AN EFFICIENT NUMERICAL PROCEDURE FOR SOLVING A MICROSscale HEAT TRANSPORT EQUATION DURING FEMTOSECOND LASER HEATING OF NANOSCALE METAL FILMS

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ABSTRACT

An alternative discretization and solution procedure is developed for implicitly solving a microscale heat transport equation during femtosecond laser heating of nanoscale metal films. The proposed numerical technique directly solves a single partial differential equation, unlike other techniques available in the literature which split the equation into a system of two equations and then apply discretization. It is shown by von Neumann stability analysis that the proposed numerical method is unconditionally stable. The numerical technique is then extended to three space dimensions, and an overall procedure for computing the transient temperature distribution during short-pulse laser heating of thin metal films is presented. Douglas-Gunn time-splitting and delta-form Douglas-Gunn time-splitting methods are employed to solve the discretized 3-D equations; a simple argument for stability is given for the split equation. The performance of the proposed numerical scheme will be compared with the numerical techniques available in the literature and it is shown that the new formulation is comparably accurate and significantly more efficient. Finally, it is shown that numerical predictions agree with available experimental data during subpicosecond laser heating.

INTRODUCTION

Fourier’s law predicts thermal disturbances propagating at infinite velocities, implying that a thermal disturbance applied at a certain location in a solid medium can be sensed immediately anywhere else in the medium (violating precepts of special relativity). In order to ensure finite propagation of thermal disturbances a hyperbolic heat conduction equation (HHCE) was proposed [1, 2]. It has been shown that in certain situations [3] the HHCE violates the second law of thermodynamics resulting in physically unrealistic temperature distribution such as the temperature overshoot phenomenon observed in a slab subject to a sudden temperature rise on its boundaries. Also, since the classical and hyperbolic models neglect the thermalization time (time for electrons and lattice to reach thermal equilibrium) and relaxation time of the electrons, their applicability to very short pulse laser heating [4, 5] becomes questionable.

Anisimov et al. [6] proposed a two-step model to describe the electron temperature $T_e$ and the lattice temperature $T_l$ during short-pulse laser heating of metals. Later, Qiu and Tien [4, 5] rigorously derived the hyperbolic two-step model from the Boltzmann transport equation for electrons. They numerically solved the equations of this model in the context of a 96/fs duration laser pulse irradiating a thin film of thickness 0.1 µm. Predicted temperature change of the electron gas during the picosecond transient agreed well with experimental data, supporting the validity of the hyperbolic two-step model for describing heat transfer mechanisms during short-pulse laser heating of metals.

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Tzou proposed the dual phase-lag (DPL) model [7–10] that reduces to diffusion, thermal wave, phonon-electron interaction [4,5], and pure phonon scattering [11] models under special values of $\tau_q$ and $\tau_T$. Over the years, various numerical methods have been investigated for the solving the DPL equation. Most early numerical studies involved only the 1-D equation, often using explicit discretization [20]. Recent studies have begun to consider 2-D and 3-D DPL equations, with implicit discretizations [15, 16, 18, 19]. Dai and Nassar [12–16] have developed an implicit finite-difference scheme in which the DPL equation is discretized using the Crank-Nicolson scheme and solved sequentially. Dai shows by the discrete energy method [12–17] that the scheme is unconditionally stable. Dai and Zhang and Zhao [18, 19] have employed the iterative techniques Gauss–Seidel, successive overrelaxation (SOR), conjugate gradient (CG), and preconditioned conjugate gradient (PCG) to solve a Dirichlet problem for the 3-D DPL equation. A recent study [23] has shown that applying Neumann boundary conditions results in a hyperbolic heat conduction equation. On the other hand, $\tau_T = 0$ results in a hyperbolic heat conduction equation.

**BRIEF REVIEW OF ORIGINS OF DPL EQUATION**

The dual phase lag concept is represented in [8] as

$$q(r,t + \tau_q) = -k \nabla T(r,t + \tau_q), \quad (1)$$

where $\tau_T$ is the phase lag of the temperature gradient, and $\tau_q$ is the phase lag of the heat flux vector. First order Taylor expansion of Eq. (1) gives

$$q(r,t) + \tau_q \frac{\partial q(r,t)}{\partial t} = -k \left( \nabla T(r,t) + \tau_T \frac{\partial (\nabla T(r,t))}{\partial t} \right). \quad (2)$$

Equation (2) coupled with the equation of energy conservation yields the DPL microscale heat conduction equation

$$\frac{\tau_q}{\alpha} \frac{\partial^2 T}{\partial t^2} + \frac{1}{\alpha} \frac{\partial T}{\partial t} - \tau_T \frac{\partial (\nabla^2 T)}{\partial t} = \nabla^2 T. \quad (3)$$

When $\tau_T$ and $\tau_q$ become zero, Eq. (3) collapses to the classical parabolic heat conduction equation. The initial and boundary conditions can be written as

$$\theta(x,t) = \frac{T(x,t) - T_i}{T_w - T_i}, \quad \beta = \frac{t}{\tau_q}, \quad \delta = \frac{x}{\sqrt{\alpha \tau_q}}, \quad (4)$$

Eq. (3) becomes

$$\frac{\partial^2 \theta}{\partial \delta^2} + Z \frac{\partial^3 \theta}{\partial \delta^3 \beta} = \frac{\partial^2 \theta}{\partial \beta^2} + \frac{\partial \theta}{\partial \beta}, \quad \text{with} \quad Z = \frac{\tau_T}{\tau_q}. \quad (5)$$

The initial and boundary conditions can be written as

$$\theta(\delta,0) = 0, \quad \frac{\partial \theta}{\partial \delta}(\delta,0) = 0 \quad \text{for} \quad \delta \in [0,\infty), \quad (6)$$

and

$$\theta(0,\beta) = 1 \quad \text{for} \quad \beta > 0, \quad \frac{\partial \theta}{\partial \delta}(\delta,\beta) = 0 \quad \delta \to \infty, \quad (7)$$

respectively.

Expressing (5) in terms of $x$ and $t$ leads to

$$\frac{\partial T}{\partial t} + \frac{\partial^2 T}{\partial t^2} - Z \frac{\partial}{\partial t} \left( \frac{\partial^2 T}{\partial x^2} \right) = \frac{\partial^2 T}{\partial x^2}. \quad (8)$$
Applying trapezoidal integration to Eq. (8) results in

\[
\begin{align*}
T_m^{n+1} - T_m^n + \left(\frac{\partial T}{\partial t}\right)_m^n + \left(\frac{\partial T}{\partial t}\right)_m^{n+1} & = -Z \left[ \left(\frac{\partial^2 T}{\partial x^2}\right)_m^{n} - \left(\frac{\partial^2 T}{\partial x^2}\right)_m^{n+1} \right] \\
& = \frac{\Delta t}{2} \left[ \left(\frac{\partial^2 T}{\partial x^2}\right)_m^{n+1} + \left(\frac{\partial^2 T}{\partial x^2}\right)_m^{n} \right].
\end{align*}
\]

(9)

We next apply a second-order backward difference for the time derivative at \( n + 1 \) and a centered difference for the time derivative at \( n \). The second-order derivatives in space are approximated using a centered-difference scheme:

\[
\begin{align*}
\left(\frac{\partial T}{\partial t}\right)_m^n & = \frac{1}{2\Delta t} \left[ 3T_m^{n+1} - 4T_m^n + T_m^{n-1} \right], \quad (10a) \\
\left(\frac{\partial T}{\partial t}\right)_m^{n+1} & = \frac{1}{2\Delta t} \left[ T_m^{n+1} - T_m^{n-1} \right], \quad (10b) \\
\frac{\partial^2 T}{\partial x^2}_m & = \frac{1}{\Delta x^2} \left[ T_m^{n+1} - 2T_m^n + T_m^{n-1} \right]. \quad (10c)
\end{align*}
\]

The discretization shown in Eqs. (10a)–(10c) renders the numerical scheme globally first-order accurate in time and second order accurate in space. After plugging Eq. (10) into Eq. (9) we obtain

\[
\begin{align*}
T_m^{n+1} - T_m^n + \left( \frac{1}{2\Delta t} \left[ 3T_m^{n+1} - 4T_m^n + T_m^{n-1} \right] \right) \\
- \left( \frac{1}{2\Delta t} \left[ T_m^{n+1} - T_m^{n-1} \right] \right) \\
- \frac{Z}{\Delta x^2} \left( \left[ T_m^{n+1} - 2T_m^n + T_m^{n-1} \right] - \left[ T_m^n - 2T_m^{n+1} + T_m^{n-1} \right] \right) \\
= \frac{\Delta t}{2\Delta x^2} \left( \left[ T_m^{n+1} - 2T_m^n + T_m^{n-1} \right] + \left[ T_m^n - 2T_m^{n+1} + T_m^{n-1} \right] \right) \quad (11)
\end{align*}
\]

After simplifications and rearrangement we obtain

\[
C_4 \left( T_{m-1}^{n+1} + T_{m+1}^{n+1} \right) + C_5 T_m^{n+1} = C_6 \left( T_{m-1}^n + T_{m+1}^n \right) + C_7 T_m^n - \frac{1}{\Delta t} T_m^{n-1}, \quad (12)
\]

where,

\[
\begin{align*}
C_4 & = - \left( Z + \frac{\Delta t}{2} \right) \frac{1}{\Delta x^2}, \quad C_6 = - \left( Z - \frac{\Delta t}{2} \right) \frac{1}{\Delta t^2}, \quad \left(13a\right) \\
C_5 & = \left( Z + \frac{\Delta t}{2} \right) \frac{2}{\Delta x^2} + \left( 1 + \frac{1}{\Delta t} \right), \quad \left(13b\right) \\
C_7 & = - \left( Z + \frac{\Delta t}{2} \right) \frac{2}{\Delta x^2} + \left( 1 + \frac{2}{\Delta t} \right). \quad \left(13c\right)
\end{align*}
\]

Notice that Eq. (12) is three-level in time. The right-hand side of Eq. (12) is a tridiagonal consists of known values, the implicit part of Eq. (12) is and is solved using familiar LU decomposition.

**STABILITY ANALYSIS**

We analyze the stability of the above scheme via a von Neumann analysis. Because the Eq. (12) is a three-level difference scheme, the von Neumann condition supplies only a necessary (and not sufficient) stability requirement in general. For the present problem we define \( \nu_m^{n+1} = T_m^n \) and replace Eq. (12) by the system

\[
C_4 \left( T_{m-1}^{n+1} + T_{m+1}^{n+1} \right) + C_5 T_m^{n+1} = C_6 \left( T_{m-1}^n + T_{m+1}^n \right) + C_7 T_m^n - \frac{1}{\Delta t} \nu_m^{n}, \quad (14)
\]

For \( \beta \in \mathbb{R} \) we can write

\[
T_{m+1}^n = e^{\beta h} T_m^n, \quad \text{and} \quad T_{m-1}^n = e^{-\beta h} T_m^n. \quad (16)
\]

Then

\[
C_4 \left( e^{\beta h} + e^{-\beta h} \right) T_m^{n+1} + C_5 T_m^{n+1} = C_6 \left( e^{\beta h} + e^{-\beta h} \right) T_m^n + C_7 T_m^n - \frac{1}{\Delta t} \nu_m^{n}, \quad (17)
\]

\[
\nu_m^{n+1} = T_m^n. \quad (18)
\]

After simplifications we have

\[
\nu_m^{n+1} = \frac{C_6 (2 \cos \beta h) + C_7}{C_4 (2 \cos \beta h) + C_5} T_m^n - \frac{1}{\Delta t} \nu_m^{n}, \quad (19)
\]
which, in matrix form can be written as

\[
\begin{bmatrix}
  T_{m}^{n+1} \\
  v_{m}^{n+1}
\end{bmatrix} =
\begin{bmatrix}
  C_6(2\cos \beta h) + C_7 & -1 \\
  C_4(2\cos \beta h) + C_5 & 1
\end{bmatrix}
\begin{bmatrix}
  T_{m}^{n} \\
  v_{m}^{n}
\end{bmatrix}.  
\] (21)

We know that the error vector must satisfy this same equation. Denoting this by \( z_{m}^{n} \in \mathbb{R}^2 \), we see that \( z_{m}^{n+1} = C z_{m}^{n} \), where

\[
C =
\begin{bmatrix}
  C_6(2\cos \beta h) + C_7 & -1 \\
  C_4(2\cos \beta h) + C_5 & 1
\end{bmatrix}
\] (22)

is the amplification matrix for the present scheme. The von Neumann necessary condition for stability is

\[
||C|| \leq 1, 
\] (23)

where \( || \cdot || \) denotes the spectral norm. Hence, we need to calculate the eigenvalues of \( C \) to analyze the stability of the method. The characteristic polynomial is

\[
\lambda^2 - \left[ \frac{C_6(2\cos \beta h) + C_7}{C_4(2\cos \beta h) + C_5} \right] \lambda + \frac{1}{\Delta t (C_4(2\cos \beta h) + C_5)} = 0
\] (24)

which has roots

\[
\lambda_{\pm} = \frac{C_6(2\cos \beta h) + C_7 \pm \sqrt{(C_6(2\cos \beta h) + C_7)^2 - 4\frac{1}{\Delta t (C_4(2\cos \beta h) + C_5)}}}{2}
\] (25)

We must determine the larger of these, and from the requirement

\[
\max(|\lambda_+|, |\lambda_-|) \leq 1, 
\] (26)

establish permissible bounds on \( \Delta t \) and \( \Delta x \). Since it is very tedious to solve Eq. (25) analytically, we solve it numerically by plugging different combinations of \( \Delta t \) and \( \Delta x \) for different wave numbers \( \beta \). Figure 1 shows the distribution of \( \lambda \) for different values of \( \Delta t \) and \( \Delta x \) at wave numbers \( \beta = 1, 4, 7 \) and \( Z = 10 \). From the figure we can see that \( \max(|\lambda_+|) \leq 1 \). It is also found that \( \max(|\lambda_-|) \leq 1 \) even though we have not shown it here. Tests were conducted for different values of \( Z \) and it was found that the stability requirement Eq. (26) is satisfied for all the values of \( Z \). This suggests that the proposed numerical scheme is unconditionally stable. The stability requirement is also met for \( Z = 0 \) (hyperbolic case) and \( Z = 1 \) (parabolic case) implying that the numerical scheme is unconditionally stable and the stability analysis can be applied for both parabolic and hyperbolic models.

**NUMERICAL SCHEME FOR SOLVING 3-D DPL EQUATION**

The governing equation used to describe the thermal behavior of microstructures in 3D is expressed as [7]

\[
\frac{\tau q}{\alpha \frac{\partial^2 T}{\partial t^2}} + \frac{1}{\alpha \frac{\partial T}{\partial t}} - \tau \frac{\partial (\nabla^2 T)}{\partial t} = \nabla^2 T + \frac{1}{k} \left( S + \tau q \frac{\partial S}{\partial t} \right). 
\] (27)
obtained by considering an alternate form of laser light intensity

describes laser heating of the electron-phonon system from a thermal
results compared to the one used by Qiu and Tien [4, 5]:

\[ S(x, t) = 0.94J \left[ 1 - \frac{R}{t_p \delta} \right] \exp \left( -\frac{x}{\delta} \frac{1.992 | t - 2t_p |}{t_p} \right) \] (28)

where laser fluence \( J = 13.7J/m^2 \), \( t_p = 96fs \) (1fs = \( 10^{-15}s \)) describes laser heating of the electron-phonon system from a thermalization state, penetration depth \( \delta = 15.3nm \) (1nm = \( 10^{-9}m \)), and reflectivity \( R = 0.93 \) [20]. The above heat source term was obtained by considering an alternate form of laser light intensity function \( I(t) \); [7–10]

\[ I(t) = I_0 e^{-a|t_p|} \quad \text{with} \quad a = 1.992, \quad t_p \geq 0 \] (29)

gives an excellent autocorrelation of laser pulse with experimental results compared to the one used by Qiu and Tien [4, 5]:

\[ I(t) = I_0 e^{-\psi(\frac{t}{t_p})^2}, \quad \psi = 4 \ln(2) \approx 2.77, \] (30)

with \( \psi \) being a constant. In three dimensions, we have extended this heat source term to

\[ S(r, t) = 0.94J \left[ 1 - \frac{R}{t_p \delta} \right] \exp \left( -\frac{(x - \frac{L_x}{2})^2 + (y - \frac{L_y}{2})^2}{2\tau^2} - \frac{z}{\delta} \frac{1.992 | t - 2t_p |}{t_p} \right) \] (31)

where \( L_x \) and \( L_y \) are the length and width of the metal film respectively, and \( r_\circ \) is the thickness of the laser beam. Applying trapezoidal integration to Eq. (27) we obtain

\[ \frac{\tau_f}{\alpha} \left[ T_{i,j,k}^{n+1} - T_{i,j,k}^n \right] + \frac{1}{\alpha} \left[ \left( \frac{\partial T}{\partial t} \right)_{i,j,k}^{n+1} - \left( \frac{\partial T}{\partial t} \right)_{i,j,k}^n \right] = \frac{\Delta t}{2} \left[ (\nabla^2 T)^{n+1} + (\nabla^2 T)^n \right] \\
+ \frac{\Delta t}{k \epsilon} \left[ \frac{S_{i,j,k}^{n+1}}{2} + S_{i,j,k}^n \right] \] (32)

Just as was done for the 1-D case, above, we apply second-order backward difference for the time derivative at \( n+1 \) and a centered difference for the time derivative at \( n \). Second-order derivatives in space are approximated using the usual centered-difference scheme. Thus we have

\[ \left( \frac{\partial^2 T}{\partial x^2} \right)_{i,j,k} = \frac{1}{\Delta x^2} \left[ T_{i+1,j,k} + T_{i-1,j,k} - 2T_{i,j,k} \right] \] (33a)

\[ \left( \frac{\partial^2 T}{\partial y^2} \right)_{i,j,k} = \frac{1}{\Delta y^2} \left[ T_{i,j+1,k} + T_{i,j-1,k} - 2T_{i,j,k} \right] \] (33b)

\[ \left( \frac{\partial^2 T}{\partial z^2} \right)_{i,j,k} = \frac{1}{\Delta z^2} \left[ T_{i,j,k+1} + T_{i,j,k-1} - 2T_{i,j,k} \right] \] (33c)

After substituting Eq. (34) into Eq. (32), followed by further simplifications, we obtain

\[ C_4 T_{i,j,k}^{n+1} + C_5 \left( T_{i,j+1,k}^{n+1} + T_{i,j-1,k}^{n+1} \right) + C_6 \left( T_{i+1,j,k}^{n+1} + T_{i-1,j,k}^{n+1} \right) \\
+ C_7 \left( T_{i,j,k+1}^{n+1} + T_{i,j,k-1}^{n+1} \right) = F^n, \] (34)

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where

\[ F^n = C_8 T^n_{i,j,k} + C_9 \left( T^n_{i+1,j,k} + T^n_{i-1,j,k} \right) \]
\[ + C_{10} \left( T^n_{i,j+1,k} + T^n_{i,j-1,k} \right) + C_{11} \left( T^n_{i,j,k+1} + T^n_{i,j,k-1} \right) \]
\[ - \frac{\tau_q}{\alpha \Delta t} T^{n-1}_{i,j,k} + \Delta G^n \]  
\[ (35) \]

\[ C_5 = - \left( \tau_T + \frac{\Delta t}{2} \right) \frac{1}{\Delta x^2}, \quad C_6 = - \left( \tau_T + \frac{\Delta t}{2} \right) \frac{1}{\Delta y^2}, \]  
\[ C_7 = - \left( \tau_T + \frac{\Delta t}{2} \right) \frac{1}{\Delta z^2}, \]  
\[ C_8 = \left( \frac{1}{\alpha} + \frac{2 \tau_q}{\alpha \Delta t} \right) - 2 (C_9 + C_{10} + C_{11}), \]  
\[ C_9 = \left( -\tau_T + \frac{\Delta t}{2} \right) \frac{1}{\Delta x^2}, \quad C_{10} = \left( -\tau_T + \frac{\Delta t}{2} \right) \frac{1}{\Delta y^2}, \]  
\[ C_{11} = \left( -\tau_T + \frac{\Delta t}{2} \right) \frac{1}{\Delta z^2}, \]  
\[ G^n = \left[ \frac{S^n_{i,j+1,k} + S^n_{i,j-1,k}}{2} + \tau_q \frac{S^n_{i+1,j,k} - S^n_{i,j,k}}{2} \right]. \]  
\[ (36a) \quad (36b) \quad (36c) \quad (36d) \quad (36e) \quad (36f) \quad (36g) \]

Equation (35) is three-level in time, and it can be efficiently solved using Douglas–Gunn time splitting method [21]. Divide both sides of Eq. (35) by

\[ \frac{1}{\alpha} + \frac{\tau_q}{\alpha \Delta t} \]  
\[ (37) \]

to obtain

\[ [1 - 2C'_5 - 2C'_6 - 2C'_7] T^{n+1}_{i,j,k} + C'_5 \left( T^{n+1}_{i+1,j,k} + T^{n+1}_{i-1,j,k} \right) \]
\[ + C'_6 \left( T^{n+1}_{i,j+1,k} + T^{n+1}_{i,j-1,k} \right) + C'_7 \left( T^{n+1}_{i,j,k+1} + T^{n+1}_{i,j,k-1} \right) = S^n, \]  
\[ (38) \]

where,

\[ S^n = \frac{F^n}{\frac{1}{\alpha} + \frac{\tau_q}{\alpha \Delta t}}, \quad C'_5 = \frac{C_5}{\frac{1}{\alpha} + \frac{\tau_q}{\alpha \Delta t}}, \]  
\[ (39a) \]
\[ C'_6 = \frac{C_6}{\frac{1}{\alpha} + \frac{\tau_q}{\alpha \Delta t}}, \quad C'_7 = \frac{C_7}{\frac{1}{\alpha} + \frac{\tau_q}{\alpha \Delta t}}, \]  
\[ (39b) \quad (39c) \]

Observe that this is now in the general form required for construction of a multilevel Douglas and Gunn time splitting [21]. We now split Eq. (38) into three equations corresponding to \( x \), \( y \) and \( z \) directions:

\[ (1 - 2C'_5) T^{n+1}_{i,j,k} + C'_5 \left( T^{n+1}_{i+1,j,k} + T^{n+1}_{i-1,j,k} \right) = S^n \]  
\[ (40a) \]
\[ (-2C'_6) T^{n+1}_{i,j,k} + C'_6 \left( T^{n+1}_{i,j+1,k} + T^{n+1}_{i,j-1,k} \right) = 0 \]  
\[ (40b) \]
\[ (-2C'_7) T^{n+1}_{i,j,k} + C'_7 \left( T^{n+1}_{i,j,k+1} + T^{n+1}_{i,j,k-1} \right) = 0. \]  
\[ (40c) \]

Applying Douglas–Gunn time-splitting technique to Eqs. (40a)–(40c) we have

\[ (I + A_x) T^{(1)} = S^n - A_y T^n - A_z T^n \]  
\[ (41a) \]
\[ (I + A_y) T^{(2)} = T^{(1)} - A_y T^n \]  
\[ (41b) \]
\[ (I + A_z) T^{(3)} = T^{(2)} - A_z T^n, \]  
\[ (41c) \]

where

\[ I + A_x = (1 - 2C'_5) T^{n+1}_{i,j,k} + C'_5 \left( T^{n+1}_{i+1,j,k} + T^{n+1}_{i-1,j,k} \right) \]  
\[ (42a) \]
\[ I + A_y = (1 - 2C'_6) T^{n+1}_{i,j,k} + C'_6 \left( T^{n+1}_{i,j+1,k} + T^{n+1}_{i,j-1,k} \right) \]  
\[ (42b) \]
\[ I + A_z = (1 - 2C'_7) T^{n+1}_{i,j,k} + C'_7 \left( T^{n+1}_{i,j,k+1} + T^{n+1}_{i,j,k-1} \right) \]  
\[ (42c) \]

\( T^{(1)}, T^{(2)} \) and \( T^{(3)} \) denote intermediate estimates of \( T^{n+1} \) with \( T^{n+1} = T^{(3)} \). The implicit part \( T^{n+1} \) of the above equations (42) is tridiagonal, and is thus easily solved using LU decomposition.

Now applying \( \delta \)-form Douglas–Gunn time-splitting [21] we can represent Eqs. (41) as follows

\[ (I + A_x) T^{(1)} = S^n - (I + A) T^n \]  
\[ (43a) \]
\[ (I + A_y) T^{(2)} = T^{(1)} \]  
\[ (43b) \]
\[ (I + A_z) T^{(3)} = T^{(2)} \]  
\[ (43c) \]
\[ T^{n+1} = T^{(3)} + T^n, \]  
\[ (43d) \]

where \( A = I + A_x + A_y + A_z \). We remark that this form is the most efficient of the forms found in the literature. Again, the implicit part of the above equations (44) is tridiagonal, and is thus easily solved using LU decomposition.

**COMPUTED RESULTS FOR SPECIFIC PROBLEM(S)**

Figure 2 shows the comparison between the numerical (explicit and implicit scheme), analytical [20] and the experimental
results of Brorson et al. [22] and Qiu and Tien [4,5] corresponding to the front surface transient response for a 0.1µm thick gold film. The laser heat source term given by Eq. (28) is used for this purpose. The thermal properties ($\alpha = 1.2 \times 10^{-4} m^2 s^{-1}$, $k = 315 W m^{-1} K^{-1}$, $\tau_T = 90 ps$, $\tau_q = 8.5 ps$) are assumed to be constant. The temperature change is normalized by the maximum value that occurs during the short-time transient. The results from the present numerical scheme compare well with experimental and analytical results. The CV wave and the parabolic models neglect the microstructural interaction effect in the short-time transient, rendering an overestimated temperature in the transient response as seen in the figure.

Figures 3–6 show the comparison of transient temperature distribution caused by a pulsating laser beam of 200nm diameter heating the top surface of the gold film (500nm long and wide and 100nm thick) at various locations of the film every 0.3ps, predicted by DPL, hyperbolic and parabolic heat conduction models. The energy absorption rate given by Eq. (31) is used to model three-dimensional laser heating. As explained earlier, $\tau_T = 90 ps$, $\tau_q = 8.5 ps \rightarrow$ DPL model; $\tau_T = 0$, $\tau_q = 0 \rightarrow$ parabolic model and $\tau_T = 8.5 ps$, $\tau_q = 0 \rightarrow$ hyperbolic model. The CV wave model and the diffusion model predict a higher temperature level in the heat affected zone than the DPL model, but the penetration depth is much shorter owing to the formation of the thermally undisturbed zone. The heat affected zone is significantly larger for the DPL model than the other models because the microstructural interaction effect incorporated in the DPL model, reflected by the delayed time for establishing the temperature gradient across a material volume ($\tau_T$) significantly extends the physical domain of the thermal penetration depth.

Following the same procedure for 1-D case the stability of the 3D numerical scheme has been performed using von Neumann analysis (not shown here). Stability properties of the Douglas–Gunn splitting method are not completely known. It is clear that von Neumann analysis will provide only necessary conditions for stability in this case.

Table 1 [23] shows the CPU time in seconds taken for the entire simulation for the explicit, Gauss–Seidel, conjugate gra-
dient, Douglas–Gunn time-splitting and δ-form Douglas–Gunn time-splitting methods using different values of the spatial discretization parameter $N$. From the table we can observe that when $N = 21$ the explicit method consumes less CPU time than the rest of the numerical techniques but for the spatial discretization parameter $N > 21$, all implicit methods except the Gauss–Seidel method perform better than the explicit method employed in this research. We are still investigating the reason for the poor performance of the Gauss–Seidel method compared to the explicit method. The δ-form Douglas-Gunn time-splitting used in the present numerical scheme consumes the least CPU time compared to all other numerical techniques available in the literature for large values of $N$.

**SUMMARY AND CONCLUSIONS**

We have developed an unconditionally stable implicit finite-difference scheme of the Crank–Nicolson type for solving the one-dimensional DPL equation as shown by the von Neumann stability analysis. Grid function convergence tests were performed to test the convergence of the numerical solution. The numerical technique was then extended to three dimensional geometry, and a numerical procedure for computing the transient temperature distribution during short pulse laser heating of thin films has been presented. The discretized 3-D microscale DPL equation has been solved using Douglas–Gunn time-splitting method and δ-form Douglas–Gunn time-splitting method. The present numerical scheme, employing the δ-form Douglas-Gunn time-splitting outperforms all the numerical techniques known to us in terms of computational time taken to complete the simulation.

**REFERENCES**


Numerical techniques | Total CPU time taken in seconds
--- | ---
Explicit Scheme | N=21 4.88 147.62 450.26 7920.00  
N=41 14.14 253.42 627.03 11343.06  
N=51 12.33 124.83 270.3 3614.69  
N=101 D-G time-splitting 9.24 82.44 165.76 1506.38
δ-form D-G 8.54 70.5 140.92 1344.4

Table 1. Performance comparison of different numerical methods for solving the discretized 3-D DPL equation [23].


