

LANDMARK UNIVERSITY, OMU-ARAN

LECTURE NOTE COLLEGE: COLLEGE OF SCIENCE AND ENGINEERING DEPARTMENT: MECHANICAL ENGINEERING *Course code: MCE521 Course title:* ADVANCED COMPUTATIONAL DYNAMICS. Credit unit: 2 UNITS. Course status: *compulsory* ENGR. ALIYU, S.J CFD CLASS WORK EXAMPLES.

3.7 Making Choices

In the previous two sections, we have introduced TSE and IOCV methods as well as explicit and implicit procedures. Here, we offer advice on the best choice of combination, keeping in mind the requirements of multidimensional problems (including convection) to be discussed in later sections. Further, we also keep in mind that coefficients AE and AW are in general not constant. This makes the discretized equations nonlinear.

1. Note that the TSE method casts the governing equations in non-conservative form whereas the IOCV method uses the as-derived conservative form. As we shall observe later, this matter is of considerable physical significance when convective problems are considered.

2. In the TSE method, coefficients AE and AW carry little physical meaning. In the IOCV method, they represent conductances.

3. In the TSE method, Scarborough's criterion may be violated. In the IOCV method, this can never happen.

4. The question of invoking explicit procedure arises only when unsteady-state problems are considered. The implicit procedure, in contrast, can be invoked for both unsteady-state as well as steady-state problems. In fact, in steady-state problems ($\Delta t = \infty$) the implicit procedure is the only one possible (Check note).

5. The explicit procedure imposes restriction on the largest time step to obtain stable solutions. The implicit procedure does not suffer from such a restriction.

In view of these comments, the best choice is to employ the IOCV method with an implicit procedure. Throughout this book, therefore, this combination will be preferred.

Note,

Some analysts employ an explicit procedure even for a steady-state problem. In this case, calculations proceed by introducing a *false* or imaginary time step. Hence, such procedures are called false transient procedures.

3.8 Dealing with Nonlinearities

Now that we have accepted a combination of IOCV with the implicit procedure, we restate the main governing discretised equation (equations 2.38 and 2.39) but in a slightly altered form:

$$(AP_{i} + SP_{i})T_{i}^{l+1} = AE_{i}T_{i+1}^{l+1} + AW_{i}T_{i-1}^{l+1} + Su_{i}, \quad i = 2, 3, \dots, N-1, \dots, 43$$

$$AP_{i} = AE_{i} + AW_{i}, \quad \dots, 44$$

$$AE_{i} = \frac{kA}{\Delta x}\Big|_{i+1/2}, \quad \dots, 45$$

$$AW_{i} = \frac{kA}{\Delta x}\Big|_{i-1/2}, \quad \dots, 46$$

$$Su_{i} = \frac{\rho\Delta V_{i}C_{i}^{0}}{\Delta t}T_{i}^{0}, SP_{i} = \frac{\rho\Delta V_{i}C_{i}^{n}}{\Delta t}, \quad \dots, 47$$

In these equations, the q''' term is deliberately ignored because it is a *problem dependent* term. The altered form shown in Equation 43 will be useful in dealing with nonlinearities. Also, a generalised computer code can be constructed around Equation 43 in such away that preserves the underlying physics. The non-linearities can emanate from three sources:

1. if q''' is a function of T

2. if conductivity k is a function of T or changes abruptly, as in a composite material and/or

3. boundary conditions at x = 0 and x = L.

In the following, we discuss methods for dealing with nonlinearities through modification of Su_i and Sp_i .

3.8.1 Nonlinear Sources

Consider a pin fin losing heat to its surroundings under *steady state* by convection with heat transfer coefficient h. Then, q''' will be given by

$$q_i^{\prime\prime\prime} = -\frac{h_i P_i \Delta x_i (T_i - T_{\infty})}{A_i \Delta x_i}, \quad \quad 48$$

where Pi is the local fin perimeter. Therefore,

$$q_i^{\prime\prime\prime} \Delta V_i = -h_i P_i \Delta x_i (T_i - T_\infty). \quad \dots \quad 49$$

When this equation is included in Equation 43, it is obvious that Ti will now appear on both sides of the equation. One can therefore write the total source term as

Source term = $Su_i + h_i P_i \Delta x_i (T_{\infty} - T_i)$ 50

This prescription can be accommodated by updating Su_i and Sp_i as

$$Su_i = Su_i + h_i P_i \Delta x_i T_{\infty}$$
,

Where Su_i and Sp_i on the RHSs are the original quantities given in Equation 47. Note that, in this case, the updated Sp_i is positive and, therefore, there is no danger of rendering AP_i + Sp_i negative. Thus, Scarborough's criterion cannot be violated. However, if we considered dissipation of heat due to an electric current or chemical reaction (as in setting of cement) then, because heat is generated within the medium, $q_i'' = a + bT_i^m$, where b is positive. In this case, Su_i = Su_i + a Δ V_i and Sp_i = Sp_i - b $T_i^{m-1}\Delta$ V_i. But now, there is a danger of violating Scarborough's criterion and, therefore, one simply sets Su_i = Su_i + $q_i''' \Delta$ V_i and Sp_i is not updated. Accounting for the source term in the manner of Equation 51 is called source term linearization. We shall discover further advantages of this form when dealing with the application of boundary conditions.

3.8.2 Nonlinear Coefficients

Coefficients AE_i and AW_i can become functions of temperature owing to thermal conductivity as in $k = a + b T + c T^2$. Thus, $k_{i+1/2}$ in AE_i (see Equation 45),

for example, may be evaluated in two ways:

$$k_{i+1/2} = a + b T_{i+1/2} + c T_{i+1/2}^2, \quad T_{i+1/2} = 0.5(T_i + T_{i+1}) \quad \dots \quad 52$$

or

Both of these representations are pragmatically acceptable but neither can be justified on the basis of the physics of conductance. To illustrate this point, let us consider a composite medium consisting of two materials with constant conductivities k_1 and k_2 (see Figure 7). In this case, we lay the grid nodes *i* and *i* + 1 in such a way that the cell face *i* + 1/2 *coincides* with the location where the two materials are joined. Thus, there is a discontinuity in conductivity at the *i* + $\frac{1}{2}$ location. Now, in spite of the discontinuity, the heat transfer $Q_{i+1/2}$ on either side of *i* + 1/2 must be the same. Therefore,

$$Q_{i+1/2} = k_1 A_{i+1/2} \frac{T_i - T_{i+1/2}}{x_{i+1/2} - x_i}, \quad k_1 = k_i, \quad \dots \quad 54$$
$$Q_{i+1/2} = k_2 A_{i+1/2} \frac{T_{i+1/2} - T_{i+1/2}}{x_{i+1} - x_{i+1/2}}, \quad k_2 = k_{i+1} \quad \dots \quad 55$$



Figure 7. Interpolation of conductivity.

Eliminating Ti+1/2 from these equations gives

$$Q_{i+1/2} = A_{i+1/2} \left[\frac{x_{i+1/2} - x_i}{k_i} + \frac{x_{i+1} - x_{i+1/2}}{k_{i+1}} \right]^{-1} (T_i - T_{i+1}). \quad \dots \dots \quad 56$$

We recall, however, that our discretised equation was derived on the basis of *linear* temperature variation between nodes i and i + 1 (see Equation 21). This implies that

$$Q_{i+1/2} = \frac{A}{\Delta x}\Big|_{i+1/2} k_{i+1/2} (T_i - T_{i+1}). \quad \dots \quad 57$$

Comparing Equations 56 and 57, leads to

$$k_{i+1/2} = \Delta x_{i+1/2} \left[\frac{x_{i+1/2} - x_i}{k_i} + \frac{x_{i+1} - x_{i+1/2}}{k_{i+1}} \right]^{-1}.$$
 (58)

If the cell face were midway between the nodes then this equation would read as

$$k_{i+1/2} = 2 \left[\frac{1}{k_i} + \frac{1}{k_{i+1}} \right]^{-1}.$$

These equations suggest that the conductivity at a cell face should be evaluated by a harmonic mean to accord with the physics of conductance. We shall regard this as a general practise and extend it to the case when thermal conductivity varies with temperature. Thus, instead of using either Equation 52 or 53, Equation 58 will be used with k_i and k_{i+1} evaluated in terms of temperatures T_i and T_{i+1} , respectively. Further, note that if conductivity is constant, $k_{i+1/2} = k_i = k_{i+1}$.

3.8.3 Boundary Conditions

In practical problems, three types of boundary conditions are encountered:

- 1. Boundary temperatures T_1 and/or T_N are specified.
- 2. Boundary heat fluxes q_1 and/or q_N are specified.
- 3. Boundary heat transfer coefficients h_1 and/or h_N are specified.

Our interest in this section lies in prescribing these boundary conditions by employing Su and Sp for the near-boundary nodes.

Boundary Temperature Specified

For the purpose of illustration, consider the i = 2 node, where T_1 is specified. Then,

Equation 43 will read as

Where Su_2 and Sp_2 are already updated to account for any source term. Equation 60 can be left as it is but we alter it via a three-step procedure in which we set

With this specification, AP_2 will now equal AE_2 because AW_2 is set to zero, but the coefficient of T_2^{l+1} remains intact because Sp_2 has been updated. Thus, the boundary condition specification is accomplished by *snapping* the boundary connection in the main discretised equation.

Heat Flux Specified

Let heat flux q_1 be specified at x = 0 (see Figure 8) Then, temperature T_1 is unknown and heat transfer will be given by

$$Q_1 = A_1 q_1 = A W_2 (T_1 - T_2), \qquad 62$$
$$T_1 = \frac{A_1 q_1}{A W_2} + T_2. \qquad 63$$

From Equation 60, it is clear that one can apply the boundary condition by employing the following sequence:

- 1. Calculate T_1 from Equation 63.
- 2. Update $Su_2 = Su_2 + A_1 q_1$ and $Sp_2 = Sp_2 + 0$.
- 3. Set $AW_2 = 0$.

The q_N -specified boundary condition can be similarly dealt with by altering AE_{N-1} and Su_{N-1} .

Heat Transfer Coefficient Specified

In this case, let h_1 be the specified heat transfer coefficient (see Figure 7 again) and let T_{∞} be the fluid temperature adjacent to the surface at x = 0. Then,

$$Q_1 = A_1 q_1 = A_1 h_1 (T_{\infty} - T_1) = A W_2 (T_1 - T_2) \dots 64$$

Therefore,



Figure 8. Flux boundary condition.

In this case, the boundary condition can be implemented via the following steps:

1. Calculate T_1 from Equation 65.

2. Update

$$Sp_2 = Sp_2 + \left[\frac{1}{A_1h_1} + \frac{1}{AW_2}\right]^{-1}$$
 and $Su_2 = Su_2 + \left[\frac{1}{A_1h_1} + \frac{1}{AW_2}\right]^{-1}T_{\infty}$.

3. Set $AW_2 = 0$.

Thus, for all types of boundary conditions, we are able to find appropriate Su and Sp augmentations and then set the boundary coefficient of the near-boundary node (AW_2 in our examples) to zero. The usefulness of this practise will become apparent when we consider the issue of convergence enhancement of the iterative solution procedures of 2D equations.

3.8.4 Underrelaxation

In a nonlinear problem, if k and/or q_i'' are strong functions of temperature then, in an iterative procedure, as the temperature field changes, the coefficients AP, AE, and AW and the source S may change very rapidly from iteration to iteration. In such highly nonlinear problems, the iterative solution may yield oscillatory or erratic convergence or may even diverge. Therefore, it is desirable to restrict the changes in temperature implied by Equation 43. Such a restriction is called underrelaxation. It can be effected by rewriting Equation 43 as

$$T_i^{l+1} = \frac{\alpha \left[AE_i T_{i+1}^{l+1} + AW_i T_{i-1}^{l+1} + Su_i \right]}{AP_i + Sp_i} + (1 + \alpha) T_i^l, \quad \dots \dots \quad 66$$

Where $0 < \alpha \le 1$. If $\alpha = 1$, no underrelaxation will be effected. If $\alpha = 0$, no change will be effected, therefore, this case is not of interest. The underrelaxation can be effected without altering the structure of Equation 43 by simply augmenting *Su* and *Sp before* every iteration. Thus,

If the coefficients AE_i and AW_i were constants and not functions of T then it is also possible to take $1 \le \alpha < 2$. This is called *overrelaxation*. Typically, compared to the case of $\alpha = 1$, the convergence rate with overrelaxation is faster up to a certain optimum α opt, but for $\alpha > \alpha$ opt, the convergence rate again slows down, so much so that it may be even slower than that with $\alpha = 1$. The magnitude of α opt is problem dependent.

3.9 Methods of Solution

When coefficients AE_i , AW_i , and AP_i are calculated and Sui and Sp_i are suitably updated to account for the effects of source linearization, boundary conditions, and underrelaxation, we are ready to solve the set of equations (43) at an iteration level l + 1. There are two extensively used methods for solving such equations.

3.9.1 Gauss-Seidel Method

The Gauss-Seidel (GS) method is extremely simple to implement on a computer.

The main steps are as follows:

1. At a given iteration level *l*, calculate coefficients *AE*, *AW*, *AP*, *Su*, and *Sp* using temperature T^l for i = 2 to N - 1

2. Hence, execute a DO loop:

100 FCMX = 0 D0 1 I = 2, N-1 TL = T(I) ANUM = AE(I)*T(I+1) + AW(I)*T(I-1) + SU(I)ADEN = AE(I) + AW(I) + SP(I)T(I) = ANUM / ADEN FC = (T(I) - TL) / TL IF (ABS(FC).GT.FCMX) FCMX = ABS(FC) 1 CONTINUE

3. If FCMX > CC, go to step 1.

The method is also called a *point-by-point* method because each node *i* is visited in succession. The method is very reliable but requires a large number of iterations and hence considerable computer time, particularly when *N* is large.

3.9.2 Tridiagonal Matrix Algorithm

In the tridiagonal matrix algorithm (TDMA), Equation 43 is rewritten as

Where,

Note that since $Sp_i \ge 0$, a_i and b_i can only be fractions. Equation 69 represents (N - 2) simultaneous algebraic equations. In matrix form, these equations can be written as [A] [T] = [C], where the coefficient matrix [A] will appear as shown in Figure 9.



Figure 9. Diagonally dominant matrix [A].

Notice that the coefficient of T_i occupies the diagonal position of the matrix with $-a_i$ and $-b_i$ occupying the neighbouring diagonal positions. All other elements of the matrix are zero. The matrix [A] thus has diagonally dominant tridiagonal structure. This structure can be exploited as follows. Let

Then

Now, substituting this equation in Equation 2.69, we can show that

$$T_{i} = \left[\frac{a_{i}}{1-b_{i}A_{i-1}}\right]T_{i+1} + \left[\frac{b_{i}B_{i-1}+c_{i}}{1-b_{i}A_{i-1}}\right].$$
(73)

Comparison of Equation 73 with Equation 71 shows that

$$A_{i} = \frac{a_{i}}{1 - b_{i}A_{i-1}}, \qquad \dots \dots 74$$
$$B_{i} = \frac{b_{i}B_{i-1} + c_{i}}{1 - b_{i}A_{i-1}}. \qquad \dots \dots 75$$

Thus, Ai and Bi can be calculated by recurrence. The implementation steps are as follows:

1. Prepare a_i , b_i , and c_i for i = 2 to N - 1 from knowledge of the T_i^l distribution.

2. From comparison of Equations 69 and 71, set $A_2 = a_2$ and $B_2 = c_2$ (because $b_2 = 0$ via the boundary condition specification). Now evaluate A_i and B_i for i = 3 to N - 1 by recurrence using Equations 74 and 75.

3. Evaluate T_i by backwards substitution using Equation 71, that is, from i = N - 1 to 2. Note that since we prescribe boundary conditions such that $AE_{N-1} = 0$, it follows that $A_{N-1} = 0$.

4. Evaluate fractional change as before and go to step 1 if the convergence criterion is not satisfied. The TDMA is essentially a forward elimination (implicit in the recurrence relations) and backward substitution procedure in which temperatures at all *i* are updated simultaneously in step 3. Hence, the TDMA is also called a *line-by-line* procedure to contrast it with the point-by-point GS procedure introduced earlier. Further, we note that if a_i , b_i , and c_i were constants and not functions of *T* then the TDMA would yield a solution in just one iteration whereas the point-by-point procedure would require several iterations even when coefficients are constants.

CLASS EXAMPLE.

1. A rectangular fin of length 2 cm, thickness 2 mm, and breadth 20 cm is attached to a plane wall as shown in Figure 6. The wall temperature $T_w = 225^{\circ}$ C and ambient temperature $T_{\infty} = 25^{\circ}$ C. For the fin material, k = 45 W/m-K and the operating h = 15 W/m²-K. Determine the heat loss from the fin and its effectiveness. Assume the tip heat loss to be negligible.



1. Table 4.1: Coefficients in the discretized equation

i	2	3	4	5	6
AW_i	0	4.5	4.5	4.5	4.5
AE_i	4.5	4.5	4.5	4.5	0
Su_i	2025.6	0.6	0.6	0.6	0.6
Sp_i	9.024	0.024	0.024	0.024	0.024

Table 4.2: Solution by Gauss – Seidel method.

1	FCMX	0 cm	0.2 cm	0.6 cm	1.0 cm	1.4 cm	1.8 cm	2.0 cm
0		225	223	219	215	211	207	205
1	0.01	225	222.65	218.31	214.15	210.08	209.1	209.1
2	0.0034	225	222.42	217.77	213.44	210.77	209.78	209.78
3	0.0021	225	222.24	217.32	213.54	211.16	210.18	210.18
3	:	:	:	:	3	÷	:	:
22	0.00012	225	222.41	218.28	215.22	213.19	212.19	212.19
23	0.00011	225	222.41	218.30	215.24	213.21	212.21	212.21
24	0.000092	225	222.42	218.31	215.25	213.23	212.23	212.23
Exact	19 <u>—</u> 51	225	222.58	218.52	215.51	213.49	212.49	212.37

Table 4.3: Solution by TDMA

x (cm)	0	0.2	0.6	1.0	1.4	1.8	2
A_i	-	0.333	0.598	0.711	0.772	0.0	
B_i		149.78	89.628	63.776	49.357	212.375	-
l = 1	225	222.45	218.40	215.38	213.37	212.37	212.37
Exact	225	222.58	218.52	215.51	213.49	212.49	212.37

SOLUTION.

Given data:

Length: 2 cm

Thickness: 2mm

Breath: 200cm

T_w: 225⁰C

 $T_{\infty}=25^0C$

k: 45W/m-k

h: 15 W/m²k

Solution.

The exact solution to this problem is

 $\frac{T - T_{\infty}}{T_w - T_{\infty}} = \frac{\cosh m(L - x)}{\cosh m L},$ $Q_{loss} = \sqrt{hPkA}(T_w - T_{\infty})tanh(m L),$ Where $m = \sqrt{hP/kA}$. Perimeter $P = 2 \times 20 = 40$ cm, Area $A = 20 \times 0.2 = 4$ cm², L = 2 cm. Therefore, m = 18.257m⁻¹ and $Q_{loss} = 23$ W. Let N = 7 and $\Delta x = 0.4$ cm $AW_2 = 45 \times 4 \times 10^{-4}/0.002 = 9$ $AW_i = 4.5 \text{ for } i = 3 \text{ to } 6.$ $AE_i = 4.5 \text{ for } i = 2 \text{ to } 5$ $AE_6 = 9.$ The boundary conditions are $T_1 = 225$ and $q_7 = 0$ (negligible tip loss). Further, $Su_i = h_i P \Delta x_i T \infty = 15 \times 0.4 \times 0.004 \times 25 = 0.6$ $Sp_i = 15 \times 0.4 \times 0.004 = 0.024.$ But $T_7 = 0 + T_6 = T_6.$ Thus, our discretised equations are $T_1 = 225,$ $[9 + 4.5 + 0.024] T_2 = 4.5 T_3 + 9 T_1 + 0.6,$ $[4.5 + 4.5 + 0.024] T_i = 4.5 T_{i+1} + 4.5 T_{i-1} + 0.6, i = 3, 4, 5,$ $[4.5 + 0.024] T_6 = 4.5 T_5 + 0.6,$ $T_7 = T_6.$

Note: Conductivity, area, perimeter and heat transfer coefficient are constant i.e

AE & AW do not change.

From the converged solution, the fin heat loss is estimated as

 $Q_{\text{loss}} = AW_2 \times (T_1 - T_2) = 9 (225 - 222.42) = 23.26 \text{ W}.$