further, $(T_e)_{ijk}^n$ is denoted as the numerical approximation of $(T_e)(r_i, \phi_j, \theta_k, t_n)$, where $t_n = n\Delta t$ and Δt is time increment. The first-order forward and backward finite difference operators are defined as follows:

$$
\nabla_r u_{ijk} = \frac{u_{i+1jk} - u_{ijk}}{\Delta r}, \quad \nabla_{\bar{r}} u_{ijk} = \frac{u_{ijk} - u_{i-1jk}}{\Delta r}.
$$

Similar notations apply for other variables.

We develop a three-level finite difference scheme for solving the above initial and boundary problem, equations (7)-(13), as follows:

$$
\begin{aligned}
C_e \frac{(T_e)_{ijk}^{n+1} - (T_e)_{ijk}^{n-1}}{2\Delta t} = & -\frac{1}{r_i^2} \nabla_r \left[r_{i-(1/2)}^2 \left(\bar{q}_e^r\right)_{i-(1/2)jk}^n \right] \\
& - \frac{1}{r_i \sin\phi_j} \nabla_\phi \left[\sin\phi_{j-(1/2)} \left(\bar{q}_e^\phi\right)_{ij-(1/2)k}^n \right] \\
& - \frac{1}{r_i \sin\phi_j} \nabla_\theta \left(\bar{q}_e^\theta\right)_{ijk-(1/2)}^n - G\left[(\bar{T}_e)_{ijk}^n - (\bar{T}_l)_{ijk}^n \right] + Q_{ijk}^n, \\
& i = 1, \ldots, N_r; \quad j = 1, \ldots, N_\phi; \quad k = 1, \ldots, N_\theta;
\end{aligned} \tag{17}
$$

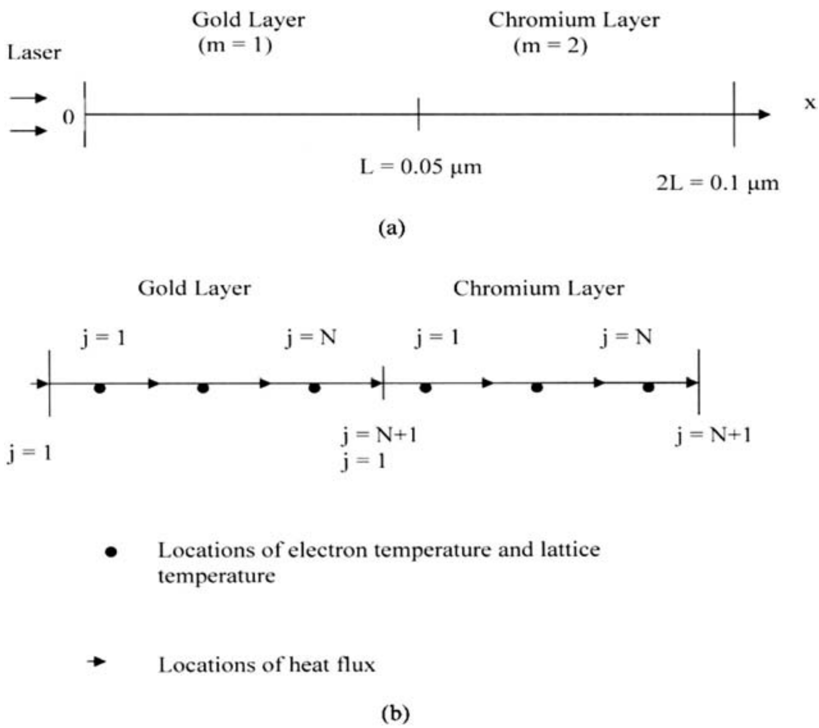

Figure 1.
A staggered grid

$$\tau_{\mathrm{e}} \frac{\left(q_{\mathrm{e}}^{r}\right)_{i-(1/2)jk}^{n+1} - \left(q_{\mathrm{e}}^{r}\right)_{i-(1/2)jk}^{n-1}}{2\Delta t} + \left(\bar{q}_{\mathrm{e}}^{r}\right)_{i-(1/2)jk}^{n} = -k_{\mathrm{e}} \nabla_{\bar{r}} (\bar{T}_{\mathrm{e}})_{ijk}^{n}, \quad i = 2, \ldots, N_r; \quad j = 1, \ldots, N_{\phi}; \quad k = 1, \ldots, N_{\theta}; \tag{18a}$$

$$\tau_{\mathrm{e}} \frac{\left(q_{\mathrm{e}}^{\phi}\right)_{ij-(1/2)k}^{n+1} - \left(q_{\mathrm{e}}^{\phi}\right)_{ij-(1/2)k}^{n-1}}{2\Delta t} + \left(\bar{q}_{\mathrm{e}}^{\phi}\right)_{ij-(1/2)k}^{n} = -\frac{k_{\mathrm{e}}}{r_i} \nabla_{\bar{\phi}} (\bar{T}_{\mathrm{e}})_{ijk}^{n}, \quad i = 1, \ldots, N_r; \quad j = 2, \ldots, N_{\phi}; \quad k = 1, \ldots, N_{\theta}; \tag{18b}$$

$$\tau_{\mathrm{e}} \frac{\left(q_{\mathrm{e}}^{\theta}\right)_{ijk-(1/2)}^{n+1} - \left(q_{\mathrm{e}}^{\theta}\right)_{ijk-(1/2)}^{n-1}}{2\Delta t} + \left(\bar{q}_{\mathrm{e}}^{\theta}\right)_{ijk-(1/2)}^{n} = -\frac{k_{\mathrm{e}}}{r_i \sin \phi_j} \nabla_{\bar{\theta}} (\bar{T}_{\mathrm{e}})_{ijk}^{n}, \quad i = 1, \ldots, N_r; \quad j = 1, \ldots, N_{\phi}; \quad k = 1, \ldots, N_{\theta}; \tag{18c}$$

and:

$$C_1\frac{(T_1)^{n+1}_{ijk}-(T_1)^{n-1}_{ijk}}{2\Delta t}=-\frac{1}{r_i^2}\nabla_r\left[r^2_{i-(1/2)}\left(\bar{q}^r_1\right)^n_{i-(1/2)jk}\right]-\frac{1}{r_i\sin\phi_j}\nabla_\phi\left[\sin\phi_{j-(1/2)}\left(\bar{q}^\phi_1\right)^n_{ij-(1/2)k}\right]-\frac{1}{r_i\sin\phi_j}\nabla_\theta\left(\bar{q}^\theta_1\right)^n_{ijk-(1/2)}+G\left[(\bar{T}_e)^n_{ijk}-(\bar{T}_1)^n_{ijk}\right],\quad(19)$$

$$i=1,\ldots,N_r;\quad j=1,\ldots,N_\phi;\quad k=1,\ldots,N_\theta;$$

$$\tau_1\frac{\left(q^r_1\right)^{n+1}_{i-(1/2)jk}-\left(q^r_1\right)^{n-1}_{i-(1/2)jk}}{2\Delta t}+\left(\bar{q}^r_1\right)^n_{i-(1/2)jk}=-k_1\nabla_{\bar{r}}(\bar{T}_1)^n_{ijk},\quad(20a)$$

$$i=2,\ldots,N_r;\quad j=1,\ldots,N_\phi;\quad k=1,\ldots,N_\theta;$$

$$\tau_1\frac{\left(q^\phi_1\right)^{n+1}_{ij-(1/2)k}-\left(q^\phi_1\right)^{n-1}_{ij-(1/2)k}}{2\Delta t}+\left(\bar{q}^\phi_1\right)^n_{ij-(1/2)k}=-\frac{k_1}{r_i}\nabla_{\bar{\phi}}(\bar{T}_1)^n_{ijk},\quad(20b)$$

$$i=1,\ldots,N_r;\quad j=2,\ldots,N_\phi;\quad k=1,\ldots,N_\theta;$$

$$\tau_1\frac{\left(q^\theta_1\right)^{n+1}_{ijk-(1/2)}-\left(q^\theta_1\right)^{n-1}_{ijk-(1/2)}}{2\Delta t}+\left(\bar{q}^\theta_1\right)^n_{ijk-(1/2)}=-\frac{k_1}{r_i\sin\phi_j}\nabla_{\bar{\theta}}(\bar{T}_1)^n_{ijk},\quad(20c)$$

$$i=1,\ldots,N_r;\quad j=1,\ldots,N_\phi;\quad k=1,\ldots,N_\theta;$$

Where the bar on T^n_e denotes $\bar{T}^n_e=\frac{1}{4}\left(T^{n+1}_e+2T^n_e+T^{n-1}_e\right)$ and so on. The initial conditions are assumed to be:

$$(\vec{q}_e)^0=(\vec{q}_1)^0=(\vec{q}_e)^1=(\vec{q}_1)^1=\vec{0},\quad (T_e)^0_{ijk}=(T_e)^1_{ijk}=(T_1)^0_{ijk}=(T_1)^1_{ijk}=T_0,\quad(21)$$

And the boundary conditions are discretized as follows:

$$\left(q^r_e\right)^n_{N_r+(1/2)jk}=0,\quad \left(q^r_1\right)^n_{N_r+(1/2)jk}=0,\quad(22a)$$

$$\left(q^\theta_e\right)^n_{ijk+(1/2)}=\left(q^\theta_e\right)^n_{ijk+(1/2)\pm N_\theta},\quad \left(q^\theta_1\right)^n_{ijk+(1/2)}=\left(q^\theta_1\right)^n_{ijk+(1/2)\pm N_\theta},\quad(22b)$$

$$\left(T^\theta_e\right)^n_{ijk}=\left(T^\theta_e\right)^n_{ijk\pm N_\theta},\quad \left(T^\theta_1\right)^n_{ijk}=\left(T^\theta_1\right)^n_{ijk\pm N_\theta},\quad(22c)$$

for any time level n.

It should be pointed out that we use a weighted average $(T^{n+1}_{ijk}+2T^n_{ijk}+T^{n-1}_{ijk})/4$ for stability. The other advantage of using the weighted average is that it is easy to handle with the temperature-dependent thermal property case, where one may evaluate these coefficients in time level n. Finally, it can be seen that the truncation errors of equations (17)-(20) are $O(\Delta t^2+\Delta r^2+\Delta\theta^2+\Delta\varphi^2)$, implying that the scheme is consistent with the partial differential equations (7)-(10).

To obtain the stability of the scheme, equations (17)-(22), with respect to the heat source, we assume that there is a small change g in the heat source Q and investigate the magnitude of the changes on $T_e, T_1, \vec{q}_e$ and $\vec{q}_1$. For simplicity, we use the same notations of $T_e, T_l, \vec{q}_e$ and $\vec{q}_l$ form the changes in the proof. We introduce the inner product and norm for mesh functions u_{ijk} and v_{ijk} as follows:

$$(u, v) = \Delta r \Delta\theta \Delta\phi \sum_{i=1}^{N_r} \sum_{j=1}^{N_\phi} \sum_{k=1}^{N_\theta} u_{ijk} v_{ijk}$$

and:

$$\|u\| = \left(\Delta r \Delta\theta \Delta\phi \sum_{i=1}^{N_r} \sum_{j=1}^{N_\phi} \sum_{k=1}^{N_\theta} u_{ijk}^2 \right)^{1/2}.$$

The following lemma 1 will be used.

Lemma 1. For any n,

$$\left(u_{ijk}^{n+1} + 2u_{ijk}^{n} + u_{ijk}^{n-1}\right) \times \left(u_{ijk}^{n+1} - u_{ijk}^{n-1}\right) = \left(u_{ijk}^{n+1} + u_{ijk}^{n}\right)^2 - \left(u_{ijk}^{n} + u_{ijk}^{n-1}\right)^2. \quad (23)$$

Theorem 2. Assume that there is a small change g in the heat source Q. Then the solutions $T_e, T_l, \vec{q}_e$ and $\vec{q}_l$ of the numerical scheme, equations (17)-(22), satisfy:

$$F(n) \le e^{3t_0} \max_{0 \le k \le n} \Phi(k), \quad 0 \le n\Delta t \le t_0, \quad (24)$$

Where:

$$\begin{aligned}
F(n) = {} & C_e \|r\sqrt{\sin\phi}[(T_e)^{n+1} + (T_e)^n]\|^2 + C_l \|r\sqrt{\sin\phi}[(T_l)^{n+1} + (T_l)^n]\|^2 \\
& + \Delta r \Delta\theta \Delta\phi \sum_{i=2}^{N_r} \sum_{j=1}^{N_\phi} \sum_{k=1}^{N_\theta} \frac{\tau_e}{k_e} r_{i-(1/2)}^2 \sin\phi_j \left[\left(q_e^r\right)_{i-(1/2)jk}^{n+1} + \left(q_e^r\right)_{i-(1/2)jk}^{n} \right]^2 \\
& + \Delta r \Delta\theta \Delta\phi \sum_{i=2}^{N_r} \sum_{j=1}^{N_\phi} \sum_{k=1}^{N_\theta} \frac{\tau_l}{k_l} r_{i-(1/2)}^2 \sin\phi_j \left[\left(q_l^r\right)_{i-(1/2)jk}^{n+1} + \left(q_l^r\right)_{i-(1/2)jk}^{n} \right]^2 \\
& + \Delta r \Delta\theta \Delta\phi \sum_{i=1}^{N_r} \sum_{j=2}^{N_\phi} \sum_{k=1}^{N_\theta} \frac{\tau_e}{k_e} r_i^2 \sin\phi_{j-(1/2)} \left[\left(q_e^\phi\right)_{ij-(1/2)k}^{n+1} + \left(q_e^\phi\right)_{ij-(1/2)k}^{n} \right]^2 \\
& + \Delta r \Delta\theta \Delta\phi \sum_{i=1}^{N_r} \sum_{j=2}^{N_\phi} \sum_{k=1}^{N_\theta} \frac{\tau_l}{k_l} r_i^2 \sin\phi_{j-(1/2)} \left[\left(q_l^\phi\right)_{ij-(1/2)k}^{n+1} + \left(q_l^\phi\right)_{ij-(1/2)k}^{n} \right]^2 \\
& + \Delta r \Delta\theta \Delta\phi \sum_{i=1}^{N_r} \sum_{j=1}^{N_\phi} \sum_{k=1}^{N_\theta} \frac{\tau_e}{k_e} r_i^2 \sin\phi_j \left[\left(q_e^\theta\right)_{ijk-(1/2)}^{n+1} + \left(q_e^\theta\right)_{ijk-(1/2)}^{n} \right]^2 \\
& + \Delta r \Delta\theta \Delta\phi \sum_{i=1}^{N_r} \sum_{j=1}^{N_\phi} \sum_{k=1}^{N_\theta} \frac{\tau_l}{k_l} r_i^2 \sin\phi_j \left[\left(q_l^\theta\right)_{ijk-(1/2)}^{n+1} + \left(q_l^\theta\right)_{ijk-(1/2)}^{n} \right]^2,
\end{aligned} \quad (25)$$

and:

$$\Phi(n) = \frac{2}{C_e} \|r\sqrt{\sin\phi} g^n\|^2 \quad (26)$$

The proof of theorem 2 can be seen in the Appendix section. Equation (24) can be considered as a discrete analogue of equation (15). The differences between equations (15) and (24) are that equation (24) gives an estimation on the changes of $T_e, T_l, \vec{q}_e$ and $\vec{q}_l$ due to a small change g in the heat source Q, and that the former uses the integral and the latter uses the summation. Equation (24) implies that the errors in $T_e, T_l, \vec{q}_e$ and $\vec{q}_l$ can be controlled by the small error in the heat source Q. Mathematically, it indicates that the scheme is stable with respect to the source term. According to the theory in numerical analysis, a consistent and stable finite difference scheme will give a numerical solution converging to the exact solution of the original problem. It should be pointed out that there is no restriction on the mesh ratios:

$$\frac{\Delta t}{\Delta r^2}, \quad \frac{\Delta t}{\Delta \phi^2} \quad \text{and} \quad \frac{\Delta t}{\Delta \theta^2}$$

implying that the scheme is unconditionally stable.

An algorithm for computing $T_e, \vec{q}_e, T_l$, and $\vec{q}_l$ at time level $n + 1$ can be written in the following steps:

(1) Solve for $(\vec{q}_e)^{n+1}$ from equations (18a)-(18c) and substitute it into equation (17) to obtain an equation that has only two unknowns $(T_e)^{n+1}$ and $(T_l)^{n+1}$. Similarly, solve for $(\vec{q}_l)^{n+1}$ from equations (20a)-(20c) and substitute it into equation (19) to obtain another equation that has only two unknowns $(T_e)^{n+1}$ and $(T_l)^{n+1}$.

(2) Set up two liner systems for $(T_e)^{n+1}$ and $(T_l)^{n+1}$, respectively, from the obtained equations in step1.

(3) Use Gauss-Seidel iterative method to solve for $(T_e)^{n+1}$ and $(T_l)^{n+1}$.

(4) Once $(T_e)^{n+1}$ and $(T_l)^{n+1}$ are obtained, $(\vec{q}_e)^{n+1}$ and $(\vec{q}_l)^{n+1}$are then obtained from equations (18a)-(18c) and equations (20a)-(20c).

Repeat the calculation until the required time steps have been achieved.

4. Numerical examples

To demonstrate the applicability of the scheme, we investigated the temperature rise in a gold sphere. The radius (R) for the gold sphere is 0.1 μm. The thermal properties of gold were chosen to be $C_e = 2.1 \times 10^{-5}\,\text{J/(mm}^3\text{K)}$, $C_l = 2.5 \times 10^{-3}\,\text{J/(mm}^3\text{K)}$, $k_e = k_l = 315\,\text{W/(mK)}$, $\tau_e = 0.04\,\text{ps}$, $\tau_l = 0.8\,\text{ps}$, $G = 2.6 \times 10^{-5}\,\text{J/(mm}^3\text{Kps)}$ (Tzou, 1996). Also, we chose $T_0 = 300\,\text{K}$.

To apply our scheme, we chose three different meshes of 25 × 20 × 20, 50 × 20 × 20 and 100 × 20 × 20 grid points in (r, θ, ϕ) coordinates. The time increment was chosen to be 0.005 ps.

In the first case, we assume the laser irradiation to be symmetric on the surface of the sphere. Thus, the heat source was chosen to be (Tzou, 1996):

$$Q(r,t) = 0.94J\left[\frac{1-R_l}{t_p\delta}\right]e^{-((R-r)/\delta)-2.77((t-2t_p)/t_p)^2} \tag{27}$$

Where $J = 13.4\,\text{J/m}^2$, $t_p = 100\,\text{fs}$ (1 fs $= 10^{-15}$ s), $\delta = 15.3\,\text{nm}$ (1 nm $= 10^{-9}$ m), and $R_l = 0.93$. Figure 2 shows the change in electron temperature $((\Delta T_e)/(\Delta T_e)\text{max})$ on the surface of the gold sphere. The maximum temperature rise of T_e (i.e. (ΔT_e)max) on the surface of the gold sphere is about 953 K. It can be seen from Figure 2 that the change in electron temperature is similar to that obtained in Chen and Beraun (2001), Tzou (1996). Also, it can be seen from Figures 2 and 3 that mesh size had no significant effect on the solution, implying that the scheme is stable. Further, we compared the solution with that obtained by the parabolic two-step model in Kaba and Dai (2005) with a mesh of 50 × 20 × 20. Figure 4 gives the electron temperature and lattice

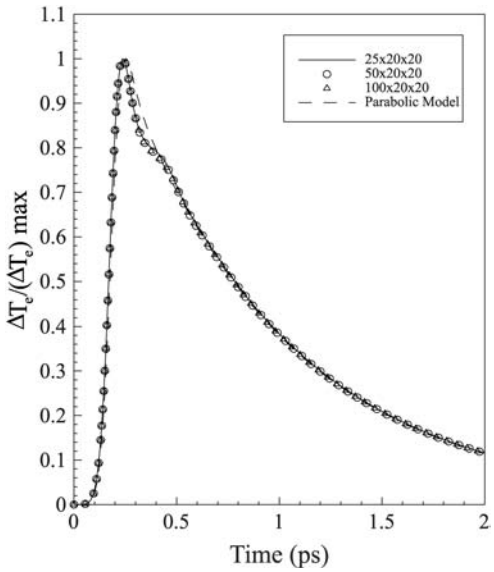

Figure 2.
Normalized electron temperature change with time on the surface of the sphere using $\Delta t = 0.005$ ps in the first example

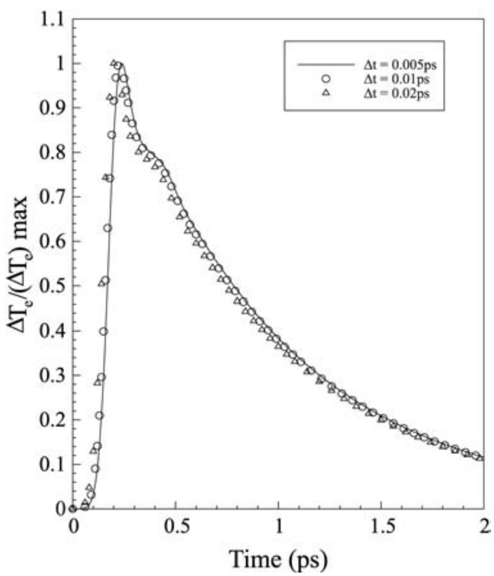

Figure 3.
Normalized electron temperature change with time on the surface of the sphere using a grid of $25 \times 20 \times 20$ in the first example

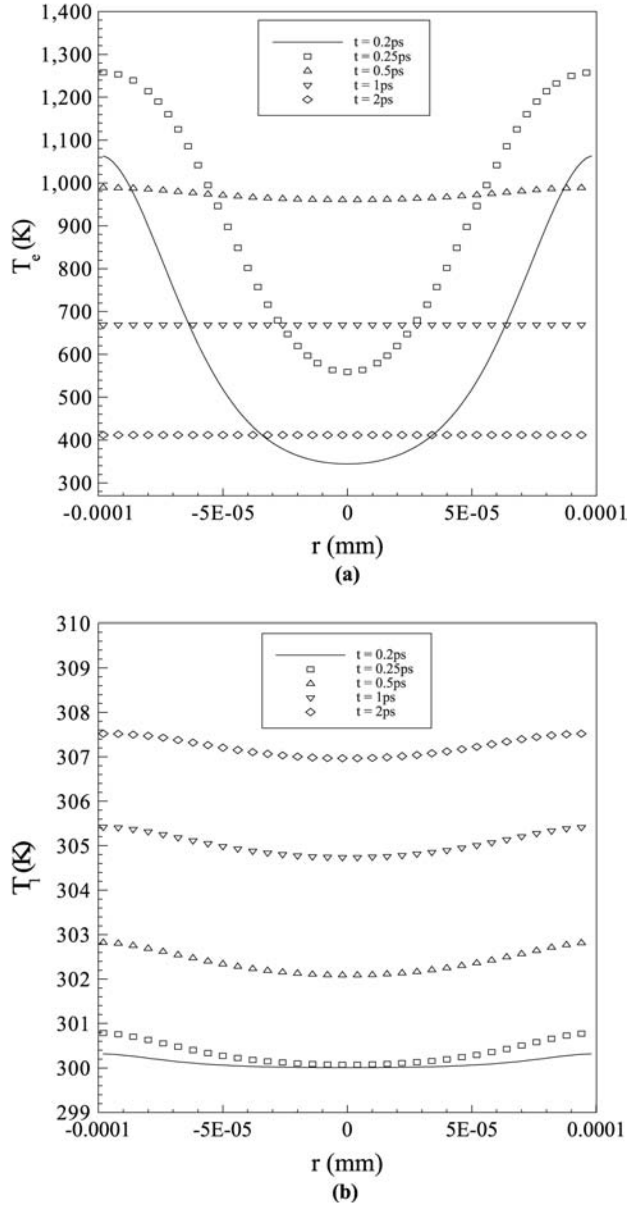

Figure 4.
Changes in electron and lattice temperatures along the *r*-axis in the first example

temperature distributions along the r-axis for different times ($t = 0.2$, 0.25, 0.5, 1.0 and 2.0 ps). It can be seen from the figure that the temperature distributions are symmetric with respect to r.

The second case assumes that the laser irradiates from top a portion $(0 < r < R, 0 \leq \theta \leq 2\pi, 0 \leq \phi \leq (\pi/2))$ of the surface of the sphere. In this case, the heat source was chosen to be:

$$Q(r, \varphi, t) = 0.94J\left[\frac{1-R}{t_p\delta}\right]e^{-((R-r)/\delta)-2.77((t-2t_p)/t_p)^2}\cos\varphi. \tag{28}$$

Figure 4 shows the change in electron temperature $((\Delta T_e)/(\Delta T_e)\text{max})$ at the point $(r = L,\ \varphi = 0)$. The maximum temperature rise of T_e (i.e. (ΔT_e)max) is about 833 K. It can be seen by comparing Figure 2 with Figure 4 that the changes in electron temperature are similar except that the change in temperature in Figure 5 drops quickly. This is because the laser irradiates only a portion of the surface and the heat is transferred from the top of the sphere to the bottom. Figure 6 gives the electron temperature and lattice temperature distributions along the r-axis with $\varphi = 0$ and π for different times ($t = 0.2$, 0.25, 0.5, 1.0 and 2.0 ps).

The third case assumes that the laser irradiates from the top a small portion $(0 < r < R, 0 \leq \theta \leq 2\pi, 0 \leq \varphi \leq \pi/4)$ of the surface of the sphere. Figure 7 shows

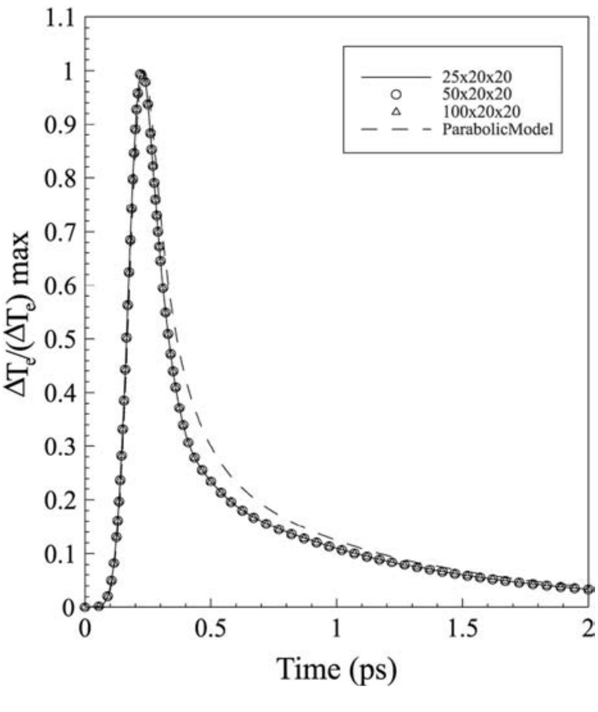

Figure 5.
Normalized electron temperature change with time at the point ($r = R$, $\phi = 0$) of the sphere in the second example

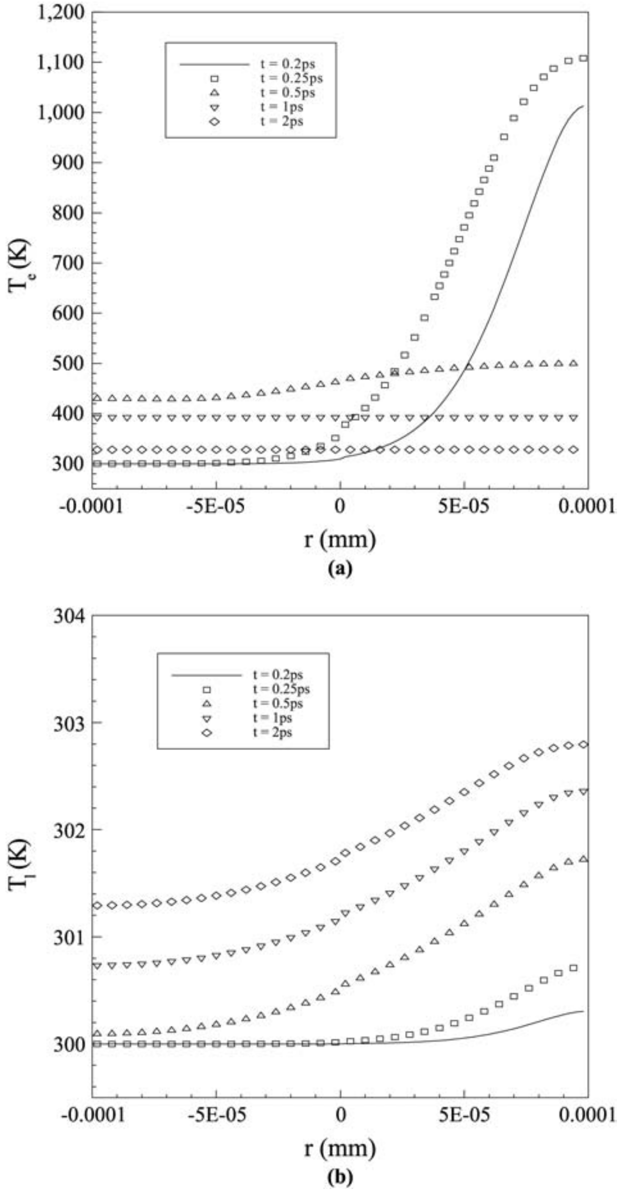

Figure 6.
Changes in electron and lattice temperatures along the r-axis with $\phi = 0$ and π in the second example

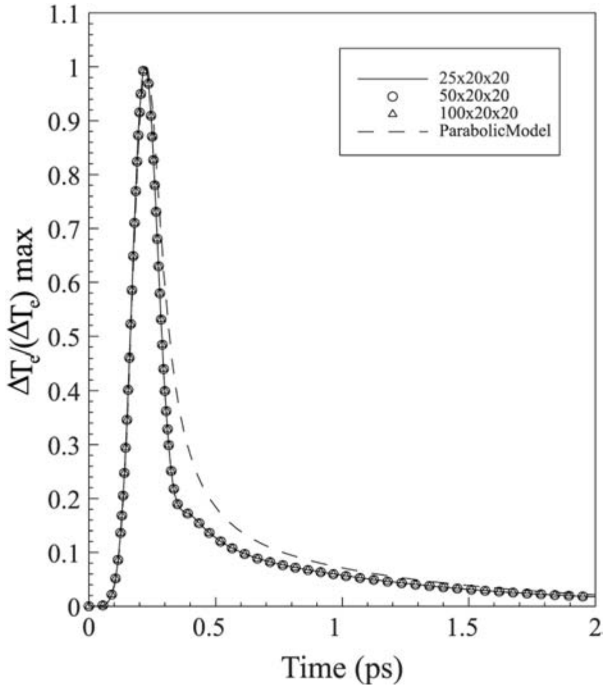

Figure 7.
Normalized electron temperature change with time at the point ($r = R$, $\phi = 0$) of the sphere in the third example

the change in electron temperature $((\Delta T_e)/(\Delta T_e)\text{max})$ at the point ($r = R$, $\varphi = 0$). The maximum temperature rise of T_e (i.e. (ΔT_e)max) is about 797 K. Again, the changes in electron temperature is similar to those in Figures 2 and 4 except that the change in electron temperature in Figure 7 drops faster. This is because the laser irradiates only a small portion of the surface and the heat is transferred from the top of the sphere to the bottom in this case. Figure 8 shows the electron temperature and lattice temperature distributions along the r-axis with $\varphi = 0$ and π for different times ($t = 0.2$, 0.25, 0.5, 1.0 and 2.0 ps).

Finally, we considered a repetitive-pulse heating case where the heat source was chosen to be:

$$Q(r,t) = 0.94J\left[\frac{1-R}{t_p\delta}\right]e^{-(R-r)/\delta}[e^{-2.77((t-2t_p)/t_p)^2} + e^{-2.77((t-4t_p)/t_p)^2}] \qquad (29)$$

with $J = 13.4\,\text{J/m}^2$, $t_{p=} 100$ fs, $\delta = 15.3$ nm, and $R = 0.93$. Figure 9 shows the change in electron temperature $((\Delta T_e)/(\Delta T_e)\text{max})$ on the surface of the gold sphere. It can be seen that there are two peaks in electron temperature because of two pulses. Also, it can be seen that mesh size had no significant effects on the solution implying that the scheme is stable. Figure 10 shows the electron temperature and lattice temperature distributions along the r-axis for different times ($t = 0.2$, 0.25, 0.5, 1.0 and 2.0 ps). Again, it can be seen from the figure that

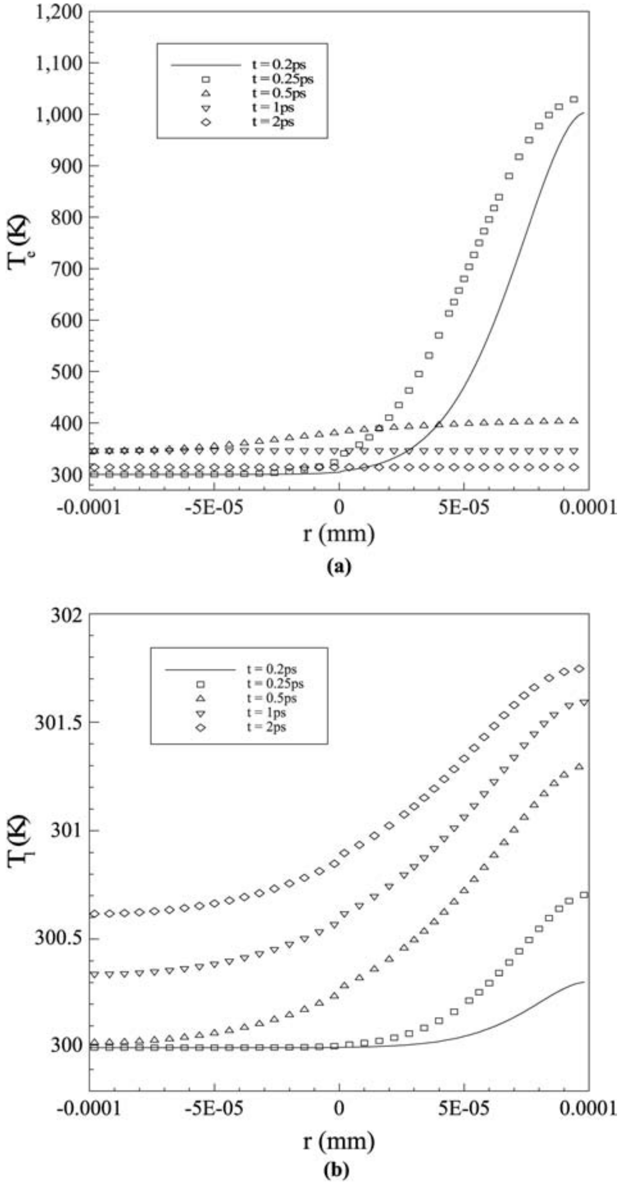

Figure 8.
Changes in electron and lattice temperatures along the r-axis with $\phi = 0$ and π in the third example

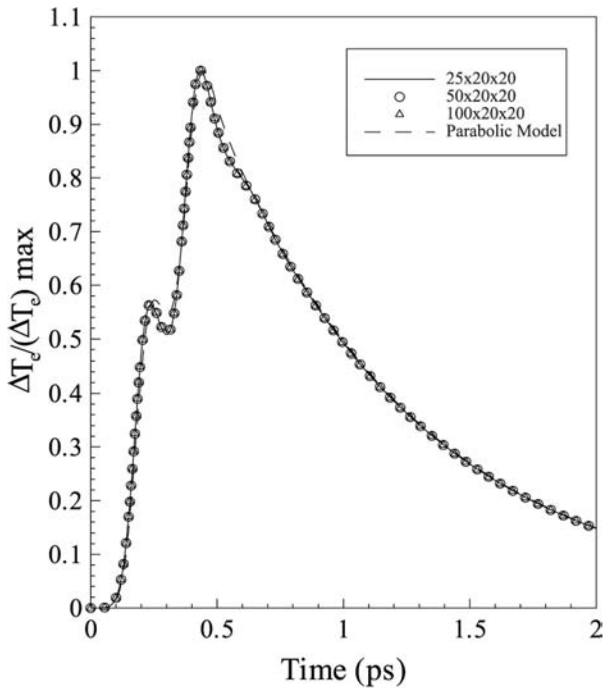

Figure 9.
Normalized electron temperature change with time on the surface of the sphere in the repetitive-pulse heating case

the temperature distributions are symmetric with respect to r, which is similar to those in Figure 4 except for the high temperature.

5. Conclusion

In this study, we have developed a three-level finite difference scheme for solving the hyperbolic two-step heat transport equations in a 3D micro-sphere heated by ultrashort-pulsed lasers. The advantages of the scheme are:

- it is second-order in truncation error;
- it satisfies a discrete energy estimation, implying that the scheme is unconditionally stable with respective to the heat source and there is no restriction on the mesh ratios $\Delta t/\Delta r^2$, $\Delta t/\Delta \phi^2$ and $\Delta t/\Delta \theta^2$; and
- it is developed in staggered grid, which prevents the solution from numerical oscillation.

Numerical examples show that the scheme is efficient.

Here, we considered the hyperbolic two-step model only with constant thermal properties. Further research will focus on the model with temperature-dependent thermal properties. The present numerical scheme can be readily generalized to the temperature-dependent property case. For example, one may evaluate C_e and k_e at time level n so that the scheme becomes a linearized finite difference scheme with the truncation error being still second-order.

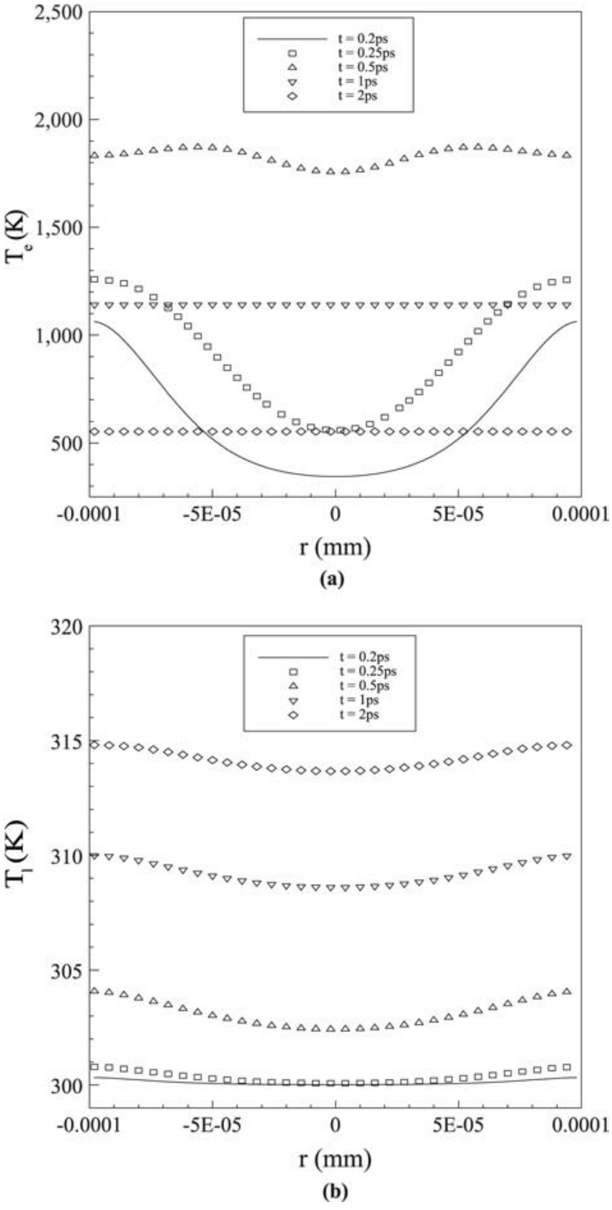

Figure 10.
Changes in electron and lattice temperatures along the *r*-axis in the repetitive-pulse heating case

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Appendix

Proof of Theorem 1. Multiplying equation (7) by $r^2 T_e \sin\phi$, and equation (9) by $r^2 T_l \sin\phi$, and integrating over the domain $\Omega = \{0 \le r \le R, 0 \le \theta \le 2\pi, 0 \le \phi \le \pi\}$ and summing the results together, we obtain:

$$\begin{aligned}
&\iiint_\Omega C_e r^2 \sin\phi \frac{\partial T_e}{\partial t} T_e \,\mathrm{d}\Omega + \iiint_\Omega C_l r^2 \sin\phi \frac{\partial T_l}{\partial t} T_l \,\mathrm{d}\Omega \\
&\quad = -\iiint_\Omega \sin\phi \frac{\partial}{\partial r}\left(r^2 q_e^r\right) T_e \,\mathrm{d}\Omega \\
&\quad - \iiint_\Omega \sin\phi \frac{\partial}{\partial r}\left(r^2 q_l^r\right) T_l \,\mathrm{d}\Omega \\
&\quad - \iiint_\Omega r \frac{\partial}{\partial \phi}\left(\sin\phi q_e^\phi\right) T_e \,\mathrm{d}\Omega \\
&\quad - \iiint_\Omega r \frac{\partial}{\partial \phi}\left(\sin\phi q_l^\phi\right) T_l \,\mathrm{d}\Omega \\
&\quad - \iiint_\Omega r \frac{\partial q_e^\theta}{\partial \theta} T_e \,\mathrm{d}\Omega \\
&\quad - \iiint_\Omega r \frac{\partial q_l^\theta}{\partial \theta} T_l \,\mathrm{d}\Omega \\
&\quad - \iiint_\Omega r^2 \sin\phi G (T_e - T_l)^2 \mathrm{d}\Omega \\
&\quad + \iiint_\Omega r^2 \sin\phi T_e Q \,\mathrm{d}\Omega,
\end{aligned} \tag{30}$$

Where $\mathrm{d}\Omega$ denotes $\mathrm{d}r\,\mathrm{d}\theta\,\mathrm{d}\phi$. The left-hand side (LHS) of equation (30) can be written as follows:

$$\mathrm{LHS} = \frac{\mathrm{d}}{\mathrm{d}t}\left[\frac{1}{2}\iiint_\Omega C_e r^2 \sin\phi T_e^2 \mathrm{d}\Omega + \frac{1}{2}\iiint_\Omega C_l r^2 \sin\phi T_l^2 \mathrm{d}\Omega\right]. \tag{31a}$$

On the other hand, one may use Green's theorem, equation (12) and the fact that $r^2 q_e^r = 0$ at $r = 0$, and then equation (8a) to simplify the first term on the right-hand side of equation (30) as follows:

$$
\begin{aligned}
-\iiint_\Omega \sin\phi \frac{\partial}{\partial r}\left(r^2 q_e^r\right) T_e \mathrm{d}\Omega &= -\int_0^{2\pi}\int_0^{\pi}\left[r^2 q_e^r T_e \sin\phi\right]_0^R \mathrm{d}\phi\,\mathrm{d}\theta \\
&\quad + \iiint_\Omega r^2 q_e^r \frac{\partial T_e}{\partial r}\sin\phi\,\mathrm{d}\Omega \\
&= \iiint_\Omega r^2 q_e^r \frac{\partial T_e}{\partial r}\sin\phi\,\mathrm{d}\Omega \\
&= -\frac{1}{k_e}\iiint_\Omega\left[\tau_e \frac{\partial q_e^r}{\partial t} + q_e^r\right] q_e^r r^2 \sin\phi\,\mathrm{d}\Omega \\
&= -\frac{\mathrm{d}}{\mathrm{d}t}\iiint_\Omega \frac{1}{2}\,\frac{\tau_e}{k_e}\left(q_e^r\right)^2 r^2\sin\phi\,\mathrm{d}\Omega \\
&\quad - \iiint_\Omega \frac{1}{k_e}\left(q_e^r\right)^2 r^2 \sin\phi\,\mathrm{d}\Omega.
\end{aligned}
\tag{31b}
$$

Similarly, the third term on the right-hand side of equation (30) can be simplified as:

$$
\begin{aligned}
-\iiint_\Omega r\frac{\partial}{\partial\phi}\left(\sin\phi q_e^\phi\right) T_e \mathrm{d}\Omega &= -\int_0^{R}\int_0^{2\pi}\left[r q_e^\phi T_e \sin\phi\right]_0^\pi \mathrm{d}\theta\,\mathrm{d}r \\
&\quad + \iiint_\Omega r q_e^\phi \frac{\partial T_e}{\partial\phi}\sin\phi\,\mathrm{d}\Omega \\
&= \iiint_\Omega r^2 q_e^\phi\left(\frac{1}{r}\,\frac{\partial T_e}{\partial\phi}\right)\sin\phi\,\mathrm{d}\Omega \\
&= -\frac{1}{k_e}\iiint_\Omega\left[\tau_e \frac{\partial q_e^\phi}{\partial t} + q_e^\phi\right] q_e^\phi r^2 \sin\phi\,\mathrm{d}\Omega \\
&= -\frac{\mathrm{d}}{\mathrm{d}t}\iiint_\Omega \frac{1}{2}\,\frac{\tau_e}{k_e}\left(q_e^\phi\right)^2 r^2\sin\phi\,\mathrm{d}\Omega \\
&\quad - \iiint_\Omega \frac{1}{k_e}\left(q_e^\phi\right)^2 r^2 \sin\phi\,\mathrm{d}\Omega,
\end{aligned}
\tag{31c}
$$

and the fifth term:

$$
\begin{aligned}
-\iiint_\Omega r\frac{\partial q_e^\theta}{\partial\theta} T_e \mathrm{d}\Omega &= -\int_0^{R}\int_0^{\pi}\left[r q_e^\theta T_e\right]_0^{2\pi} \mathrm{d}r\,\mathrm{d}\phi + \iiint_\Omega r q_e^\theta \frac{\partial T_e}{\partial\theta}\,\mathrm{d}\Omega \\
&= \iiint_\Omega r^2 q_e^\theta\left(\frac{1}{r\sin\phi}\,\frac{\partial T_e}{\partial\theta}\right)\sin\phi\,\mathrm{d}\Omega \\
&= -\frac{1}{k_e}\iiint_\Omega\left[\tau_e \frac{\partial q_e^\theta}{\partial t} + q_e^\theta\right] q_e^\theta r^2 \sin\phi\,\mathrm{d}\Omega \\
&= -\frac{\mathrm{d}}{\mathrm{d}t}\iiint_\Omega \frac{1}{2}\,\frac{\tau_e}{k_e}\left(q_e^\theta\right)^2 r^2\sin\phi\,\mathrm{d}\Omega - \iiint_\Omega \frac{1}{k_e}\left(q_e^\theta\right)^2 r^2 \sin\phi\,\mathrm{d}\Omega.
\end{aligned}
\tag{31d}
$$

Using a similar argument, we obtain:

$$
\begin{aligned}
-\iiint_\Omega \sin\phi \frac{\partial}{\partial r}\left(r^2 q_l^r\right) T_l \mathrm{d}\Omega &= -\frac{\mathrm{d}}{\mathrm{d}t}\iiint_\Omega \frac{1}{2}\,\frac{\tau_l}{k_l}\left(q_l^r\right)^2 r^2\sin\phi\,\mathrm{d}\Omega \\
&\quad - \iiint_\Omega \frac{1}{k_l}\left(q_l^r\right)^2 r^2 \sin\phi\,\mathrm{d}\Omega,
\end{aligned}
\tag{31e}
$$

$$-\iiint_{\Omega} r\frac{\partial}{\partial\phi}\left(\sin\phi q_1^{\phi}\right)T_1\mathrm{d}\Omega = -\frac{\mathrm{d}}{\mathrm{d}t}\iiint_{\Omega}\frac{1}{2}\frac{\tau_1}{k_1}\left(q_1^{\phi}\right)^2 r^2\sin\phi\,\mathrm{d}\Omega - \iiint_{\Omega}\frac{1}{k_1}\left(q_1^{\phi}\right)^2 r^2\sin\phi\,\mathrm{d}\Omega, \tag{31f}$$

and:

$$-\iiint_{\Omega} r\frac{\partial q_1^{\theta}}{\partial\theta}T_1\mathrm{d}\Omega = -\frac{\mathrm{d}}{\mathrm{d}t}\iiint_{\Omega}\frac{1}{2}\frac{\tau_1}{k_1}\left(q_1^{\theta}\right)^2 r^2\sin\phi\,\mathrm{d}\Omega - \iiint_{\Omega}\frac{1}{k_1}\left(q_1^{\theta}\right)^2 r^2\sin\phi\,\mathrm{d}\Omega. \tag{31g}$$

Furthermore, we have by Cauchy-Schwartz's inequality:

$$\iiint_{\Omega} r^2\sin\phi T_e Q\,\mathrm{d}\Omega \le \frac{1}{2}\iiint_{\Omega} C_e T_e^2 r^2\sin\phi\,\mathrm{d}\Omega + \frac{1}{2C_e}\iiint_{\Omega} Q^2 r^2\sin\phi\,\mathrm{d}\Omega. \tag{31h}$$

Substituting equations (31a)-(31h) into equation (30) gives:

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t}\iiint_{\Omega}\frac{1}{2}\left[C_e T_e^2 + C_1 T_1^2\right] r^2\sin\phi\,\mathrm{d}\Omega \\
&\quad + \frac{\mathrm{d}}{\mathrm{d}t}\iiint_{\Omega}\frac{1}{2}\frac{\tau_e}{k_e}\left[\left(q_e^r\right)^2 + \left(q_e^{\phi}\right)^2 + \left(q_e^{\theta}\right)^2\right] r^2\sin\phi\,\mathrm{d}\Omega \\
&\quad + \frac{\mathrm{d}}{\mathrm{d}t}\iiint_{\Omega}\frac{1}{2}\frac{\tau_1}{k_1}\left[\left(q_1^r\right)^2 + \left(q_1^{\phi}\right)^2 + \left(q_1^{\theta}\right)^2\right] r^2\sin\phi\,\mathrm{d}\Omega \\
&\quad + \iiint_{\Omega}\frac{1}{k_e}\left[\left(q_e^r\right)^2 + \left(q_e^{\phi}\right)^2 + \left(q_e^{\theta}\right)^2\right] r^2\sin\phi\,\mathrm{d}\Omega \\
&\quad + \iiint_{\Omega}\frac{1}{k_1}\left[\left(q_1^r\right)^2 + \left(q_1^{\phi}\right)^2 + \left(q_1^{\theta}\right)^2\right] r^2\sin\phi\,\mathrm{d}\Omega \\
&\quad + \iiint_{\Omega} G(T_e - T_1)^2 r^2\sin\phi\,\mathrm{d}\Omega \\
&\le \frac{1}{2}\iiint_{\Omega} C_e T_e^2 r^2\sin\phi\,\mathrm{d}\Omega + \frac{1}{2C_e}\iiint_{\Omega} Q^2 r^2\sin\phi\,\mathrm{d}\Omega.
\end{aligned} \tag{32}$$

Dropping the fourth, fifth and sixth terms on the LHS and using the notations of $F(t)$ and $\Phi(t)$. Equation (32) can be simplified as follows:

$$F'(t) \le F(t) + \Phi(t). \tag{33}$$

By Gronwall's inequality (Evens, 1998), we obtain that:

$$F(t) \le \mathrm{e}^t\left[F(0) + \int_0^{\mathrm{t}}\Phi(s)\mathrm{d}s\right],$$

which completes the proof.

Proof of Theorem 2. Multiplying equation (17) by $16\Delta r\Delta\theta\Delta\phi\Delta t r_i^2\sin\phi_j(\bar{T}_e)_{ijk}^n$ and equation (19) by $16\Delta r\Delta\theta\Delta\phi\Delta t r_i^2\sin\phi_j(\bar{T}_1)_{ijk}^n$, summing over i, j, k with $1 \le i \le N_r$, $1 \le j \le N_{\phi}$, $1 \le k \le N_{\phi}$, and adding the results together, we obtain by lemma 1:

$$
\begin{aligned}
&2C_{\mathrm{e}}\Big\{\|r\sqrt{\sin\phi}\big[(T_{\mathrm{e}})^{n+1}+(T_{\mathrm{e}})^{n}\big]\|^2-\|r\sqrt{\sin\phi}\big[(T_{\mathrm{e}})^{n}+(T_{\mathrm{e}})^{n-1}\big]\|^2\Big\}\\
&\quad+2C_{\mathrm{l}}\Big\{\|r\sqrt{\sin\phi}\big[(T_{\mathrm{l}})^{n+1}+(T_{\mathrm{l}})^{n}\big]\|^2-\|r\sqrt{\sin\phi}\big[(T_{\mathrm{l}})^{n}+(T_{\mathrm{l}})^{n-1}\big]\|^2\Big\}\\
&\quad=-16\Delta r\Delta\theta\Delta\phi\Delta t\sum_{i=1}^{N_r}\sum_{j=1}^{N_\phi}\sum_{k=1}^{N_\theta}\sin\phi_j\nabla_r\Big[r^2_{i-(1/2)}\big(\bar{q}^r_{\mathrm{e}}\big)^n_{i-(1/2)jk}\Big](\bar{T}_{\mathrm{e}})^n_{ijk}\\
&\quad-16\Delta r\Delta\theta\Delta\phi\Delta t\sum_{i=1}^{N_r}\sum_{j=1}^{N_\phi}\sum_{k=1}^{N_\theta}\sin\phi_j\nabla_r\Big[r^2_{i-(1/2)}\big(\bar{q}^r_{\mathrm{l}}\big)^n_{i-(1/2)jk}\Big](\bar{T}_{\mathrm{l}})^n_{ijk}\\
&\quad-16\Delta r\Delta\theta\Delta\phi\Delta t\sum_{i=1}^{N_r}\sum_{j=1}^{N_\phi}\sum_{k=1}^{N_\theta}r_i\nabla_\phi\Big[\sin\phi^2_{j-(1/2)}\big(\bar{q}^\phi_{\mathrm{e}}\big)^n_{ij-(1/2)k}\Big](\bar{T}_{\mathrm{e}})^n_{ijk}\\
&\quad-16\Delta r\Delta\theta\Delta\phi\Delta t\sum_{i=1}^{N_r}\sum_{j=1}^{N_\phi}\sum_{k=1}^{N_\theta}r_i\nabla_\phi\Big[\sin\phi^2_{j-(1/2)}\Big(\bar{q}^\phi_{\mathrm{l}}\Big)^n_{ij-(1/2)k}\Big](\bar{T}_{\mathrm{l}})^n_{ijk}\\
&\quad-16\Delta r\Delta\theta\Delta\phi\Delta t\sum_{i=1}^{N_r}\sum_{j=1}^{N_\phi}\sum_{k=1}^{N_\theta}r_i\nabla_\theta\big(\bar{q}^\theta_{\mathrm{e}}\big)^n_{ijk-(1/2)}(\bar{T}_{\mathrm{e}})^n_{ijk}\\
&\quad-16\Delta r\Delta\theta\Delta\phi\Delta t\sum_{i=1}^{N_r}\sum_{j=1}^{N_\phi}\sum_{k=1}^{N_\theta}r_i\nabla_\theta\big(\bar{q}^\theta_{\mathrm{l}}\big)^n_{ijk-(1/2)}(\bar{T}_{\mathrm{l}})^n_{ijk}\\
&\quad-16G\,\Delta t\|r\sqrt{\sin\phi}[(\bar{T}_{\mathrm{e}})^n-(\bar{T}_{\mathrm{l}})^n\|^2+16\Delta t(g^n,r^2\sin\phi(\bar{T}_{\mathrm{e}})^n),
\end{aligned}
\tag{34}
$$

We now simplify the first term on the right-hand side of equation (34) using the boundary condition, equation (22a) and the fact that $r_{(1/2)}=((1/2)-(1/2))\Delta r=0$, and then equation (20a) as well as lemma 1 as follows:

$$
\begin{aligned}
&\Delta r\sum_{i=1}^{N_r}\nabla_r\Big[r^2_{i-(1/2)}\big(\bar{q}^r_{\mathrm{e}}\big)^n_{i-(1/2)jk}\Big](\bar{T}_{\mathrm{e}})^n_{ijk}\\
&\quad=\sum_{i=1}^{N_r}r^2_{i+(1/2)}\big(\bar{q}^r_{\mathrm{e}}\big)^n_{i+(1/2)jk}(\bar{T}_{\mathrm{e}})^n_{ijk}-\sum_{i=1}^{N_r}r^2_{i-(1/2)}\big(\bar{q}^r_{\mathrm{e}}\big)^n_{i-(1/2)jk}(\bar{T}_{\mathrm{e}})^n_{ijk}\\
&\quad=\sum_{i=2}^{N_r}r^2_{i-(1/2)}\big(\bar{q}^r_{\mathrm{e}}\big)^n_{i-(1/2)jk}(\bar{T}_{\mathrm{e}})^n_{i-1jk}-\sum_{i=2}^{N_r}r^2_{i-(1/2)}\big(\bar{q}^r_{\mathrm{e}}\big)^n_{i-(1/2)jk}(\bar{T}_{\mathrm{e}})^n_{ijk}\\
&\quad=-\sum_{i=2}^{N_r}r^2_{i-(1/2)}\big(\bar{q}^r_{\mathrm{e}}\big)^n_{i-(1/2)jk}\cdot\nabla_{\bar{r}}(\bar{T}_{\mathrm{e}})^n_{ijk}\cdot\Delta r\\
&\quad=\frac{\tau_{\mathrm{e}}\Delta r}{2k_{\mathrm{e}}\Delta t}\sum_{i=2}^{N_r}r^2_{i-(1/2)}\big(\bar{q}^r_{\mathrm{e}}\big)^n_{i-(1/2)jk}\Big[\big(q^r_{\mathrm{e}}\big)^{n+1}_{i-(1/2)jk}-\big(q^r_{\mathrm{e}}\big)^{n-1}_{i-(1/2)jk}\Big]\\
&\qquad+\frac{\Delta r}{k_{\mathrm{e}}}\sum_{i=2}^{N_r}r^2_{i-(1/2)}\Big[\big(\bar{q}^r_{\mathrm{e}}\big)^n_{i-(1/2)jk}\Big]^2\\
&\quad=\frac{\tau_{\mathrm{e}}\Delta r}{8k_{\mathrm{e}}\Delta t}\sum_{i=2}^{N_r}r^2_{i-(1/2)}\Big\{\Big[\big(q^r_{\mathrm{e}}\big)^{n+1}_{i-(1/2)jk}+\big(q^r_{\mathrm{e}}\big)^{n}_{i-(1/2)jk}\Big]^2-\Big[\big(q^r_{\mathrm{e}}\big)^{n}_{i-(1/2)jk}+\big(q^r_{\mathrm{e}}\big)^{n-1}_{i-(1/2)jk}\Big]^2\Big\}\\
&\qquad+\frac{\Delta r}{k_{\mathrm{e}}}\sum_{i=2}^{N_r}r^2_{i-(1/2)}\Big[\big(\bar{q}^r_{\mathrm{e}}\big)^n_{i-(1/2)jk}\Big]^2.
\end{aligned}
\tag{35a}
$$

Similarly, we use the face that $\sin\phi_{(1/2)} = \sin 0 = \sin\phi_{N_\phi+(1/2)} = \sin\pi = 0$, and then equation (20b) as well as lemma 1 to obtain

$$\begin{aligned}
&\Delta\phi\sum_{j=1}^{N_\phi} r_i\nabla_\phi\left[\sin\phi_{j-(1/2)}\left(\bar{q}_{\rm e}^{\phi}\right)_{ij-(1/2)k}^{n}\right](\bar{T}_{\rm e})_{ijk}^{n}\\
&= -\Delta\phi\sum_{j=2}^{N_\phi} r_i\sin\phi_{j-(1/2)}\left(\bar{q}_{\rm e}^{\phi}\right)_{ij-(1/2)k}^{n}\nabla_{\bar{\phi}}(\bar{T}_{\rm e})_{ijk}^{n}\\
&= \frac{\tau_{\rm e}\Delta\phi}{8k_{\rm e}\Delta t}\sum_{j=2}^{N_\phi} r_i^2\sin\phi_{j-(1/2)}\left\{\left[\left(q_{\rm e}^{\phi}\right)_{ij-(1/2)k}^{n+1} + \left(q_{\rm e}^{\phi}\right)_{ij-(1/2)k}^{n}\right]^2\right.\\
&\quad\left.-\left[\left(q_{\rm e}^{\phi}\right)_{ij-(1/2)k}^{n} + \left(q_{\rm e}^{\phi}\right)_{ij-(1/2)k}^{n-1}\right]^2\right\}\\
&\quad+\frac{\Delta\phi}{k_{\rm e}}\sum_{j=2}^{N_\phi} r_i^2\sin\phi_{j-(1/2)}\left[\left(\bar{q}_{\rm e}^{\phi}\right)_{ij-\frac{1}{2}k}^{n}\right]^2,
\end{aligned}\tag{35b}$$

and use the boundary condition, equations (22b)-(22c), and then equation (20c) as well as lemma 1 to obtain:

$$\begin{aligned}
\Delta\theta\sum_{k=1}^{N_\theta} r_i\nabla_\theta\left(\bar{q}_{\rm e}^{\theta}\right)_{ijk-(1/2)}^{n}(\bar{T}_{\rm e})_{ijk}^{n} &= \sum_{k=2}^{N_\theta+1} r_i\left(\bar{q}_{\rm e}^{\theta}\right)_{ijk-(1/2)}^{n}(\bar{T}_{\rm e})_{ijk-1}^{n} - \sum_{k=1}^{N_\theta} r_i\left(\bar{q}_{\rm e}^{\theta}\right)_{ijk-(1/2)}^{n}(\bar{T}_{\rm e})_{ijk-1}^{n}\\
&= -\Delta\theta\sum_{k=2}^{N_\theta} r_i\left(\bar{q}_{\rm e}^{\theta}\right)_{ijk-(1/2)}^{n}\nabla_{\bar{\theta}}(\bar{T}_{\rm e})_{ijk}^{n} + r_i\left(\bar{q}_{\rm e}^{\theta}\right)_{ijN_\theta+(1/2)}^{n}(\bar{T}_{\rm e})_{ijN_\theta}^{n}\\
&\quad - r_i\left(\bar{q}_{\rm e}^{\theta}\right)_{ij(1/2)}^{n}(\bar{T}_{\rm e})_{ij1}^{n}\\
&= -\Delta\theta\sum_{k=1}^{N_\theta} r_i\left(\bar{q}_{\rm e}^{\theta}\right)_{ijk-(1/2)}^{n}\nabla_{\bar{\theta}}(\bar{T}_{\rm e})_{ijk}^{n}\\
&= \frac{\tau_{\rm e}\Delta\theta}{8k_{\rm e}\Delta t}\sum_{k=1}^{N_\theta} r_i^2\sin\phi_j\left\{\left[\left(q_{\rm e}^{\theta}\right)_{ijk-(1/2)}^{n+1} + \left(q_{\rm e}^{\theta}\right)_{ijk-(1/2)}^{n}\right]^2\right.\\
&\quad\left.-\left[\left(q_{\rm e}^{\theta}\right)_{ijk-(1/2)}^{n} + \left(q_{\rm e}^{\theta}\right)_{ijk-(1/2)}^{n-1}\right]^2\right\}\\
&\quad+\frac{\Delta\theta}{k_{\rm e}}\sum_{k=1}^{N_\theta} r_i^2\sin\phi_j\left[\left(\bar{q}_{\rm e}^{\theta}\right)_{ijk-(1/2)}^{n}\right]^2,
\end{aligned}\tag{35c}$$

Where $(\bar{T}_{\rm e})_{ijN_\theta}^{n}$ is denoted as $(\bar{T}_{\rm e})_{ij0}^{n}$. Using a similar argument, we have:

$$\begin{aligned}
\Delta r\sum_{i=1}^{N_r}\nabla_r\left[r_{i-(1/2)}^2\left(\bar{q}_1^{r}\right)_{i-(1/2)jk}^{n}\right](\bar{T}_1)_{ijk}^{n} &= \frac{\tau_1\Delta r}{8k_1\Delta t}\sum_{i=2}^{N_r} r_{i-(1/2)}^2\left\{\left[\left(q_1^{r}\right)_{i-(1/2)jk}^{n+1} + \left(q_1^{r}\right)_{i-(1/2)jk}^{n}\right]^2\right.\\
&\quad\left.-\left[\left(q_1^{r}\right)_{i-(1/2)jk}^{n} + \left(q_1^{r}\right)_{i-(1/2)jk}^{n-1}\right]^2\right\}\\
&\quad+\frac{\Delta r}{k_1}\sum_{i=2}^{N_r} r_{i-(1/2)}^2\left[\left(\bar{q}_1^{r}\right)_{i-(1/2)jk}^{n}\right]^2,
\end{aligned}\tag{35d}$$

$$\Delta\phi\sum_{j=1}^{N_\phi} r_i\nabla_\phi\left[sin\phi_{j-(1/2)}\left(\bar{q}_1^\phi\right)^n_{ij-(1/2)k}\right]\left(\bar{T}_1\right)^n_{ijk}$$
$$= \frac{\tau_1\Delta\phi}{8k_1\Delta t}\sum_{j=2}^{N_\phi} r_i^2 \sin\phi_{j-(1/2)}\left\{\left[\left(q_1^\phi\right)^{n+1}_{ij-(1/2)k} + \left(q_1^\phi\right)^n_{ij-(1/2)k}\right]^2\right. \tag{35e}$$
$$\left.-\left[\left(q_1^\phi\right)^n_{ij-\frac{1}{2}k} + \left(q_1^\phi\right)^{n-1}_{ij-(1/2)k}\right]^2\right\} + \frac{\Delta\phi}{k_1}\sum_{j=2}^{N_\phi} r_i^2 \sin\phi_{j-(1/2)}\left[\left(\bar{q}_1^\phi\right)^n_{ij-(1/2)k}\right]^2,$$

and:

$$\Delta\theta\sum_{k=1}^{N_\theta} r_i\nabla_\theta\left[\left(\bar{q}_1^\theta\right)^n_{ijk-(1/2)}\right]\left(\bar{T}_1\right)^n_{ijk} = \frac{\tau_1\Delta\theta}{8k_1\Delta t}\sum_{k=1}^{N_\theta} r_i^2 \sin\phi_j\left\{\left[\left(q_1^\theta\right)^{n+1}_{ijk-(1/2)} + \left(q_1^\theta\right)^n_{ijk-(1/2)}\right]^2\right.$$
$$\left.-\left[\left(q_1^\theta\right)^n_{ijk-(1/2)} + \left(q_1^\theta\right)^{n-1}_{ijk-(1/2)}\right]^2\right\} \tag{35f}$$
$$+\frac{\Delta\theta}{k_1}\sum_{k=1}^{N_\theta} r_i^2 \sin\phi_j\left[\left(\bar{q}_1^\theta\right)^n_{ijk-(1/2)}\right]^2.$$

By Cauchy-Schwartz's inequality, we have:

$$8(g^n, r^2\sin\phi(\bar{T}_e)^n) = 2(g^n, r^2\sin\phi[(T_e)^{n+1} + 2(T_e)^n + (T_e)^{n-1}])$$
$$= 2\Delta r\Delta\theta\Delta\varphi\sum_{i=1}^{N_r}\sum_{j=1}^{N_\phi}\sum_{k=1}^{N_\theta}\left(r_i\sqrt{\sin\phi_j}g^n_{ijk}\right)\cdot r_i\sqrt{\sin\phi_j}\left[(T_e)^{n+1}_{ijk} + (T_e)^n_{ijk}\right]$$
$$+2\Delta r\Delta\theta\Delta\varphi\sum_{i=1}^{N_r}\sum_{j=1}^{N_\phi}\sum_{k=1}^{N_\theta}\left(r_i\sqrt{\sin\phi_j}g^n_{ijk}\right)\cdot r_i\sqrt{\sin\phi_j}\left[(T_e)^n_{ijk} + (T_e)^{n-1}_{ijk}\right] \tag{36}$$
$$\leq \frac{1}{C_e}\|r\sqrt{\sin\phi}g^n\|^2 + C_e\|r\sqrt{\sin\phi}[(T_e)^{n+1} + (T_e)^n]\|^2$$
$$+\frac{1}{C_e}\|r\sqrt{\sin\phi}g^n\|^2 + C_e\|r\sqrt{\sin\phi}[(T_e)^n + (T_e)^{n-1}]\|^2.$$

Substituting equations (35a)-(35f) and equation (36) into equation (34), dropping some nonnegative terms, and then using the notations of $F(n)$ and $\Phi(n)$, we obtain:

$$(1 - \Delta t)F(n) \leq (1 + \Delta t)F(n-1) + \Delta t\Phi(n). \tag{37}$$

Thus, we have:

$$
\begin{aligned}
F(n) &\le \frac{(1+\Delta t)}{(1-\Delta t)} F(n-1) + \frac{\Delta t}{(1-\Delta t)} \Phi(n) \\
&\le \frac{(1+\Delta t)}{(1-\Delta t)} \left[\frac{(1+\Delta t)}{(1-\Delta t)} F(n-2) + \frac{\Delta t}{(1-\Delta t)} \Phi(n-1) \right] + \frac{\Delta t}{(1-\Delta t)} \Phi(n) \\
&\le \cdots \\
&\le \left(\frac{1+\Delta t}{1-\Delta t} \right)^n F(0) + \frac{\Delta t}{(1-\Delta t)} \left[1 + \left(\frac{1+\Delta t}{1-\Delta t} \right) + \left(\frac{1+\Delta t}{1-\Delta t} \right)^2 \right. \\
&\quad \left. + \cdots + \left(\frac{1+\Delta t}{1-\Delta t} \right)^{n-1} \right] \max_{0 \le k \le n} \Phi(k) \\
&\le \left(\frac{1+\Delta t}{1-\Delta t} \right)^n F(0) + \frac{\Delta t}{(1-\Delta t)} \left[\frac{1 - \left(\frac{1+\Delta t}{1-\Delta t} \right)^n}{1 - \left(\frac{1+\Delta t}{1-\Delta t} \right)} \right] \max_{0 \le k \le n} \Phi(k) \\
&\le \left(\frac{1+\Delta t}{1-\Delta t} \right)^n F(0) - \frac{1}{2} \left[1 - \left(\frac{1+\Delta t}{1-\Delta t} \right)^n \right] \max_{0 \le k \le n} \Phi(k) \\
&\le \left(\frac{1+\Delta t}{1-\Delta t} \right)^n \left[F(0) + \max_{0 \le k \le n} \Phi(k) \right].
\end{aligned}
\tag{38}
$$

Using the inequalities $(1+\varepsilon)^n \le e^{n\varepsilon} \mathit{for}\ \varepsilon > 0$, and $(1-\varepsilon)^{-1} \le e^{2\varepsilon}$ when $0 < \varepsilon \le \frac{1}{2}$, we let $\varepsilon = \Delta t$ and obtain:

$$
\begin{aligned}
F(n) &\le e^{n\Delta t} \cdot e^{2n\Delta t} \left[F(0) + \max_{0 \le k \le n} \Phi(k) \right] \\
&\le e^{3t_0} \left[F(0) + \max_{0 \le k \le n} \Phi(k) \right],
\end{aligned}
\tag{39}
$$

when $\Delta t \le \frac{1}{2}$. From equation (21) and the assumption of no changes in the initial conditions, we obtain that $F(0) = 0$ and hence $F(n) \le e^{3t_0} \max_{0 \le k \le n} \Phi(k)$, which completes the proof.

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