A generalized two-cycle componentwise splitting method for solving three-dimensional parabolic differential equations with variable coefficients on multilayers

Received July 1996
Revised November 1996

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1. Introduction

Parabolic differential equations in three dimensions and on multilayers often arise in engineering processes. An example is the rapid thermal processing (RTP). With the decrease of dimensional scale, one of the essential problems in the RTP is to control the dynamical temperature in order to reduce temperature nonhomogenenities during heating up and cooling down which are responsible for layer nonhomogenenities and slip generation (Leitz *et al.,* 1993; Lie *et al.,* 1993). Another example is x-ray lithography, an important technology in micromanufacturing (Ameel *et al.*, 1994). The process consists of x-ray irradiation of a photoresist, such as polymethylmethacrylate (PMMA), deposited on a silicon substrate. Prediction of the temperature distribution in three dimensions in the photoresist and substrate is essential for determining the effect of high flux x-ray exposure on distortions in the photoresist owing to thermal expansion and on bonding between resist and substrate. A thorough understanding of the problem has been hampered by the difficulties involved in solving the differential equations describing temperature profiles in multilayers (Cole and McGahan, 1993; Kant, 1988; Madison and McDaniel, 1989). These difficulties include the unknown value at the interface between layers, and the small spatial scale measured in micron. In applications of numerical methods for solving parabolic differential equations on multilayers, the common approach, to overcome the interface problem, is to apply the iteration method. As such, the unknown value at the interface between layers is replaced by the value at the previous time step, and is iterated until the solution is obtained. However, the iteration method in the three-dimensional case requires too much computational time. Furthermore, the small spatial scale results in a fine spatial grid size

This research is supported by a Louisiana Educational Quality Support Fund (LEQSF) grant. Contract No: 72- 6000792.

International Journal of Numerical Methods for Heat & Fluid Flow
Vol. 7 No. 8, 1997, pp. 863–879.

compared with the time increment. Thus, the mesh ratio is large, which causes many second-order accurate schemes, such as the Crank-Nicolson scheme and two-cycle componentwise splitting method (Marchuk, 1989), to converge slowly to the steady-state solution. Recently, we developed a generalized three-dimensional Douglas ADI scheme for solving three-dimensional parabolic differential equations on multilayers (Dai and Nassar, 1997). It avoids iteration at each time step and is suited for either simulating fast transient phenomena or for numerical computations on fine spatial meshes. To overcome the problem with the unknown value at the interface between layers, the generalized "divide and conquer" procedure for solving tridiagonal linear systems is applied. As such, the computational procedure is simple and efficient.

In this paper, we generalize our three-dimensional numerical procedure to the case of solving parabolic differential equations with variable coefficients on multilayers. For many practical problems, conductivity is not constant, in which case the heat conduction equations have variable coefficients. Since the differential operators with variable coefficients are not commutative, the generalized Douglas ADI scheme cannot be used. Therefore, we develop a generalized two-cycle componentwise splitting scheme, which is unconditionally stable, almost second-order accurate and is suitable for either simulating fast transient phenomena or for numerical computations on fine spatial meshes. A numerical model for multilayers that employ this scheme is formulated.

2. Generalized two-cycle componentwise splitting scheme

Consider the three-dimensional parabolic equation with variable coefficients

$$\frac{\partial U}{\partial t} = \frac{\partial}{\partial x}\left(K(x, y, z, t)\frac{\partial U}{\partial x}\right) + \frac{\partial}{\partial y}\left(K(x, y, z, t)\frac{\partial U}{\partial y}\right) + \frac{\partial}{\partial z}\left(K(x, y, z, t)\frac{\partial U}{\partial z}\right) + f(x, y, z, t), \tag{1}$$

where $k(x, y, z, t) \geq a > 0$ is the diffusivity coefficient. Let

$$AU \equiv -\frac{\partial}{\partial x}\left(K\frac{\partial U}{\partial x}\right) - \frac{\partial}{\partial y}\left(K\frac{\partial U}{\partial y}\right) - \frac{\partial}{\partial z}\left(K\frac{\partial U}{\partial z}\right) = A_1U + A_2U + A_3U, \tag{2}$$

where

$$A_1U = -\frac{\partial}{\partial x}\left(K\frac{\partial U}{\partial x}\right), \quad A_2U = -\frac{\partial}{\partial y}\left(K\frac{\partial U}{\partial y}\right) \quad \text{and} \quad A_3U = -\frac{\partial}{\partial z}\left(K\frac{\partial U}{\partial z}\right).$$

Obviously, $A_iA_jU \neq A_jA_iU$, $i \neq j$, i.e. operators A_α, $\alpha = 1, 2, 3$, are not commutative.

We denote u_{ijk}^n as the approximation to $U(i\Delta x, j\Delta y, k\Delta z, n\Delta t)$, where Δx, Δy and Δz are the grid sizes in the x, y and z directions respectively, Δt is the time increment $i = 0, \ldots, N_x + 1$, $j = 0, \ldots, N_y + 1$, and $k = 0, \ldots, N_z + 1$. For convenience, we write $\Delta x = \Delta y = \Delta z = h$ and $\Delta t = \tau$. We use the centred-difference equation,

$$\Lambda_1^n u_{ijk}^n = -\frac{1}{h}\left(K^n_{i+\frac{1}{2}jk} \frac{u^n_{i+1jk} - u^n_{ijk}}{h} - K^n_{i-\frac{1}{2}jk} \frac{u^n_{ijk} - u^n_{i-1jk}}{h} \right),$$

to approximate, $\partial/\partial x \left(K \times \partial U/\partial x \right)$ where $\wedge_1^n$ represents a tridiagonal matrix, and so on. Then, the three-dimensional two-cycle componentwise splitting scheme can be written as follows (Marchuk, 1989):

$$\left[I + \tfrac{1}{2}\tau \Lambda_1^n \right] u^{n-\frac{3}{4}} = \left[I - \tfrac{1}{2}\tau \Lambda_1^n \right] u^{n-1}, \tag{3a}$$

$$\left[I + \tfrac{1}{2}\tau \Lambda_2^n \right] u^{n-\frac{2}{4}} = \left[I - \tfrac{1}{2}\tau \Lambda_2^n \right] u^{n-\frac{3}{4}}, \tag{3b}$$

$$\left[I + \tfrac{1}{2}\tau \Lambda_3^n \right] u^{n-\frac{1}{4}} = \left[I - \tfrac{1}{2}\tau \Lambda_3^n \right] u^{n-\frac{2}{4}}, \tag{3c}$$

$$u^{n+\frac{1}{4}} = u^{n-\frac{1}{4}} + 2\tau f^n, \tag{3d}$$

$$\left[I + \tfrac{1}{2}\tau \Lambda_3^n \right] u^{n+\frac{2}{4}} = \left[I - \tfrac{1}{2}\tau \Lambda_3^n \right] u^{n+\frac{1}{4}}, \tag{3e}$$

$$\left[I + \tfrac{1}{2}\tau \Lambda_2^n \right] u^{n+\frac{3}{4}} = \left[I - \tfrac{1}{2}\tau \Lambda_2^n \right] u^{n+\frac{2}{4}}, \tag{3f}$$

$$\left[I + \tfrac{1}{2}\tau \Lambda_1^n \right] u^{n+1} = \left[I - \tfrac{1}{2}\tau \Lambda_1^n \right] u^{n+\frac{3}{4}}, \tag{3g}$$

where I is an identity matrix. The above scheme is unconditionally stable and second-order accurate. Based on the idea in Dai and Nassar (1997) and Samarskii and Vabishchevich (1994), we develop a generalized two-cycle componentwise splitting scheme as follows:

$$\left[I + \tfrac{1}{2}(1+\varepsilon)\tau \Lambda_1^n \right] u^{n-\frac{3}{4}} = \left[I - \tfrac{1}{2}(1-\varepsilon)\tau \Lambda_1^n \right] u^{n-1}, \tag{4a}$$

$$\left[I + \tfrac{1}{2}(1+\varepsilon)\tau \Lambda_2^n \right] u^{n-\frac{2}{4}} = \left[I - \tfrac{1}{2}(1-\varepsilon)\tau \Lambda_2^n \right] u^{n-\frac{3}{4}}, \tag{4b}$$

$$\left[I + \tfrac{1}{2}(1+\varepsilon)\tau \Lambda_3^n \right] u^{n-\frac{1}{4}} = \left[I - \tfrac{1}{2}(1-\varepsilon)\tau \Lambda_3^n \right] u^{n-\frac{2}{4}}, \tag{4c}$$

$$u^{n+\frac{1}{4}} = u^{n-\frac{1}{4}} + 2\tau f^n, \tag{4d}$$

$$\left[I + \tfrac{1}{2}(1+\varepsilon)\tau\Lambda_3^n\right]u^{n+\frac{2}{4}} = \left[I - \tfrac{1}{2}(1-\varepsilon)\tau\Lambda_3^n\right]u^{n+\frac{1}{4}}, \tag{4e}$$

$$\left[I + \tfrac{1}{2}(1+\varepsilon)\tau\Lambda_2^n\right]u^{n+\frac{3}{4}} = \left[I - \tfrac{1}{2}(1-\varepsilon)\tau\Lambda_2^n\right]u^{n+\frac{2}{4}}, \tag{4f}$$

$$\left[I + \tfrac{1}{2}(1+\varepsilon)\tau\Lambda_1^n\right]u^{n+1} = \left[I - \tfrac{1}{2}(1-\varepsilon)\tau\Lambda_1^n\right]u^{n+\frac{3}{4}}, \tag{4g}$$

where $\varepsilon \leq 1$ is a small positive number. When $\varepsilon = 0$, the above scheme reduces to the scheme (3).

For investigating the stability of the system, we eliminate the medium values and simplify the scheme (4) as follows:

$$\begin{aligned}
u^{n+1} = {} & \left[I+\tfrac{1}{2}(1+\varepsilon)\tau\Lambda_1^n\right]^{-1}\left[I - \tfrac{1}{2}(1-\varepsilon)\tau\Lambda_1^n\right] \\
& \cdot\left[I+\tfrac{1}{2}(1+\varepsilon)\tau\Lambda_2^n\right]^{-1}\left[I - \tfrac{1}{2}(1-\varepsilon)\tau\Lambda_2^n\right] \\
& \cdot\left[I+\tfrac{1}{2}(1+\varepsilon)\tau\Lambda_3^n\right]^{-1}\left[I - \tfrac{1}{2}(1-\varepsilon)\tau\Lambda_3^n\right] \\
& \cdot\left[I+\tfrac{1}{2}(1+\varepsilon)\tau\Lambda_3^n\right]^{-1}\left[I - \tfrac{1}{2}(1-\varepsilon)\tau\Lambda_3^n\right] \\
& \cdot\left[I+\tfrac{1}{2}(1+\varepsilon)\tau\Lambda_2^n\right]^{-1}\left[I - \tfrac{1}{2}(1-\varepsilon)\tau\Lambda_2^n\right] \\
& \cdot\left[I+\tfrac{1}{2}(1+\varepsilon)\tau\Lambda_1^n\right]^{-1}\left[I - \tfrac{1}{2}(1-\varepsilon)\tau\Lambda_1^n\right]u^{n-1} \\
& +2\tau\left[I+\tfrac{1}{2}(1+\varepsilon)\tau\Lambda_1^n\right]^{-1}\left[I - \tfrac{1}{2}(1-\varepsilon)\tau\Lambda_1^n\right] \\
& \cdot\left[I+\tfrac{1}{2}(1+\varepsilon)\tau\Lambda_2^n\right]^{-1}\left[I - \tfrac{1}{2}(1-\varepsilon)\tau\Lambda_2^n\right] \\
& \cdot\left[I+\tfrac{1}{2}(1+\varepsilon)\tau\Lambda_3^n\right]^{-1}\left[I - \tfrac{1}{2}(1-\varepsilon)\tau\Lambda_3^n\right]f^n \\
= {} & T^n u^{n-1} + 2\tau T_1^n T_2^n T_3^n f^n,
\end{aligned} \tag{5}$$

where $T^n = T^n{}_1 T^n{}_2 T^n{}_3 T^n{}_3 T^n{}_2 T^n{}_1$ and $T_\alpha^n = [I + \frac{1}{2}(1+\varepsilon)\tau\Lambda_\alpha^n]^{-1}[I - \frac{1}{2}(1-\varepsilon)\tau\Lambda_\alpha^n]$. The discussion of the stability of scheme (5) can be seen in the Appendix. We obtain from (A5-A6) in the Appendix that $\| T \| \leq 1$, where $\| T \| = \underset{n}{Max}\{ \| T^n \|$,

$\| T^{n-1} \|, \ldots, \| T^1 \| \}$, and $\| u^{n+1} \| \leq \| g \| + 2_{t0} \| f \|$, where $u^\circ = g$, $\| f \| = \underset{j}{Max} \| f^j \|$. Hence, the scheme (5) is unconditionally stable.

Further, to investigate the behaviour of the scheme when the mesh ratio is large, we consider the constant coefficient case ($K(x, y, z, t) \equiv K$ = constant) for convenience. The amplification factor of G the generalized scheme (5) can be obtained

$$G^2 = \frac{\left[1-\frac{1}{2}(1-\varepsilon)\tau\lambda_1\right]^2\left[1-\frac{1}{2}(1-\varepsilon)\tau\lambda_2\right]^2\left[1-\frac{1}{2}(1-\varepsilon)\tau\lambda_3\right]^2}{\left[1+\frac{1}{2}(1+\varepsilon)\tau\lambda_1\right]^2\left[1+\frac{1}{2}(1+\varepsilon)\tau\lambda_2\right]^2\left[1+\frac{1}{2}(1+\varepsilon)\tau\lambda_3\right]^2}, \tag{6}$$

where $\lambda_\alpha (\alpha = 1, 2, 3$ is an eigenvalue of Λ_α. When $\tau\lambda_\alpha$ is large, we obtain from (6)

$$G \sim \frac{(1-\varepsilon)^3}{(1+\varepsilon)^3} < 1 \qquad \text{if } 0 < \varepsilon < 1, \tag{7}$$

while $G \sim 1$ if $\varepsilon = 0$. Thus G^n in the two-cycle componentwise splitting scheme ($\varepsilon = 0$, $G \sim 1$) goes to zero very slowly as $n \to \infty$. On the other hand, G^n in the generalized scheme ($\varepsilon > 0$, $G < 1$) goes to zero much faster. A large $\tau\lambda_\alpha$ may arise from a large mesh ratio $\tau K/h^2$. This can occur as a result of a large K or a fine spatial grid size compared with the time increment, implying that the two-cycle componentwise splitting scheme is not well suited for either simulating a fast transient phenomenon or for computations on a fine spatial mesh.

To determine the accuracy of the generalized scheme, we calculate T^n to obtain, if $\frac{1}{2}(1+\varepsilon)\tau\| \Lambda_\alpha^n \| < 1$,

$$\begin{aligned}
T^n = &\left[I - \tfrac{1}{2}(1+\varepsilon)\tau\Lambda_1^n + \tfrac{1}{4}(1+\varepsilon)^2\tau^2\left(\Lambda_1^n\right)^2 + 0(\tau^3)\right]\left[I - \tfrac{1}{2}(1-\varepsilon)\tau\Lambda_1^n\right] \\
&\cdot\left[I - \tfrac{1}{2}(1+\varepsilon)\tau\Lambda_2^n + \tfrac{1}{4}(1+\varepsilon)^2\tau^2\left(\Lambda_2^n\right)^2 + 0(\tau^3)\right]\left[I - \tfrac{1}{2}(1-\varepsilon)\tau\Lambda_2^n\right] \\
&\cdot\left[I - \tfrac{1}{2}(1+\varepsilon)\tau\Lambda_3^n + \tfrac{1}{4}(1+\varepsilon)^2\tau^2\left(\Lambda_3^n\right)^2 + 0(\tau^3)\right]\left[I - \tfrac{1}{2}(1-\varepsilon)\tau\Lambda_3^n\right] \\
&\cdot\left[I - \tfrac{1}{2}(1+\varepsilon)\tau\Lambda_3^n + \tfrac{1}{4}(1+\varepsilon)^2\tau^2\left(\Lambda_3^n\right)^2 + 0(\tau^3)\right]\left[I - \tfrac{1}{2}(1-\varepsilon)\tau\Lambda_3^n\right] \\
&\cdot\left[I - \tfrac{1}{2}(1+\varepsilon)\tau\Lambda_2^n + \tfrac{1}{4}(1+\varepsilon)^2\tau^2\left(\Lambda_2^n\right)^2 + 0(\tau^3)\right]\left[I - \tfrac{1}{2}(1-\varepsilon)\tau\Lambda_2^n\right] \\
&\cdot\left[I - \tfrac{1}{2}(1+\varepsilon)\tau\Lambda_1^n + \tfrac{1}{4}(1+\varepsilon)^2\tau^2\left(\Lambda_1^n\right)^2 + 0(\tau^3)\right]\left[I - \tfrac{1}{2}(1-\varepsilon)\tau\Lambda_1^n\right] \\
&= \left\{I - \tau\Lambda^n + \tfrac{1}{2}\tau^2\left[\left(\Lambda_1^n\right)^2 + \left(\Lambda_2^n\right)^2 + \left(\Lambda_3^n\right)^2 + 2\Lambda_1^n\Lambda_2^n + 2\Lambda_1^n\Lambda_3^n + 2\Lambda_2^n\Lambda_3^n\right]\right.
\end{aligned}$$

$$+\tfrac{1}{2}\varepsilon\tau^2\left[(\Lambda_1^n)^2+(\Lambda_2^n)^2+(\Lambda_3^n)^2\right]+0(\tau^3)\Big\}$$

$$\cdot\Big\{I-\tau\Lambda^n+\tfrac{1}{2}\tau^2\left[(\Lambda_1^n)^2+(\Lambda_2^n)^2+(\Lambda_3^n)^2+2\Lambda_2^n\Lambda_1^n+2\Lambda_3^n\Lambda_1^n+2\Lambda_3^n\Lambda_2^n\right]$$

$$+\tfrac{1}{2}\varepsilon\tau^2\left[(\Lambda_1^n)^2+(\Lambda_2^n)^2+(\Lambda_3^n)^2\right]+0(\tau^3)\Big\}$$

$$=I-2\tau\Lambda^n+\tfrac{1}{2}(2\tau)^2(\Lambda^n)^2+\varepsilon\tau^2\left[(\Lambda_1^n)^2+(\Lambda_2^n)^2+(\Lambda_3^n)^2\right]+0(\tau^3), \quad (8)$$

where $\Lambda^n = \Lambda_1^n + \Lambda_2^n + \Lambda_3^n$. The scheme is first-order in accuracy when $\varepsilon \neq 0$. However, if ε is small, accuracy will be high. This raises the question as to how small ε should be chosen if both the stability and accuracy are considered. To obtain a G value ($G \sim 1/\sqrt{2} = 0.707$) similar to that of the generalized Douglas ADI scheme when the mesh ratio is large (Dai and Nassar, 1997), we choose $\varepsilon = 0.05$, which gives, from (7), $G \sim 0.741$. In practice, the time step τ is usually chosen not to be very small. Therefore, with $\varepsilon = 0.05$, the accuracy of the generalized two-cycle componentwise splitting scheme is almost second-order.

3. Generalized divide and conquer procedure

Consider solving a tridiagonal linear system

$$\begin{cases} -b_i x_{i-1} + a_i x_i - c_i x_{i+1} = d_i, \quad i = 1, \cdots, n, \\ x_o = x_{n+1} = 0. \end{cases} \quad (9)$$

The usual approach for solving the above tridiagonal linear system is the Gaussian elimination technique. This approach results in a procedure called the "divide and conquer" procedure, shown as follows:

$$\beta_k = \frac{c_k}{a_k - b_k \beta_{k-1}}, \quad \beta_o = 0, \quad (10a)$$

$$\nu_k = \frac{d_k + b_k \nu_{k-1}}{a_k - b_k \beta_{k-1}}, \ \nu_o = 0; \quad k = 1, \cdots, n, \quad (10b)$$

$$x_k = \beta_k x_{k+1} + \nu_k, \quad x_{n+1} = 0; \quad k = n, \cdots, 1. \quad (10c)$$

In the above procedure, β_k, ν_k are calculated from $k = 1$ to $k = n$, while x_k is computed from $k = n$ to $k = 1$. A similar procedure that is opposite in direction can be expressed as

$$\tilde{\beta}_k = \frac{b_k}{a_k - c_k \tilde{\beta}_{k+1}}, \quad \tilde{\beta}_{n+1} = 0, \tag{11a}$$

$$\tilde{\nu}_k = \frac{d_k + c_k \tilde{\nu}_{k+1}}{a_k - c_k \tilde{\beta}_{k+1}}, \quad \tilde{\nu}_{n+1} = 0;\ k = n, \cdots, 1, \tag{11b}$$

$$x_k = \tilde{\beta}_k x_{k-1} + \tilde{\nu}_k, \quad x_o = 0;\ k = 1, \cdots, n. \tag{11c}$$

Combining procedures (10) and (11), one can develop a generalized "divide and conquer" procedure. To this end, let $n = 2N + 1$ for convenience and divide the system (9) into two subsystems, which consist of the first N equations and the last N equations, with the $(N+1)$th equation denoting the interface. As such, the procedure can be described as follows:

Divide and conquer procedure

Step 1. Calculate $\left\{ \begin{array}{l} \beta_k, \nu_k, \ k = 1, \cdots, N \\ \\ \tilde{\beta}_k, \tilde{\nu}_k, \ k = 2N+1, \cdots, N+2 \end{array} \right\}$.

Step 2. Substitute $x_N = \beta_N x_{N+1} + \nu_N$ and $x_{N+2} = \tilde{\beta}_{N+2} x_{N+1} + \tilde{\nu}_{N+2}$ into

$$-b_{N+1} x_N + a_{N+1} x_{N+1} - c_{N+1} x_{N+2} = d_{N+1}, \text{ then solve}$$

$$x_{N+1} = \frac{d_{N+1} + b_{N+1} \nu_N + c_{N+1} \tilde{\nu}_{N+2}}{a_{N+1} - b_{N+1} \beta_N - c_{N+1} \tilde{\beta}_{N+2}}.$$

Step 3. Solve $\left\{ \begin{array}{l} x_k = \beta_k x_{k+1} + \nu_k, \ k = N, \cdots, 1 \\ x_k = \tilde{\beta}_k x_{k-1} + \tilde{\nu}_k, \ k = N+2, \cdots, 2N+1 \end{array} \right\}$.

The idea of the above generalized "divide and conquer" procedure can be applied to a tridiagonal linear system which is divided into many subsystems. It should be pointed out that the generalized "divide and conquer" procedure is one type of the domain decomposition methods (Ottega, 1988). Therefore, it is characterized by a high inherent parallelism.

4. Numerical models for solving parabolic equations on multilayers

Consider a three-dimensional domain with two layers for convenience, as shown in Figure 1. Three-dimensional parabolic differential equations on two layers can be expressed as follows:

$$\frac{\partial U_1}{\partial t} = \frac{\partial}{\partial x}\left(K_1(x, y, z, t) \frac{\partial U_1}{\partial x} \right) + \frac{\partial}{\partial y}\left(K_1(x, y, z, t) \frac{\partial U_1}{\partial y} \right) \tag{12a}$$

$$\frac{\partial U_2}{\partial t} = \frac{\partial}{\partial x}\left(K_2(x,y,z,t)\frac{\partial U_2}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_2(x,y,z,t)\frac{\partial U_2}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_2(x,y,z,t)\frac{\partial U_2}{\partial z}\right) + f_2(x,y,z,t). \tag{12b}$$

We assume that the flux across the interface does not change. That is, at $z = H$,

$$-K_1\frac{\partial U_1}{\partial z} = -K_2\frac{\partial U_2}{\partial z},\ U_1 = U_2\ . \tag{13}$$

To obtain the numerical solution in the three-dimensional case, we assume that there is a mesh grid of $N_x \times N_y \times N_z$ for each of the layers with the same grid size Δx, Δy and Δz, where $(N_x + 1)\Delta x = L$, $(N_y + 1)\Delta y = L$ and $(N_z + 1)\Delta z = H$. We employ the generalized two-cycle componentwise splitting scheme in Section 2 to solve equations (12). As such,

$$\left[I + \tfrac{1}{2}(1+\varepsilon_l)\tau(\Lambda^l)_1^n\right](u_l)^{n-\frac{3}{4}} = \left[I - \tfrac{1}{2}(1-\varepsilon_l)\tau(\Lambda^l)_1^n\right](u_l)^{n-1}, \tag{14a}$$

$$\left[I + \tfrac{1}{2}(1+\varepsilon_l)\tau(\Lambda^l)_2^n\right](u_l)^{n-\frac{2}{4}} = \left[I - \tfrac{1}{2}(1-\varepsilon_l)\tau(\Lambda^l)_2^n\right](u_l)^{n-\frac{3}{4}}, \tag{14b}$$

$$\left[I + \tfrac{1}{2}(1+\varepsilon_l)\tau(\Lambda^l)_3^n\right](u_l)^{n-\frac{1}{4}} = \left[I - \tfrac{1}{2}(1-\varepsilon_l)\tau(\Lambda^l)_3^n\right](u_l)^{n-\frac{2}{4}}, \tag{14c}$$

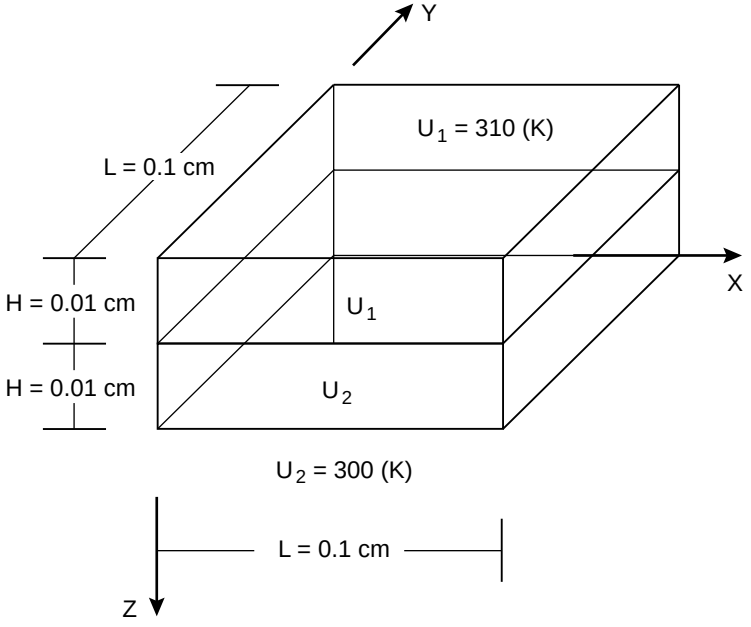

Figure 1.
Three-dimensional domain with two layers for equations (12a) and (12b) and for example of equations (20a) and (20b) in the text

$$(u_l)^{n+\frac{1}{4}} = (u_l)^{n-\frac{1}{4}} + 2\tau(f_l)^n, \tag{14d}$$

$$\left[I + \tfrac{1}{2}(1+\varepsilon_l)\tau(\Lambda^l)_3^n\right](u_l)^{n+\frac{2}{4}} = \left[I - \tfrac{1}{2}(1-\varepsilon_l)\tau(\Lambda^l)_3^n\right](u_l)^{n+\frac{1}{4}}, \tag{14e}$$

$$\left[I + \tfrac{1}{2}(1+\varepsilon_l)\tau(\Lambda^l)_2^n\right](u_l)^{n+\frac{3}{4}} = \left[I - \tfrac{1}{2}(1-\varepsilon_l)\tau(\Lambda^l)_2^n\right](u_l)^{n+\frac{2}{4}} \tag{14f}$$

$$\left[I + \tfrac{1}{2}(1+\varepsilon_l)\tau(\Lambda^l)_1^n\right](u_l)^{n+1} = \left[I - \tfrac{1}{2}(1-\varepsilon_l)\tau(\Lambda^l)_1^n\right](u_l)^{n+\frac{3}{4}}, \tag{14g}$$

where l represents the (l)th layer (l = 1, 2). For the interfacial equations, we let, at any time step n,

$$-K_1\left(\frac{(u_1)^n_{ijN_z+1} - (u_1)^n_{ijN_z}}{\Delta z}\right) = -K_2\left(\frac{(u_2)^n_{ij1} - (u_2)^n_{ij0}}{\Delta z}\right), \quad (u_1)^n_{ijN_z+1} = (u_2)^n_{ij0}. \tag{15}$$

Hence, the computational procedure of the three-dimensional model is as follows:

Step 1 is to determine

$$\left\{(u_1)^{n-\frac{3}{4}}_{ijk}\right\}$$

and

$$\left\{(u_2)^{n-\frac{3}{4}}_{ijk}\right\}$$

by using equation (14a). To this end, we solve two tridiagonal linear systems to obtain

$$\left\{(\vec{u}_1)^{n-\frac{3}{4}}_{jk}\right\}$$

and

$$\left\{(\vec{u}_2)^{n-\frac{3}{4}}_{jk}\right\},$$

$j = 1, \ldots, N_y$, $k = 1, \ldots, N_z$, independently, then, we substitute

$$(u_1)^{n-\frac{3}{4}}_{ijN_z}$$

and

$$(u_2)^{n-\frac{3}{4}}_{ij1}$$

into equation (15) to obtain

$$(u_1)^{n-\frac{3}{4}}_{ijN_z+1}$$

and

$$(u_2)_{ijo}^{n-\frac{3}{4}}$$

Similarly, step 2 is to determine

$$\left\{(u_1)_{ijk}^{n-\frac{2}{4}}\right\}$$

and

$$\left\{(u_2)_{ijk}^{n-\frac{2}{4}}\right\}$$

by using equation (14b).

Step 3 is to determine

$$\left\{(u_1)_{ijk}^{n-\frac{1}{4}}\right\}$$

and

$$\left\{(u_2)_{ijk}^{n-\frac{1}{4}}\right\}$$

by using equation (14c). As such, we express equations (14c), with $l = 1, 2$, as three tridiagonal linear systems.

$$-b_k^1(u_1)_{ijk-1}^{n-\frac{1}{4}} + a_k^1(u_1)_{ijk}^{n-\frac{1}{4}} - c_k^1(u_1)_{ijk+1}^{n-\frac{1}{4}} = d_{ijk}^1, \quad k = 1, \cdots, N_z, \tag{16a}$$

$$-b_k^2(u_2)_{ijk-1}^{n-\frac{1}{4}} + a_k^2(u_2)_{ijk}^{n-\frac{1}{4}} - c_k^2(u_2)_{ijk+1}^{n-\frac{1}{4}} = d_{ijk}^2, \quad k = 1, \cdots, N_z, \tag{16b}$$

where $i = 1, \ldots, N_x$ and $j = 1, \ldots, N_y$. Since u_l ($l = 1, 2$) at the $(n-\frac{1}{4})\Delta t$ time step is unknown at the interface between layers, the above two tridiagonal linear systems cannot be solved. To overcome this difficulty, we apply the generalized divide and conquer procedure, and calculate the coefficients listed in step 1 of the procedure, then, substitute the following two equations

$$\begin{cases} (u_1)_{ijN_z}^{n-\frac{1}{4}} = \beta_{N_z}^{(1)}(u_1)_{ijN_z+1}^{n-\frac{1}{4}} + \nu_{N_z}^{(1)} \\ (u_2)_{ij1}^{n-\frac{1}{4}} = \tilde{\beta}_1^{(2)}(u_2)_{ijo}^{n-\frac{1}{4}} + \tilde{\nu}_1^{(2)} \end{cases} \tag{17}$$

into the interfacial equation (15) to obtain

$$(u_1)_{ijN_z+1}^{n-\frac{1}{4}}$$

and

$(u_2)_{ijo}^{n-\frac{1}{4}}$

Finally, we solve for the rest of the unknowns in

$$\left\{(u_1)_{ijk}^{n-\frac{1}{4}}\right\}$$

and

$$\left\{(u_2)_{ijk}^{n-\frac{1}{4}}\right\}$$

by step 3 of the procedure.

Step 4 is to determine

$$\left\{(u_1)_{ijk}^{n+\frac{1}{4}}\right\}$$

and

$$\left\{(u_2)_{ijk}^{n+\frac{1}{4}}\right\}$$

by using equation (14d).

Similar to step 3, step 5 is to determine

$$\left\{(u_1)_{ijk}^{n+\frac{2}{4}}\right\}$$

and

$$\left\{(u_2)_{ijk}^{n+\frac{2}{4}}\right\}$$

by using equation (14e).

Similar to step 2, step 6 is to determine

$$\left\{(u_1)_{ijk}^{n+\frac{3}{4}}\right\}$$

and

$$\left\{(u_2)_{ijk}^{n+\frac{3}{4}}\right\}$$

by using equation (14f).

Similar to step 1, step 7 is to determine

$$\left\{(u_1)_{ijk}^{n+1}\right\}$$

and

$$\left\{(u_2)_{ijk}^{n+1}\right\}$$

by using equation (14g).

The above iterations are continued until the steady state solution is obtained.

It should be pointed out that the above procedure is one type of the domain decomposition methods for solving parabolic differential equations (Chan, 1994).

5. Numerical examples

To illustrate the advantage of the generalized two-cycle componentwise splitting scheme, we first consider a three-dimensional parabolic differential equation

$$\frac{\partial U}{\partial t} = \frac{\partial}{\partial x}\left(K(x,y,z)\frac{\partial U}{\partial x}\right) + \frac{\partial}{\partial y}\left(K(x,y,z)\frac{\partial U}{\partial y}\right) + \frac{\partial}{\partial z}\left(K(x,y,z)\frac{\partial U}{\partial z}\right) + f(x,y,z,t), \quad 0 < x,y,z < 1, t > 0; \tag{18}$$

where $K(x, y, z) = \mu(x^2 + y^2 + z^2 + 1)$ and $f(x, y, z, t) = -70\mu xyz\, e^{-\mu t}$. Its exact solution is given as

$$U(x,y,z,t) = 10\,xyze^{-\mu t}, \quad 0 \le x,y,z \le 1, t > 0. \tag{19}$$

Initial and boundary conditions are obtained from the exact solution. From (19), it is seen that for large μ, the solution converges fast to the steady state solution (which is zero) as time increases. Hence, the equation in (18) has a fast transient phenomenon.

Equation (18) was solved by using the generalized two-cycle componentwise splitting scheme (4). In our calculation, we first chose $\Delta x = \Delta y = \Delta z = h = 0.02$ and $\Delta t = 0.02$. To obtain the steady state solution, the time iteration was continued until $max|u| \le 10^{-3}$ was satisfied. The number of iterations for different μ values 5, 20 and 100 are compared with that of the two-cycle componentwise splitting scheme (3) (Table I).

From Table I, it can be seen that the solution from the two-cycle componentwise splitting scheme converges very slowly when μ is large. Convergence of the numerical solutions from the generalized scheme was much faster than that from scheme (3). This shows that the new scheme is suitable for simulating fast transient phenomena.

We then chose $\Delta t = 0.02$ with difference grid sizes, $h = 0.05$, 0.02 and 0.01. Again, to obtain the steady state solution (which is zero), the time iteration was continued until $max|u| \le 10^{-3}$ was satisfied. The number of iterations for $\mu = 5.0$ is compared with that of the scheme (3) (Table II).

Table I.
Number of iterations, for different μ values n ($n\Delta t = t$)

ADI schemes	$n(\mu = 5)$	$n(\mu = 20$	$n(\mu = 100)$
Scheme (3)	90	98	428
Scheme (4) ($\varepsilon = 0.05$)	90	44	16
Exact solution	90	22	4

From Table II, it can be seen that the solution from the two-cycle componentwise splitting scheme converges very slowly when the spatial grid is fine. Convergence of the numerical solutions from the generalized scheme was much faster than that from the two-cycle componentwise splitting scheme. For $h = 0.01$, the two-cycle componentwise splitting scheme took 182 minutes of CPU time on a SUN workstation while the generalized scheme only took 43 minutes. This shows that the new scheme is suitable for computations on fine spatial meshes, which makes it applicable to micromanufacturing, such as the prediction of the temperature profile in x-ray lithography.

ADI schemes	$n(h = 0.05)$	$n(h = 0.02)$	$n(h = 0.01)$
Scheme (3)	90	184	396
Scheme (4) ($\varepsilon = 0.05$)	90	90	90
Exact solution	90	90	90

Table II. Number of iterations, for different h values n ($n\Delta t = t$)

We now consider the three-dimensional heat conduction on two layers.

$$\frac{\partial U_1}{\partial t} = \frac{\partial}{\partial x}\left(K_1(x, y, z)\frac{\partial U_1}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_1(x, y, z)\frac{\partial U_1}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_1(x, y, z)\frac{\partial U_1}{\partial z}\right), \tag{20a}$$

$$\frac{\partial U_2}{\partial t} = \frac{\partial}{\partial x}\left(K_2(x, y, z)\frac{\partial U_2}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_2(x, y, z)\frac{\partial U_2}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_2(x, y, z)\frac{\partial U_2}{\partial z}\right), \tag{20b}$$

where $K_1(x, y, z) = \mu_1(x^2 + y^2 + z^2 + 1)$, $K_2(x, y, z) = \mu_2(x^2 + y^2 + z^2 + 1)$. This situation may be encountered in x-ray lithography, used in micromanufacturing. The two layers are composed of a photoresist and a substrate. For this example, it is of interest to predict the temperature profile in each of the layers. Each layer is chosen to be of dimension 0.1cm × 0.1cm × 0.01cm as shown in Figure 1. The initial and boundary value problem with homogeneous conditions ($U_m = 300$ (K), $m = 1, 2$) except $U_1 = 310.0$ (K) at $z = 0.0$ is considered. Problem (20) with initial and boundary conditions is computed by using the numerical procedure described in Section 4. In this calculation, we chose $\Delta x = \Delta y = 0.002$cm, $\Delta z = 0.0002$cm and $\Delta t = 0.02$second. To obtain the steady state solution, the time iteration was continued until

$$\max_{i,j,k} |(u_1)_{ijk}^{n+1} - (u_1)_{ijk}^{n-1}| \leq 0.0005$$

was satisfied. We chose $\mu_1 = \mu_2 = 5.0$ (Wcm^2/J) and $\varepsilon_1 = \varepsilon_2 = 0.05$. The steady state solution was obtained when the number of iterations is 30. The maximum temperature rise in the first layer is 3.18 (K). The contours of the temperature profile in the cross section at $y = 0.05$ cm are plotted in Figure 2. We also chose the procedure with $\varepsilon_1 = \varepsilon_2 = 0.0$. The steady state solution was obtained when the number of iterations is 2,174. Furthermore, the contours of the temperature profile in the cross section at $y = 0.05$cm are oscillatory, as shown in Figure 3. This shows that the two-cycle componentwise scheme is not suitable for the problem with microscale in dimension.

6. Conclusion

A generalized two-cycle componentwise splitting method for solving three-dimensional parabolic differential equations with variable coefficients has been developed based on the idea of the regularized difference scheme. The method is shown to be unconditionally stable, and suitable for simulating fast transient phenomena and for computations on fine spatial meshes. A numerical procedure that employs this method was developed to solve three-dimensional parabolic differential equations with variable coefficients on multilayers. In the procedure, the generalized "divide and conquer" method for solving tridiagonal linear systems is applied, in order to overcome the problem with the unknown value at the interface between layers. Numerical results show that the

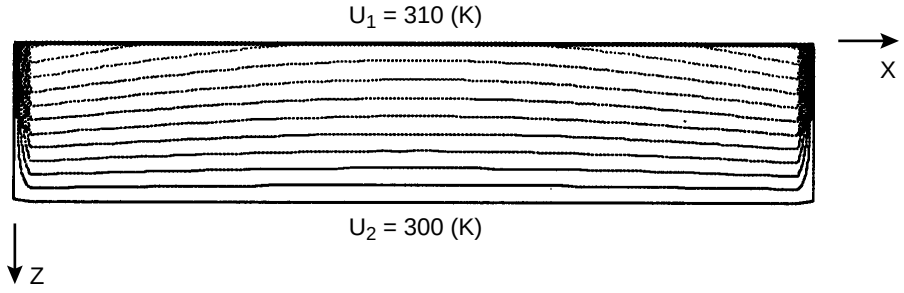

Figure 2.
Contour of the temperature distribution in the cross-section at $y = 0.05$cm ($\varepsilon_1 = \varepsilon_2 = 0.05$)

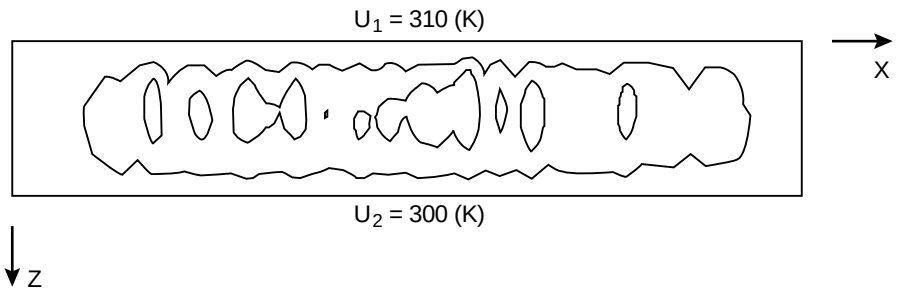

Figure 3.
Contour of the temperature distribution in the cross-section at $y = 0.05$cm ($\varepsilon_1 = \varepsilon_2 = 0.0$)

generalized two-cycle componentwise splitting scheme is accurate and the numerical procedure is efficient.

References

Ameel, T.A., Warrington, R.O., Yu, D. and Dahlbacka, G. (1994), "Thermal analysis of X-ray irradiated thick resists to determine induced structural deformations", *Heat Transfer,* Vol. 4, pp. 313-8.

Chan, T.F. (1994), "Domain decomposition algorithms", *Acta Numerica*, pp. 61-143.

Cole, K.D. and McGahan, W.A. (1993), "Theory of multilayers heated by laser absorption", *Journal of Heat Transfer,* Vol. 115, pp. 767-71.

Dai, W. and Nassar, R. (1997), "A generalized Douglas ADI method for solving three- dimensional parabolic differential equations on multilayers", *Int. J. Numerical Methods for Heat & Fluid Flow,* Vol. 7 No. 7, pp. 659-74.

Dean, J. and Glowinski, R. (1993), "On some finite element methods for the numerical simulation of incompressible viscous flow", in Gunzburger, M.D. and Nicolaides, R.A. (Eds), *Incompressible Computational Fluid Dynamics,* Cambridge University Press, Cambridge.

Kant, R. (1988), "Laser-induced heating of a multilayered medium resting on a half- space: part I – stationary source", *Journal of Applied Mechanics*, Vol. 55, pp. 93-7.

Leitz, G., Pezoldt, J., Patzschke, I., Zollner, J.-P. and Eichhorn, G. (1993), "Investigation of dynamical temperature behaviour in RTP", *Mat. Res. Soc. Symp. Proc.,* Vol. 303, pp. 171-82.

Lie, K.-H., Merchant, T.P. and Jensen, K.F. (1993), "Simulation of rapid thermal processing equipment and processes", *Mat. Res. Soc. Symp. Proc.,* Vol. 303, pp. 197-209.

Madison, M.R. and McDaniel, T.W. (1989), "Temperature distributions produced in an N-layer by static or scanning laser or electron beam with application to magneto-optical media", *Journal of Applied Physics,* Vol. 66, pp. 5738-48.

Marchuk, G.I. (1989), "Splitting and alternating direction methods", in Ciarlet, P.G. and Lions, J.L. (Eds), *Handbook of Numerical Analysis*, Vol. 1, pp. 197-465, North-Holland, New York, NY.

Ottega, J.M. (1988), *Introduction to Parallel and Vector Solution of Linear Systems*, Plenum Press, New York, NY.

Samarskii, A.A. and Vabishchevich, P.N. (1994), "Regularized difference schemes", *MMCE*, Vol. 1, pp. 44-50.

Appendix

Consider the three-dimensional parabolic equation with variable coefficients

$$\frac{\partial U}{\partial t} = \frac{\partial}{\partial x}\left(K(x, y, z, t)\frac{\partial U}{\partial x}\right) + \frac{\partial}{\partial y}\left(K(x, y, z, t)\frac{\partial U}{\partial y}\right)$$

$$+ \frac{\partial}{\partial z}\left(K(x, y, z, t)\frac{\partial U}{\partial z}\right) + f(x, y, z, t), \qquad \text{in } \Omega \times [0, t_o], \tag{A1a}$$

$$U = 0 \quad \text{on } \partial\Omega, \quad \text{and} \quad U = g, \quad t = 0, \tag{A1b}$$

where $K(x, y, z, t) \geq a > 0$ is the diffusivity coefficient. Let

$$AU \equiv -\frac{\partial}{\partial x}\left(K\frac{\partial U}{\partial x}\right) - \frac{\partial}{\partial y}\left(K\frac{\partial U}{\partial y}\right) - \frac{\partial}{\partial z}\left(K\frac{\partial U}{\partial z}\right) \tag{A2}$$

$$= A_1 U + A_2 U + A_3 U,$$

where $A_1 U = -\frac{\partial}{\partial x}\left(K\frac{\partial U}{\partial x}\right)$, $A_2 U = -\frac{\partial}{\partial y}\left(K\frac{\partial U}{\partial y}\right)$ and $A_3 U = -\frac{\partial}{\partial z}\left(K\frac{\partial U}{\partial z}\right)$

Obviously, $A_i A_j U \neq A_j A_i U$, $i \neq j$, i.e. operators A_α, $\alpha = 1, 2, 3$, are not commutative.

Let F be the Hilbert space of the real function $L_2(\Omega)$ with the inner product $(u, v) = \int_\Omega uv d\Omega$ and the norm $\|u\| = (u, u)^{\frac{1}{2}}$. Denote by Φ the set of functions that are continuous in $\bar{\Omega} = \Omega + \partial\Omega$ and that have continuous first and second derivatives in Ω. Let the elements of $\bar{\Omega}_h = \Omega_h + \partial\Omega_h = \{(xi, yj, zk); 0 \le i \le N_x + 1, 0 \le j \le N_y + 1, 0 \le k \le N_z + 1\}$. Define the inner products and the norms as follows:

$$(u, v)_h = h^3 \sum_{i=0}^{N_x+1} \sum_{j=0}^{N_y+1} \sum_{k=0}^{N_z+1} u_{ijk} v_{ijk}, \quad \|u\|_h^2 = (u, u)_h$$

$$(u, v)_{ho} = h^3 \sum_{i=1}^{N_x} \sum_{j=1}^{N_y} \sum_{k=1}^{N_z} u_{ijk} v_{ijk}, \text{ and } \|u\|_{ho}^2 = (u, u)_{ho}.$$

Two properties for stability are:

Property 1. Operator in A in (A.2) is semi-positive definite.

Proof. $$(AU, U) = \left(-\frac{\partial}{\partial x}\left(K\frac{\partial U}{\partial x}\right) - \frac{\partial}{\partial y}\left(K\frac{\partial U}{\partial y}\right) - \frac{\partial}{\partial z}\left(K\frac{\partial U}{\partial z}\right), U\right)$$

$$= \int_\Omega \left[K\left(\frac{\partial U}{\partial x}\right)^2 + K\left(\frac{\partial U}{\partial y}\right)^2 + K\left(\frac{\partial U}{\partial z}\right)^2\right] d\Omega \ge 0.$$

Property 2. If A is semi-positive definite in real Hilbert space Φ, then

$$\left\|[I + (1+\varepsilon)\sigma A]^{-1}[I - (1-\varepsilon)\sigma A]\right\| \le 1, \tag{A3}$$

where σ is a positive constant and $\varepsilon \le 1$ is a positive number.

Proof. Let $T = [I - (1-\varepsilon)\sigma A][I + (1+\varepsilon)\sigma A]^{-1}$. Then

$$\|T\|^2 = \sup_\varphi \frac{(T\varphi, T\varphi)}{(\varphi, \varphi)}$$

$$= \sup_\psi \frac{([I - (1-\varepsilon)\sigma A]\psi, [I - (1-\varepsilon)\sigma A]\psi)}{([I + (1+\varepsilon)\sigma A]\psi, [I + (1+\varepsilon)\sigma A]\psi)}$$

$$= \sup_\psi \frac{(\psi, \psi) - 2(1-\varepsilon)\sigma(A\psi, \psi) + (1-\varepsilon)^2\sigma^2(A\psi, A\psi)}{(\psi, \psi) + 2(1+\varepsilon)\sigma(A\psi, \psi) + (1+\varepsilon)^2\sigma^2(A\psi, A\psi)} \le 1.$$

Using the identity, $[I + \alpha A]^{-1} A = \frac{1}{\alpha}\left[I - [I + \alpha A]^{-1}\right] = A[I + \alpha A]^{-1}$,

one can obtain

$$\left\|[I + (1+\varepsilon)\sigma A]^{-1}[I - (1-\varepsilon)\sigma A]\right\| = \left\|[I - (1-\varepsilon)\sigma A][I + (1+\varepsilon)\sigma A]^{-1}\right\| \le 1.$$

We now discuss the stability of the system (5), $u^{n+1} = T^n u^{n-1} + 2\tau T_1^n T_2^n T_3^n f^n$, with $u^\circ = g$. Consider an odd integer n. Then

$$u^{n+1} = T^n \left(T^{n-2} u^{n-3} + 2\tau T_1^{n-2} T_2^{n-2} T_3^{n-2} f^{n-2} \right) + 2\tau T_1^n T_2^n T_3^n f^n$$

$$= T^n T^{n-2} \cdots T^1 g + 2\tau T_1^n T_2^n T_3^n f^n + \cdots + 2\tau T^n T^{n-2} \cdots T^1 T_1^1 T_2^1 T_3^1 f^1$$

Hence,

$$\|u^{n+1}\|_h \le \|T\|^n \|g\|_h + 2\tau \sum_{i=1}^{m} \|T\|^{m-i} \left\| f^{2i-1} \right\|_{h_0}, \tag{A4}$$

where $\|T\| = max\{\|T^n\|, \ldots, \|T^1\|\}$ and $m = \frac{n+1}{2}$ is the number of factors $\{T^k\}$ in $T^n T^{n-2} \ldots T^1$. Here we use the fact that $\|T_\alpha^k\| \le 1$ by property 2. Further, we obtain by property 2

$$\|T\| \le \left\| \left[I + (1+\varepsilon)\sigma \Lambda_1 \right]^{-1} \left[I - (1-\varepsilon)\sigma \Lambda_1 \right] \right\|^2$$

$$\cdot \left\| \left[I + (1+\varepsilon)\sigma \Lambda_2 \right]^{-1} \left[I - (1-\varepsilon)\sigma \Lambda_2 \right] \right\|^2 \tag{A5}$$

$$\cdot \left\| \left[I + (1+\varepsilon)\sigma \Lambda_3 \right]^{-1} \left[I - (1-\varepsilon)\sigma \Lambda_3 \right] \right\|^2 \le 1.$$

Hence, (A4) becomes

$$\|u^{n+1}\|_h \le \|g\|_h + 2m\tau \|f\|$$

$$\le \|g\|_h + 2t_0 \|f\|, \tag{A6}$$

where $\|f\| = \max_j \|f^j\|_{h_0}$. Hence, we conclude that the scheme (5) is unconditionally stable.