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A Fast Computing Technique for Diffusion-type Equations

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A fast computing technique is presented for numerical solutions of diffusion-type equations. The essence of this technique consists of performing the numerical computation using about a half number of variables without loss of numerical stability and accuracy by making use of analytical relations under the governing equation. Numerical stability of the present scheme is superior to usual schemes. Test calculations for a thermal transient problem with 100 meshes show that the computing time is decreased to about $\frac{1}{3}$ as compared with a usual method.

1. INTRODUCTION

Recently, there has been a growing need for the application of numerical analysis of diffusion and convection problems in complicated systems with large geometries such as thermohydraulic problems in connection with detailed hot spot temperature analyses in a nuclear reactor core under both normal and off-normal operating conditions [1, 2].

In the convection problems, there have been presented some of accelerated computing techniques such as methods using a parabolic flow approximation for fluid flows with one primary flow direction [3], and introducing the velocity-correction factors and cell boundary conditions parameters in the pressure iteration procedure [1]. In the diffusion problems, there have been presented some of accelerated computing techniques for discrete Poisson equations such as SOR (successive over-relaxation) method [4, 5] and TDM (tridiagonal-matrix) method [6] in the explicit scheme, and fast matrix transpose method [7, 8] and fast Poisson-solver method [9, 10, 11] in the implicit scheme.

The purpose of this paper is to present a fast computing technique for the diffusion-type equations. In this technique, the numerical computation is performed by making use of about a half number of variables without loss of numerical stability and accuracy based on analytical relations under the governing equation. Numerical stability in the present scheme is investigated based on the linear theory by von Neumann [12].

To demonstrate the effectiveness of this technique, the computing time is compared with that using a usual method for a thermal transient problem.

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To simplify the discussion, we present the scheme here in the context of a 2-dimensional thermal problem, but the extension to three dimensions is immediate. Moreover, the idea of the present method could be applied to the more general linear differential equations and be used in conjunction with the usual accelerated computing techniques.

2. Technique for Diffusion-type Equations

We will consider the following heat conduction equation as an example of diffusion type equations:

$$\frac{\partial}{\partial t}(\rho C T) = \operatorname{div}(k \operatorname{grad} T) + Q, \tag{1}$$

where T, ρ, C, and k are temperature, density, specific heat, and thermal conductivity of material, respectively. Q is heat source per unit volume and unit time.

Figure 1 shows the computational region which is divided into a set of quadrilateral cells with spacings Δx_i and Δy_j in the x and y directions in the 2-dimensional Cartesian coordinate system, respectively. Cells are labeled with an index (i, j), which denotes the cell number as counted from the origin in the x and y directions, respectively. $\phi_{i,j}$ denotes $\phi(x_i, y_j)$ defined at the cell center, where ϕ is a dummy symbol representing any one of the dependent variables.

Using the Laossonen type difference scheme [13] (i.e., backward difference) with respect to time and the central difference scheme with respect to space, an approximate solution can be obtained by the following modified difference equation as being exclusive of the nearest neighbor temperatures $(T_{i\pm1,j}, T_{i,j\pm1})$:

$$\begin{aligned}
&\left(\frac{\rho_{i,j}C_{i,j}T_{i,j} - \rho'_{i,j}C'_{i,j}T'_{i,j}}{\Delta t}\right)\Delta V_{i,j} \\
&\quad = \lambda_{i,j}^{i-1,j}\alpha_{i-1,j}^{(1)}T_{i-2,j} \\
&\qquad + (\lambda_{i,j}^{i-1,j}\alpha_{i-1,j}^{(3)} + \lambda_{i,j}^{i,j-1}\alpha_{i,j-1}^{(1)})\,T_{i-1,j-1} \\
&\qquad + (\lambda_{i,j}^{i-1,j}\alpha_{i-1,j}^{(4)} + \lambda_{i,j}^{i,j+1}\alpha_{i,j+1}^{(1)})\,T_{i-1,j+1} + \lambda_{i,j}^{i,j-1}\alpha_{i,j-1}^{(3)}T_{i,j-2} \\
&\qquad + [\lambda_{i,j}^{i-1,j}(\alpha_{i-1,j}^{(2)} - 1) + \lambda_{i,j}^{i+1,j}(\alpha_{i+1,j}^{(1)} - 1) \\
&\qquad + \lambda_{i,j}^{i,j-1}(\alpha_{i,j-1}^{(4)} - 1) + \lambda_{i,j}^{i,j+1}(\alpha_{i,j+1}^{(3)} - 1)]\,T_{i,j} \\
&\qquad + \lambda_{i,j}^{i,j+1}\alpha_{i,j+1}^{(4)}T_{i,j+2} \\
&\qquad + (\lambda_{i,j}^{i+1,j}\alpha_{i+1,j}^{(3)} + \lambda_{i,j}^{i,j-1}\alpha_{i,j-1}^{(2)})\,T_{i+1,j-1} \\
&\qquad + (\lambda_{i,j}^{i+1,j}\alpha_{i+1,j}^{(4)} + \lambda_{i,j}^{i,j+1}\alpha_{i,j+1}^{(2)})\,T_{i+1,j+1} \\
&\qquad + \lambda_{i,j}^{i+1,j}\alpha_{i+1,j}^{(2)}T_{i+2,j} \\
&\qquad + \lambda_{i,j}^{i-1,j}\alpha_{i-1,j}^{(5)} + \lambda_{i,j}^{i+1,j}\alpha_{i+1,j}^{(5)} + \lambda_{i,j}^{i,j-1}\alpha_{i,j-1}^{(5)} \\
&\qquad + \lambda_{i,j}^{i,j+1}\alpha_{i,j+1}^{(5)} + Q_{i,j}\Delta V_{i,j}.
\end{aligned} \tag{2}$$

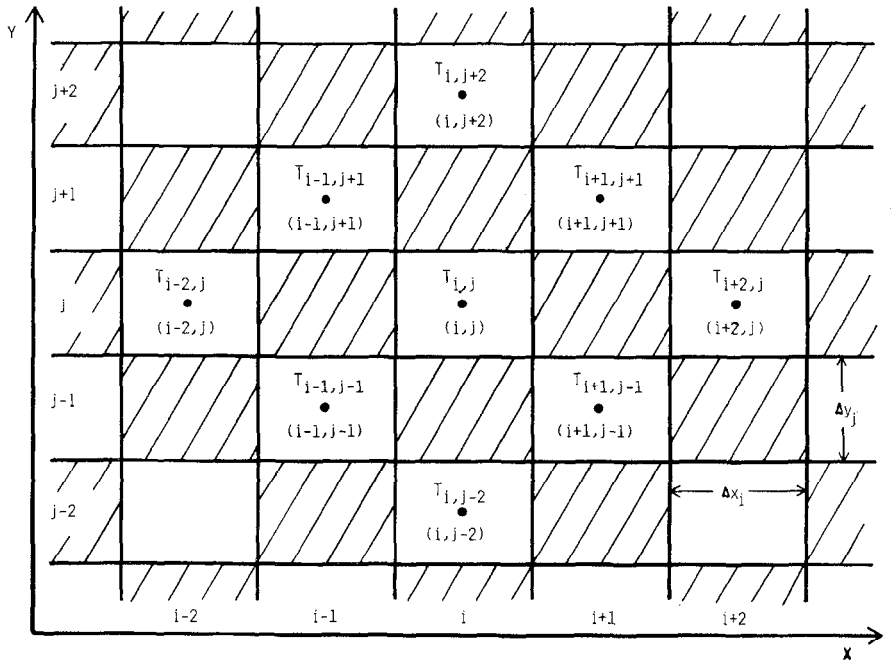

FIG. 1. Cell arrangement in a computational region. With respect to the cell (i,j) under consideration, the indexes of the nearest neighbor cells with hatched lines are $(i-1,j)$, $(i,j-1)$, $(i,j+1)$, and $(i+1,j)$, and those of the next nearest neighbor cells are $(i-2,j)$, $(i-1,j-1)$, $(i-1,j+1)$, $(i,j-2)$, $(i,j+2)$, $(i+1,j-1)$, $(i+1,j+1)$, and $(i+2,j)$.

Here

$$\alpha_{i,j}^{(1)} \equiv \lambda_{i,j}^{i-1,j}/\Lambda_{i,j}, \qquad \alpha_{i,j}^{(2)} \equiv \lambda_{i,j}^{i+1,j}/\Lambda_{i,j},$$

$$\alpha_{i,j}^{(3)} \equiv \lambda_{i,j}^{i,j-1}/\Lambda_{i,j}, \qquad \alpha_{i,j}^{(4)} \equiv \lambda_{i,j}^{i,j+1}/\Lambda_{i,j},$$

$$\alpha_{i,j}^{(5)} \equiv \left(Q_{i,j} + \frac{\rho'_{i,j} C'_{i,j} T'_{i,j}}{\Delta t} \right) \Delta V_{i,j}/\Lambda_{i,j},$$

$$\Lambda_{i,j} \equiv \lambda_{i,j}^{i-1,j} + \lambda_{i,j}^{i+1,j} + \lambda_{i,j}^{i,j-1} + \lambda_{i,j}^{i,j+1} + (\rho_{i,j} C_{i,j} \Delta V_{i,j}/\Delta t),$$

$$\lambda_{i,j}^{i',j} \equiv \frac{S_{i,j}^{i',j}}{[(\Delta x_i/2)/k_{i,j}] + [(\Delta x_{i'}/2)/k_{i',j}]} \qquad (\text{for } i' = i-1 \text{ and } i+1),$$

$$\lambda_{i,j}^{i,j'} \equiv \frac{S_{i,j}^{i,j'}}{[(\Delta y_j/2)/k_{i,j}] + [(\Delta y_{j'}/2)/k_{i,j'}]} \qquad (\text{for } j' = j-1 \text{ and } j+1),$$

where $\Delta V_{i,j}$ is the volume of cell (i,j) $(\Delta V_{i,j} = \Delta x_i \cdot \Delta y_j \cdot 1)$, Δt is time increment, $S_{i,j}^{i',j'}$ is the interface between the cell (i,j) and the cell (i',j') and dependent variables with a prime represent the values at the old time $t - \Delta t$.

Equation (2) is nothing but an expression for the temperature $T_{i,j}$ under consideration in terms of the next nearest neighbor temperatures, except that the nearest neighbor termperatures are included as known values at old time step and implicity included through material properties. Equation (2) is derived (1) by expressing the nearest neighbor temperatures in terms of $T_{i,j}$ and the next nearest neighbor temperatures using the original Laossonen-type difference equation [13], and (2) by substituting these expressions into original difference equation (see Appendix A).

By Eq. (2), we can efficiently perform the numerical computation using about a half number of variables composed of the next nearest neighbor temperatures without loss of numerical accuracy.

In the latter sections, we will put forward discussions on this finite difference equation in both the explicit scheme and the implicit scheme.

3. Investigation

3.1. *Stability in the Explicit Scheme*

3.1.1. *Steady State*

We will investigate the numerical stability for the steady state solution of Eq. (2) in use of the SOR (successive over-relaxation) iterative method with the Liebman method [14], which is a typical example of explicitly solving procedures.

Based on the von Neumann stability theory in case of constant material properties and a regular ($\Delta x_i = \Delta x$, $\Delta y_j = \Delta y$) system with periodic boundary conditions, the amplification factor $G_s(\theta_x, \theta_y)$ for the Fourier components of the deviation error from the true difference solution with phase angles θ_x and θ_y is given by the following equation (see Appendix B):

$$G_s(\theta_x, \theta_y) = \left(\frac{g_2(\theta_x, \theta_y)}{g_1(\theta_x, \theta_y)} \right)^{1,2}, \tag{3a}$$

where

$$\begin{aligned} g_1(\theta_x, \theta_y) \equiv & \left[1 - \frac{\omega}{1 + 4\beta^2 + \beta^4} \left(\frac{1}{2} \cos 2\theta_x + \beta^2 \cos(\theta_x + \theta_y) \right. \right. \\ & \left. \left. + \beta^2 \cos(\theta_x - \theta_y) + \frac{\beta^4}{2} \cos 2\theta_y \right) \right]^2 \\ & + \left[\frac{\omega}{1 + 4\beta^2 + \beta^4} \left(\frac{1}{2} \sin 2\theta_x + \beta^2 \sin(\theta_x + \theta_y) \right. \right. \\ & \left. \left. + \beta^2 \sin(\theta_x - \theta_y) + \frac{\beta^4}{2} \sin 2\theta_y \right) \right]^2, \end{aligned} \tag{3b}$$

$$g_2(\theta_x, \theta_y) \equiv \left[1-\omega+\frac{\omega}{1+4\beta^2+\beta^4}\left(\frac{1}{2}\cos 2\theta_x+\beta^2\cos(\theta_x+\theta_y)\right.\right.$$
$$\left.+\beta^2\cos(\theta_x-\theta_y)+\frac{\beta^4}{2}\cos 2\theta_y\right)\Bigg]^2$$
$$+\left[\frac{\omega}{1+4\beta^2+\beta^4}\left(\frac{1}{2}\sin 2\theta_x+\beta^2\sin(\theta_x+\theta_y)\right.\right.$$
$$\left.\left.+\beta^2\sin(\theta_x-\theta_y)+\frac{\beta^2}{2}\sin 2\theta_y\right)\right]^2, \tag{3c}$$

with $\beta = \Delta x/\Delta y$. From the stability condition $G_s(\theta_x, \theta_y) \leqslant 1$, we get the following inequality:

$$\omega(2-\omega)[(\cos 2\theta_x - 1) + 2\beta^2(\cos(\theta_x+\theta_y)$$
$$+\cos(\theta_x-\theta_y)-2)+\beta^4(\cos 2\theta_y - 1)] \leqslant 0. \tag{4}$$

Since the value in the above square bracket is always less than zero, we get

$$0 < \omega \leqslant 2,$$

for all phase angles and all values of β. The above stability condition for the accelerating factor ω is the same as that for the usual scheme using the nearest neighbor variables. Thus, it was shown that the numerical stability condition in the present scheme is not restricted as compared with the usual scheme.

In the above SOR iteration, the temperature of the nearest neighbor cells removed in the iteration step can be calculated in terms of the next nearest neighbor temperatures and the material properties of all cells needed in the calculation may be calculated with a relevant interval in the iteration according to the necessity. Especially, this explicit scheme is effective for the weak dependency of material properties on temperatures.

3.1.2. *Transient State*

In a similar manner to the steady state, the amplification factor $G_t(\theta_x, \theta_y)$ for the transient state solution in use of the fully explicity scheme is given as follows (see Appendix C):

$$G_t(\theta_x, \theta_y) = 1+\frac{1}{1+\beta^2}\left(\frac{k\,\Delta t}{\rho C\,\Delta x^2}\right)[(\cos 2\theta_x - 1)+2\beta^2(\cos(\theta_x+\theta_y)$$
$$+\cos(\theta_x-\theta_y)-2)+\beta^4(\cos 2\theta_y - 1)]. \tag{5}$$

From the stability condition such that $-1 \leqslant G_t(\theta_x, \theta_y) \leqslant 1$ for all phase angles, we get the following criterion for the time step Δt:

$$0 < \Delta t \leqslant \left(\frac{1+\beta^2}{1+4\beta^2+\beta^4}\right)\left(\frac{\rho C\,\Delta x^2}{k}\right). \tag{6}$$

On the other hand, the time step criterion for the usual scheme using the nearest neighbor variables is

$$0 < \Delta t \leqslant \frac{1}{2(1+\beta^2)}\left(\frac{\rho C\,\Delta x^2}{k}\right). \tag{7}$$

The ratio of the maximum value of Δt in the present scheme to that in the usual scheme is

$$\frac{2(1+\beta^2)^2}{1+4\beta^2+\beta^4}.$$

This value is always larger than unity for all values of β. For instance, in case of $\beta = 1$ ($\Delta x = \Delta y$), a $\frac{4}{3}$ times larger value of Δt than that for the usual scheme is allowable for the present scheme. When $\beta \to 0$ or $\beta \to \infty$, twice the value of Δt is allowable as compared with the usual scheme. These limiting cases correspond to a 1-dimensional problem. Then, it is considered that the diffusion time in the present scheme is twice as large as that in the usual scheme, since the adjacent cells are treated implicitly in the present numerical calculation.

3.2. *Implicit Scheme*

The heat balance equations in the form of Eq. (2) for the whole computational region can be rearranged and combined into the following matrix form:

$$[A]\cdot[T] = [B], \tag{8}$$

where elements of the column vector $[T]$ are composed of the temperatures at a location and its next nearest neighbors.

Let the temperatures put in order such that ..., $T_{i-2,j}$,..., $T_{i-1,j-1}$, $T_{i-1,j+1}$,..., $T_{i,j-2}$, $T_{i,j}$, $T_{i,j+2}$,..., $T_{i+1,j-1}$,... in $[T]^t$. Then, in case of a quadrilateral computational region, there are the following relations between the sequential number $n_{i,j}$ of matrix elements arranged in $[T]$ and the sequential number $m_{i,j}$ through the whole cells:

$$n_{i,j} = \frac{m_{i,j}}{2} + \frac{1-(-1)^{m_{i,j}}}{4}, \tag{9a}$$

$$m_{i,j} = (i-1)\,j_M + j, \tag{9b}$$

with j_M being the maximum number of j. Non-zero elements corresponding to the row number $s = n_{i,j}$ in the square matrix $[A] = [a_{s,t}]$ and the column vector $[B] = [b_s]$ are as follows:

$$
\begin{aligned}
a_{s,t_1} &= -\lambda_{i,j}^{i-1,j}\alpha_{i-1,j}^{(1)},\\
a_{s,t_2} &= -\lambda_{i,j}^{i-1,j}\alpha_{i-1,j}^{(3)} - \lambda_{i,j}^{i,j-1}\alpha_{i,j-1}^{(1)},\\
a_{s,t_2+1} &= -\lambda_{i,j}^{i-1,j}\alpha_{i-1,j}^{(4)} - \lambda_{i,j}^{i,j+1}\alpha_{i,j+1}^{(1)},\\
a_{s,s-1} &= -\lambda_{i,j}^{i,j-1}\alpha_{i,j-1}^{(3)},\\
a_{s,s} &= (1-\alpha_{i-1,j}^{(2)})\,\lambda_{i,j}^{i-1,j} + (1-\alpha_{i+1,j}^{(1)})\,\lambda_{i,j}^{i+1,j}\\
&\quad (1-\alpha_{i,j-1}^{(4)})\,\lambda_{i,j}^{i,j-1} + (1-\alpha_{i,j+1}^{(3)})\,\lambda_{i,j}^{i,j+1} + \rho_{i,j}C_{i,j}\Delta V_{i,j}/\Delta t, \qquad (10a)\\
a_{s,s+1} &= -\lambda_{i,j}^{i,j+1}\alpha_{i,j+1}^{(4)},\\
a_{s,t_3} &= -\lambda_{i,j}^{i+1,j}\alpha_{i+1,j}^{(3)} - \lambda_{i,j}^{i,j-1}\alpha_{i,j-1}^{(2)},\\
a_{s,t_3+1} &= -\lambda_{i,j}^{i+1,j}\alpha_{i+1,j}^{(4)} - \lambda_{i,j}^{i,j+1}\alpha_{i,j+1}^{(2)},\\
a_{s,t_4} &= -\lambda_{i,j}^{i+1,j}\alpha_{i+1,j}^{(2)},\\
b_s &= Q_{i,j}\Delta V_{i,j} + \dot{\rho}_{i,j}\dot{C}_{i,j}\dot{T}_{i,j}\Delta V_{i,j}/\Delta t,
\end{aligned}
$$

where

$$
\begin{aligned}
t_1 &\equiv n_{i-2,j},\\
t_2 &\equiv n_{i-1,j-1},\\
t_3 &\equiv n_{i+1,j-1},\\
t_4 &\equiv n_{i+2,j}.
\end{aligned} \qquad (10b)
$$

When the next nearest neighbor cells are outside the computational region, the above matrix elements are to be slighty modified according to the appropriate boundary conditions explained in Appendix A.

Thus, the size of a matrix can be almost halved as compared with the usual scheme. The temperature of the nearest neighbor cells removed from the matrix elements can be calculated in terms of the next nearest neighbor temperatures included in the matrix elements. Then the material properties of all cells needed in the matrix calculation at the advanced time step are to be calculated.

4. Test Calculations

To demonstrate the effectiveness of the present technique, test calculations for a thermal transient problem. Both the maximum mesh number i_M and j_M are 10. Adiabatic boundary conditions and heat transfer boundary conditions are employed on the boundaries at the both end sides of x-axis and on the boundaries at the both end sides of y-axis, respectively.

Two FORTRAN programs were run on the computer NEAC-ACOS S 1000 for the above test problem during 300 s after the initiation of the transient. One is the

previously developed RCT program [14] in which temperatures of all the computational cells are explicitly treated, resulting in use of 100×100 matrix. The other is based on the present scheme in which the nearest neighbor cells are removed from the matrix elements by applying the present idea, resulting in use of 50×50 matrix. Alost the same results were obtained between the two programs. The RCT program required 135 s of CPU time, while the present program requied 47 s of CPU time. The greater the mesh number, the more decrease in the computing time.

5. Conclusions

Results obtained through the present study are summarized as follows:

(1) A fast computing technique for numerical solutions of diffusion-type equations was proposed. In the present technique, the numerical computation can be performed by using about a half number of variables based on the analytical relations under the governing equations.

(2) Numerical stability of the present scheme was investigated based on the von Neumann linear theory. As compared with the usual schemes, the stability condition in the SOR iteration is not restricted and a larger time increment for transient solutions is allowable.

(3) Test calculations for the thermal transient problem with 100 meshes showed that the computing time was decreased to about $\frac{1}{3}$ as compared with a usual method.

Appendix A

Using the continuity condition of heat flux on the boundary between adjacent cells in Fig. 1, the incoming heat flux from cell (i', j) into cell (i, j) through the interface $S_{i,j}^{i',j}$ with the unit length in the z direction is given by

$$q_{i,j}^{i',j} = \frac{S_{i,j}^{i',j}}{[(\Delta x_i/2)/k_{i,j}] + [(\Delta x_{i'}/2)/k_{i',j}]} (T_{i',j} - T_{i,j}) \tag{A1}$$

(for $i' = i-1$ and $i+1$) with corresponding expression for $q_{i,j}^{i,j'}$ ($j' = j-1$ and $j+1$) having Δy_j in place of Δx_i. When the adjacent cell (i', j) is outside the computational region, the second term in the denominator and $T_{i',j}$ in Eq. (A1) are to be slightly modified corresponding to boundary conditions. For example, in case of Dirichlet type boundary conditions $T_{i',j}$ is to be replaced by the specified temperature; in case of heat transfer boundary condition the second term in the denominator is to be replaced by $1/h$, where h is heat transfer coefficient between the computational boundary and its environmental fluid; in case of adiabatic boundary conditions the limit that h approaches to zero is to be performed. Thus, an

approximate solution of Eq. (1) is obtained by the following finite difference equation using the differencing scheme of the Laossonen type [13]:

$$\left(\frac{\rho_{i,j}C_{i,j}T_{i,j}-\rho'_{i,j}C'_{i,j}T'_{i,j}}{\Delta t}\right)\Delta V_{i,j}=\sum_{(i',j')} q^{i',j'}_{i,j}+Q_{i,j}\Delta V_{i,j} \tag{A2a}$$

$$\begin{aligned}&=\lambda^{i-1,j}_{i,j}(T_{i-1,j}-T_{i,j})+\lambda^{i+1,j}_{i,j}(T_{i+1,j}-T_{i,j})\\&\quad+\lambda^{i,j-1}_{i,j}(T_{i,j-1}-T_{i,j})+\lambda^{i,j+1}_{i,j}(T_{i,j+1}-T_{i,j})\\&\quad+Q_{i,j}\Delta V_{i,j}.\end{aligned} \tag{A2b}$$

From Eq. (A2b), $T_{i,j}$ of the cell (i,j) under consideration at time t is given by

$$T_{i,j}=\alpha^{(1)}_{i,j}T_{i-1,j}+\alpha^{(2)}_{i,j}T_{i+1,j}+\alpha^{(3)}_{i,j}T_{i,j-1}+\alpha^{(4)}_{i,j}T_{i,j+1}+\alpha^{(5)}_{i,j}, \tag{A3}$$

where

$$\alpha^{(1)}_{i,j}\equiv\lambda^{i-1,j}_{i,j}/\Lambda_{i,j},\qquad \alpha^{(2)}_{i,j}\equiv\lambda^{i+1,j}_{i,j}/\Lambda_{i,j},$$

$$\alpha^{(3)}_{i,j}\equiv\lambda^{i,j-1}_{i,j}/\Lambda_{i,j},\qquad \alpha^{(4)}_{i,j}\equiv\lambda^{i,j+1}_{i,j}/\Lambda_{i,j},$$

$$\alpha^{(5)}_{i,j}\equiv\left(Q_{i,j}+\frac{\rho'_{i,j}C'_{i,j}T'_{i,j}}{\Delta t}\right)\Delta V_{i,j}/\Lambda_{i,j},$$

$$\Lambda_{i,j}\equiv\lambda^{i-1,j}_{i,j}+\lambda^{i+1,j}_{i,j}+\lambda^{i,j-1}_{i,j}+\lambda^{i,j+1}_{i,j}+(\rho_{i,j}C_{i,j}\Delta V_{i,j}/\Delta t).$$

$T_{i,j}$ in a steady state (or initial state) is given by removing the terms including Δt in Eq. (A3). In Eq. (A3), $T_{i,j}$ is expressed in terms of the temperatures of the nearest neighbor cells $(i\pm1,j)$, $(i,j\pm1)$ adjacent to the cell (i,j) under consideration. Next, we will express $T_{i,j}$ in terms of only the next nearest neighbor temperatures, which are shown in Fig. 1. Expressing $T_{i\pm1,j}$ and $T_{i,\pm1}$ in terms of $T_{i,j}$ and the next nearest neighbor temperatures ($T_{i-2,j}$, $T_{i-1,j-1}$, $T_{i-1,j+1}$, $T_{i,j-2}$, $T_{i,j+2}$, $T_{i+1,j-1}$, $T_{i+1,j+1}$, and $T_{i+2,j}$) using Eq. (A3) and substituting those expressions into $T_{i\pm1,j}$ and $T_{i,j\pm1}$ in the right-hand side of Eq. (A2b), we obtain Eq. (1).

Appendix B

From Eq. (2), $T_{i,j}$ under consideration in the steady state is given by

$$\begin{aligned}T_{i,j}&=\xi^{(1)}_{i,j}T_{i-2,j}+\xi^{(2)}_{i,j}T_{i-1,j-1}+\xi^{(3)}_{i,j}T_{i-1,j+1}+\xi^{(4)}_{i,j}T_{i,j-2}\\&\quad+\xi^{(5)}_{i,j}T_{i,j+2}+\xi^{(6)}_{i,j}T_{i+1,j-1}+\xi^{(7)}_{i,j}T_{i+1,j+1}+\xi^{(8)}_{i,j}T_{i+2,j}+\xi^{(9)}_{i,j}\end{aligned} \tag{B1a}$$

$$T_{i,j}\equiv f(T_{i-2,j},\ T_{i-1,j-1},\ T_{i-1,j+1},\ T_{i,j-2},\ T_{i,j+2},\ T_{i+1,j-1},\ T_{i+1,j+1},\ T_{i+2,j}), \tag{B1b}$$

where

$$
\begin{aligned}
\xi_{i,j}^{(1)} &\equiv \lambda_{i,j}^{i-1,j}\alpha_{i-1,j}^{(1)}/\Sigma_{i,j},\\
\xi_{i,j}^{(2)} &\equiv (\lambda_{i,j}^{i-1,j}\alpha_{i-1,j}^{(3)} + \lambda_{i,j}^{i,j-1}\alpha_{i,j-1}^{(1)})/\Sigma_{i,j},\\
\xi_{i,j}^{(3)} &\equiv (\lambda_{i,j}^{i-1,j}\alpha_{i-1,j}^{(4)} + \lambda_{i,j}^{i,j+1}\alpha_{i,j+1}^{(1)})/\Sigma_{i,j},\\
\xi_{i,j}^{(4)} &\equiv \lambda_{i,j}^{i,j-1}\alpha_{i,j-1}^{(3)}/\Sigma_{i,j},\\
\xi_{i,j}^{(5)} &\equiv \lambda_{i,j}^{i,j+1}\alpha_{i,j+1}^{(4)}/\Sigma_{i,j},\\
\xi_{i,j}^{(6)} &\equiv (\lambda_{i,j}^{i+1,j}\alpha_{i+1,j}^{(3)} + \lambda_{i,j}^{i,j-1}\alpha_{i,j-1}^{(2)})/\Sigma_{i,j},\\
\xi_{i,j}^{(7)} &\equiv (\lambda_{i,j}^{i+1,j}\alpha_{i+1,j}^{(4)} + \lambda_{i,j}^{i,j+1}\alpha_{i,j+1}^{(2)})/\Sigma_{i,j},\\
\xi_{i,j}^{(8)} &\equiv \lambda_{i,j}^{i+1,j}\alpha_{i+1,j}^{(2)}/\Sigma_{i,j},\\
\xi_{i,j}^{(9)} &\equiv [\lambda_{i,j}^{i-1,j}\alpha_{i-1,j}^{(5)} + \lambda_{i,j}^{i+1,j}\alpha_{i+1,j}^{(5)} + \lambda_{i,j}^{i,j-1}\alpha_{i,j-1}^{(5)}\\
&\qquad + \lambda_{i,j}^{i,j+1}\alpha_{i,j+1}^{(5)} + Q_{i,j}\Delta V_{i,j}]/\Sigma_{i,j},\\
\Sigma_{i,j} &\equiv (1-\alpha_{i-1,j}^{(2)})\,\lambda_{i,j}^{i-1,j} + (1-\alpha_{i,j+1}^{(1)})\,\lambda_{i,j}^{i+1,j}\\
&\qquad + (1-\alpha_{i,j-1}^{(4)})\,\lambda_{i,j}^{i,j-1} + (1-\alpha_{i,j+1}^{(3)})\,\lambda_{i,j}^{i,j+1},
\end{aligned}
\tag{B2}
$$

and f represents the function defined by Eq. (B1).

In the SOR method, the temperature of cell (i,j) at the $(l+1)$th iteration is corrected by a weighted residue in terms of an accelerating factor ω as follows:

$$T_{i,j}^{l+1} = T_{i,j}^{l} + \omega[f^{l+1}(T_{i-2,j},\ldots,T_{i+2,j}) - T_{i,j}^{l}] \tag{B3a}$$

$$
\begin{aligned}
&= T_{i,j}^{l} + \omega[\xi_{i,j}^{(1)}T_{i-2,j}^{l+1} + \xi_{i,j}^{(2)}T_{i-1,j-1}^{l+1} + \xi_{i,j}^{(3)}T_{i-1,j+1}^{l+1}\\
&\quad + \xi_{i,j}^{(4)}T_{i,j-2}^{l+1} + \xi_{i,j}^{(5)}T_{i,j+2}^{l} + \xi_{i,j}^{(6)}T_{i+1,j-1}^{l}\\
&\quad + \xi_{i,j}^{(7)}T_{i+1,j+1}^{l} + \xi_{i,j}^{(8)}T_{i+2,j}^{l} + \xi_{i,j}^{(9)} - T_{i,j}^{l}].
\end{aligned}
\tag{B3b}
$$

In the above equation, the temperature of the cells $(i-2,j)$, $(i-1,j-1)$, $(i-1,j+1)$, and $(i,j-2)$ are replaced by the latest values at the $(l+1)$th iteration while sweeping in the direction of increasing i and j in use of the Liebman method [4]. In case of constant material properties and regular space meshes ($\Delta x_i = \Delta x$, $\Delta y_j = \Delta y$), $\xi_{i,j}^{(1)},\ldots,\xi_{i,j}^{(8)}$ are as follows:

$$
\begin{aligned}
\xi_{i,j}^{(1)} &= \frac{1}{2A}, & \xi_{i,j}^{(2)} &= \frac{\beta^2}{A},\\
\xi_{i,j}^{(3)} &= \frac{\beta^2}{A}, & \xi_{i,j}^{(4)} &= \frac{\beta^4}{2A},\\
\xi_{i,j}^{(5)} &= \frac{\beta^4}{2A}, & \xi_{i,j}^{(6)} &= \frac{\beta^2}{A},\\
\xi_{i,j}^{(7)} &= \frac{\beta^2}{A}, & \xi_{i,j}^{(8)} &= \frac{1}{2A},
\end{aligned}
\tag{B4}
$$

where

$$A \equiv 1 + 4\beta^2 + \beta^4,$$

$$\beta \equiv \Delta x/\Delta y.$$

Since both the exact solution and the numerical solution of Eq. (B3) satisfy the same difference equation, the error, δT, of the numerical solution due to accumulation of round-off errors satisfies the same equation as Eq. (B3) except the source term introducing no errors. The general solution for δT with periodic boundary conditions is

$$\delta T_{i,j} = \sum_{(\theta_x, \theta_y)} V^l(\theta_x, \theta_y)\, e^{\sqrt{-1}(i\theta_x + j\theta_y)}, \tag{B5}$$

where θ_x and θ_y are any phase angles of the Fourier component. The variation of the amplitude $V^l(\theta_x, \theta_y)$ vs iteration l is governed by the following amplification factor:

$$G_y(\theta_x, \theta_y) \equiv \left| \frac{V(\theta_x, \theta_y)^{l+1}}{V(\theta_x, \theta_y)^l} \right|. \tag{B6}$$

In a straightforward calculation with substitution of Eqs. (B3) and (B4) into the error equation (i.e., Eq. (B3b) without the source term), we get Eq. (3) in Chapter 3 for the amplification factor.

Appendix C

From Eq. (2), $T_{i,j}$ under consideration in a transient state is given in the fully explicit scheme as follows:

$$\begin{aligned} T^{n+1}_{i,j} = {} & \psi^{(1)}_{i,j} T^n_{i-2,j} + \psi^{(2)}_{i,j} T^n_{i-1,j-1} + \psi^{(3)}_{i,j} T^n_{i-1,j+1} \\ & + \psi^{(4)}_{i,j} T^n_{i,j-2} + \psi^{(5)}_{i,j} T^n_{i,j} + \psi^{(6)}_{i,j} T^n_{i,j+2} + \psi^{(7)}_{i,j} T^n_{i+1,j-1} \\ & + \psi^{(8)}_{i,j} T^n_{i+1,j+1} + \psi^{(9)}_{i,j} T^n_{i+2,j} + \psi^{(10)}_{i,j}, \end{aligned} \tag{C1}$$

where

$$\psi^{(1)}_{i,j} \equiv \lambda^{i-1,j}_{i,j} \alpha^{(1)}_{i-1,j} \Delta t/(\rho_{i,j} C_{i,j} \Delta V_{i,j}),$$

$$\psi^{(2)}_{i,j} \equiv (\lambda^{i-1,j}_{i,j} \alpha^{(3)}_{i-1,j} + \lambda^{i,j-1}_{i,j} \alpha^{(1)}_{i,j-1})\, \Delta t/(\rho_{i,j} C_{i,j} \Delta V_{i,j}),$$

$$\psi^{(3)}_{i,j} \equiv (\lambda^{i-1,j}_{i,j} \alpha^{(4)}_{i-1,j} + \lambda^{i,j+1}_{i,j} \alpha^{(1)}_{i,j+1})\, \Delta t/(\rho_{i,j} C_{i,j} \Delta V_{i,j}),$$

$$\psi^{(4)}_{i,j} \equiv \lambda^{i,j-1}_{i,j} \alpha^{(3)}_{i,j-1} \Delta t/(\rho_{i,j} C_{i,j} \Delta V_{i,j}),$$

$$\begin{aligned} \psi^{(5)}_{i,j} \equiv {} & [\lambda^{i-1,j}_{i,j} (\alpha^{(2)}_{i-1,j} - 1) + \lambda^{i+1,j}_{i,j} (\alpha^{(1)}_{i+1,j} - 1) + \lambda^{i,j-1}_{i,j} (\alpha^{(4)}_{i,j-1}) \\ & + \lambda^{i,j+1}_{i,j} (\alpha^{(3)}_{i,j+1} - 1)]\, \Delta t/(\rho_{i,j} C_{i,j} \Delta V_{i,j}) + \dot{\rho}_{i,j} \dot{C}_{i,j}/(\rho_{i,j} C_{i,j}) \end{aligned}$$

$$\psi_{i,j}^{(6)} \equiv \lambda_{i,j}^{i,j+1}\alpha_{i,j+1}^{(4)}\Delta t/(\rho_{i,j}C_{i,j}\Delta V_{i,j}),$$

$$\psi_{i,j}^{(7)} \equiv (\lambda_{i,j}^{i+1,j}\alpha_{i+1,j}^{(3)} + \lambda_{i,j}^{i,j-1}\alpha_{i,j-1}^{(2)})\,\Delta t/(\rho_{i,j}C_{i,j}\Delta V_{i,j}),$$

$$\psi_{i,j}^{(8)} \equiv (\lambda_{i,j}^{i+1,j}\alpha_{i+1,j}^{(4)} + \lambda_{i,j}^{i,j+1}\alpha_{i,j+1}^{(2)})\,\Delta t/(\rho_{i,j}C_{i,j}\Delta V_{i,j}),$$

$$\psi_{i,j}^{(9)} \equiv \lambda_{i,j}^{i+1,j}\alpha_{i+1,j}^{(2)}\Delta t/(\rho_{i,j}C_{i,j}\Delta V_{i,j}),$$

$$\psi_{i,j}^{(10)} \equiv (\lambda_{i,j}^{i-1,j}\alpha_{i-1,j}^{(5)} + \lambda_{i,j}^{i+1,j}\alpha_{i+1,j}^{(5)} + \lambda_{i,j}^{i,j-1}\alpha_{i,j-1}^{(5)} + \lambda_{i,j}^{i,j+1}\alpha_{i,j+1}^{(5)} + Q_{i,j}\Delta V_{i,j})\,\Delta t/(\rho_{i,j}C_{i,j}\Delta V_{i,j}).$$

Here, an index n denotes the time step number as counted from the initial state.

For the constant material properties and regular meshes, $\psi_{i,j}^{(1)},\ldots,\psi_{i,j}^{(9)}$ are as follows:

$$\psi_{i,j}^{(1)} = \frac{1}{2(1+\beta^2)}\left(\frac{k}{\Delta x^2}\right)\left(\frac{\Delta t}{\rho C}\right), \qquad \psi_{i,j}^{(2)} = \frac{\beta^2}{1+\beta^2}\left(\frac{k}{\Delta x^2}\right)\left(\frac{\Delta t}{\rho C}\right),$$

$$\psi_{i,j}^{(3)} = \frac{\beta^2}{1+\beta^2}\left(\frac{k}{\Delta x^2}\right)\left(\frac{\Delta t}{\rho C}\right), \qquad \psi_{i,j}^{(4)} = \frac{\beta^4}{2(1+\beta^2)}\left(\frac{k}{\Delta x^2}\right)\left(\frac{\Delta t}{\rho C}\right),$$

$$\psi_{i,j}^{(5)} = 1 - \frac{1}{(1+\beta^2)}(1+4\beta^2+\beta^4)\left(\frac{k}{\Delta x^2}\right)\left(\frac{\Delta t}{\rho C}\right),$$

$$\psi_{i,j}^{(6)} = \frac{\beta^4}{2(1+\beta^2)}\left(\frac{k}{\Delta x^2}\right)\left(\frac{\Delta t}{\rho C}\right), \qquad \psi_{i,j}^{(7)} = \frac{\beta^2}{1+\beta^2}\left(\frac{k}{\Delta x^2}\right)\left(\frac{\Delta t}{\rho C}\right),$$

$$\psi_{i,j}^{(8)} = \frac{\beta^2}{1+\beta^2}\left(\frac{k}{\Delta x^2}\right)\left(\frac{\Delta t}{\rho C}\right), \qquad \psi_{i,j}^{(9)} = \frac{1}{2(1+\beta^2)}\left(\frac{k}{\Delta x^2}\right)\left(\frac{\Delta t}{\rho C}\right).$$

Based on the von Neumann linear theory, we get Eq. (5) for the amplification factor $G_t(\theta_x, \theta_y)$ in a similar manner to $G_s(\theta_x, \theta_y)$ for the steady state.

REFERENCES

1. K. SAKAI, *J. Comput. Phys.* **40** No. 2, 509 (1981).
2. K. SAKAI, M. YANO AND H. TEZUKA, *Nucl. Eng. Des.* **73**, 373 (1983).
3. S. V. PATANKER AND D. B. SPALDING, *Int. J. Heat Mass Transfer* **15**, 1787 (1972).
4. S. P. FRANKEL, *Math Tables Aids Comput.* **4**, 65 (1950).
5. D. YOUNG, *Trans. Amer. Math. Soc.* **76**, 92 (1954).
6. H. M. DOMANUS ET AL., ANL Report ANL–81–10, 1980, p. 55.
7. U. SCHUMANN, *Angew. Inform.* **5**, 213 (1972).
8. U. SCHUMANN, *IEEE Trans. Comput.* **C-22**, 542 (1973).
9. B. L. BUZBEE, *IEEE Trans. Comput.* **C–22**, 793 (1973).
10. R. W. HOCKNEY, *J. Assoc. Comput. Mach.* **12**, 95 (1965).
11. D. M. BURRIDGE AND C. TEMPERTON, *J. Comput. Phys.* **30**, 145 (1979).
12. P. J. ROACHE, *Computational Fluid Dynamics*, (Hermosa, Albuquerque, 1972).
13. R. D. RICHTMYER AND K. W. MORTON, *Difference Method for Initial-Value Problem* (Wiley, New York, 1967), p. 189.
14. K. SAKAI AND T. SEKIYA, *Technol. Rep. Osaka Univ.* **33**, No. 1709, 221 (1983).