ADVANCES IN COMPUTER METHODS FOR PARTIAL DIFFERENTIAL EQUATIONS

Proceedings of the AICA International Symposium
on Computer Methods for Partial Differential Equations
held at Lehigh University - Bethlehem, Pennsylvania, U.S.A.
June 17-19, 1975

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Published by AICA
1975

AICA
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Rutgers University
New Brunswick, N. J. 08903 U.S.A.

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University of Ghent
533 Coupure Links
B-9000 Ghent, Belgium

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PUBL. A I C A - 1975

FINITE DIFFERENCE MODELLING OF THE HEAT CONDUCTION EQUATION IN GENERAL ORTHOGONAL CURVILINEAR COORDINATES USING TAYLOR SERIES EXPANSION

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Abstract

In the analytic solution of heat conduction and other potential field problems, it is often advantageous to employ an orthogonal curvilinear coordinate system. Advantages similar to those obtained in analytic solutions can also be gained through their use in numerical solutions. Using a Taylor series expansion to approximate the spatial derivatives appearing in the general heat conduction equation with appropriate consideration of the heat generation and time dependent terms, general expressions are derived which define the finite difference coefficients for use in finite difference analyses. The ease of applicability of the resultant coefficients is demonstrated by example for the circular cylinder coordinate system. A second example employing oblate spheroidal coordinates is also given. Two references cited illustrate its successful usage on practical problems. The generalized finite difference coefficients can provide substantial flexibility, accuracy, and economy to finite difference solutions when appropriate selection of the coordinate system is made.

Nomenclature

a	=	generating disk radius of oblate spheroidal coordinate system
A	=	area
C_1,C_2,C_3	=	finite difference (f.d.) coefficients
C_4,C_5,C_6,C_s	=	finite difference (f.d.) coefficients
C_p	=	specific heat at constant pressure
D	=	constant, defined in equation (17)
Fo	=	Fourier modulus, $\alpha t/a^2$
g_1,g_2,g_3,g	=	metric coefficients (defined in text)
i,j,k	=	subscripts denoting three principal directions
P	=	heat generation rate per unit volume
r	=	radial coordinate of circular cylinder system
t	=	time
T	=	temperature
u_1,u_2,u_3	=	three principal generalized coordinate directions
V	=	volume
y,z	=	coordinate directions in cartesian frame
α	=	thermal diffusivity, $\alpha = \lambda/\rho C_p$
η	=	oblate spheroidal coordinate
θ	=	oblate spheroidal coordinate
λ	=	thermal conductivity
ρ	=	mass density
ϕ	=	angular coordinate of circular cylinder system
ψ	=	oblate spheroidal coordinate

Introduction

In the solution of heat conduction and other potential field problems, the governing differential equation can always be written in terms of the three conventional coordinate systems; cartesian, circular cylinder or spherical coordinates. This is so since the governing equation is concerned with satisfying an energy balance imposed on a differential volume element. Since the volume element is of differential dimensions, its specification need not be tied to the geometry of the bounding surfaces and as a result the governing equation can be formulated in either of the three conventional coordinate systems. Where the bounding surfaces of the region under consideration lend themselves to a cartesian, circular cylinder or spherical frame, many solutions are available[1].

It is sometimes possible, however, to set up a system of coordinates 'more natural' to the vector field of interest, in this work that of heat conduction, whose coordinate surfaces conform to the lines of flow and the potential surfaces[2]. In the solution of many of these problems, the nature of the resultant field is determined by the specification of its behavior at its bounding surfaces, by specifying the nature and position of its singularities, or by a combination of these two influences. The resulting field specification may often have a simple and tractable form in terms of these 'natural' coordinates[3] whereas in terms of the three conventional systems the problem specification may be complex and its solution intractable.

It is for these reasons that it has become increasingly important for the heat conduction analyst to be proficient in the use of orthogonal curvilinear coordinate systems in the solution of heat conduction problems. However, while many multi-directional problems can be reduced through their use to problems dependent upon a single curvilinear coordinate, there still remains a wide variety of problems which cannot be so reduced but for which the flow of heat is predominately uni-directional in nature. Where possible, analytic solutions to these problems are desirable since the effect of changes in the various solution parameters can immediately be evaluated by examination of the functional form of the solution. Unfortunately, however, the scope of problems which lend themselves to such analytic solutions, whether approximate or exact, is limited to those having relatively simple boundary conditions. The vast majority of two and three dimensional problems in conduction heat transfer have no known analytic solution due to irregular boundary geometries and/or inconvenient boundary condition specifications. In such cases it may be advisable to use a numerical method to obtain an 'adequate' solution more simply and efficiently than to labor with an analytic method which may not admit a solution within the time frame allowed for the problem. The finite difference method is a numerical solution procedure popular in the solution of heat transfer problems(4-10). The spatial discretization process inherent to the method leads to a system of simultaneous algebraic equations which must be solved to determine the temperatures at discretized locations in the field, the nodal values.

Determination of the coefficients multiplying the nodal temperatures in these algebraic equations is of considerable concern since approximations made there directly influence the accuracy of the results. In the excellent work by Clausing(4), the three conventional coordinate systems are treated and their corresponding finite difference coefficients obtained. The major limitation of his analysis, however, lies in the restriction to the three conventional coordinate systems. In fact, in his and other finite difference analyses (4-10), not only is the restriction to the three conventional coordinate systems made, but for each of the three, a completely independent development has been required. Recently, an examination of a specialized coordinate system has been made and the resulting coefficients used successfully in finite difference solutions(11,12). Throughout the remaining literature dealing with the subject, however, attention has been restricted to the three conventional coordinate systems.

Convinced that advantages similar to those available when using the most appropriate coordinate system in an analytic solution, are possible when performing a numerical solution, this work is aimed at providing a generalized development of the finite difference coefficients for use with any orthogonal curvilinear coordinate system in the numerical description of the heat conduction equation. This will be accomplished by employing a Taylor series expansion in the vicinity of the current node of interest to describe the local temperature field. In this way the required derivatives can be approximated and substituted into the governing differential equation thereby developing the difference equations controlling the flow of heat within the discretized spatial domain.

Preliminary Remarks

In a general orthogonal curvilinear coordinate system, (u_1, u_2, u_3), the heat conduction equation can be written as (2)

$$\frac{\partial}{\partial u_1}\left[\frac{\lambda_1\sqrt{g}}{g_1}\frac{\partial T}{\partial u_1}\right] + \frac{\partial}{\partial u_2}\left[\frac{\lambda_2\sqrt{g}}{g_2}\frac{\partial T}{\partial u_2}\right] + \frac{\partial}{\partial u_3}\left[\frac{\lambda_3\sqrt{g}}{g_3}\frac{\partial T}{\partial u_3}\right] + P\sqrt{g} = \frac{\partial}{\partial t}\left(\sqrt{g}\,\rho C_p\,T\right) \qquad (1)$$

where the metric coefficients relating the curvilinear system to the cartesian frame are defined by(2)

$$g_i \equiv \left(\frac{\partial x}{\partial u_i}\right)^2 + \left(\frac{\partial y}{\partial u_i}\right)^2 + \left(\frac{\partial z}{\partial u_i}\right)^2, \quad i = 1,2,3 \qquad (2)$$

with $\sqrt{g} \equiv \sqrt{g_1 \cdot g_2 \cdot g_3}$ (3)

Since a general solution of equation (1) with arbitrary boundary condition specification is not yet possible, many problems of practical interest must remain unresolved if only analytic solutions are considered. This realization has led to increased usage of the finite difference methods for solving certain heat conduction problems.

The finite difference method is concerned with the approximation of equation (1) for use in a numerical computational scheme and reduces the problem from that of finding solutions to equation (1) to that of solving a system of simultaneous equations of the form

$$C_1 T_{i-1,j,k} + C_2 T_{i+1,j,k} + C_3 T_{i,j-1,k} + C_4 T_{i,j+1,k} + C_5 T_{i,j,k-1} + C_6 T_{i,j,k+1} + C_s T_{i,j,k} + D = 0 \qquad (4)$$

where the subscripts refer to locations within the decretized spatial domain. The constant term D contains information regarding the heat generation as well as temperatures from the time planes preceding the one under consideration. Equation (4) can be written once for each location of the discretized spatial domain yielding a system of simultaneous equations which require solution. In general, the coefficients of equation (4) must also be allowed to vary from location to location in the field. It is the basic problem, then, for any finite difference analysis to determine the coefficients and constants appearing in equation (4) for use with the particular coordinate system under consideration. An analysis is presented herein which examines this problem in a general fashion so that the results are applicable for any orthogonal coordinate system provided the associated metric coefficients are known.

General Considerations

Figure 1 illustrates a typical volume element in a general orthogonal curvilinear coordinate system having coordinate directions u_1, u_2 and u_3. The physical dimensions of the volume element are related to the variation in the coordinate value through the metric coefficients by the relation(2)

$$ds_i = \sqrt{g_i}\, du_i, \quad i = 1, 2, 3 \qquad (5)$$

Using (5), area elements are given by

$$dA_i = \sqrt{g_j g_k}\, du_j du_k, \quad i,j,k = 1,2,3, \; i \neq j \neq k \qquad (6)$$

where the convention has been used that the direction associated with the area element be normal to the plane in which it lies. Similarly the element of volume is determined from

$$dV = \sqrt{g}\, du_1\, du_2\, du_3 \qquad (7)$$

The control volume width surrounding node u_i is characterized by Δu_i where u_i is a generalized orthogonal curvilinear coordinate. Extension of this nomenclature to other coordinate directions is taken directly but it should be noted that Δu_i corresponds to a change in the orthogonal coordinate u_i and may not reflect directly the physical distances involved.

Taylor Series Expansion

Considering the discretization of space as illustrated in Figure 2, the subscript i shall be used to denote the u_1 direction; j for the u_2 direction, and k for the u_3 direction.

The first term of equation (1) can be expanded by performing the indicated differentiation to give

$$\frac{\partial}{\partial u_1}\left[\frac{\lambda_1\sqrt{g}}{g_1}\frac{\partial T}{\partial u_1}\right] = \frac{\lambda_1\sqrt{g}}{g_1}\frac{\partial^2 T}{\partial u_1^2} + \frac{\partial}{\partial u_1}\left[\frac{\lambda_1\sqrt{g}}{g_1}\right]\frac{\partial T}{\partial u_1} \quad (8)$$

Similar terms will be present for the conduction terms in the other two principal directions.

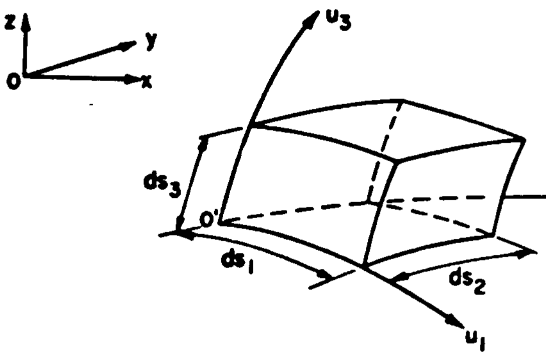

Fig. 1 Typical Volume Element in Curvilinear Coordinates

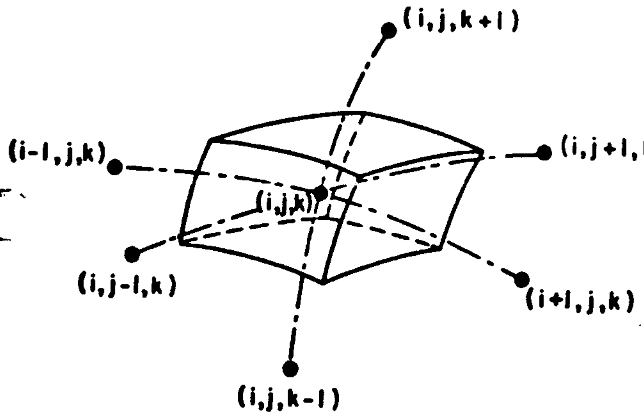

Fig. 2 Internodal Linkage of Discretized Curvilinear Space

Expressing the variation in temperature in the u_1 direction in a Taylor series expansion about node (i,j,k), the temperature at nodes (i+1, j, k) and (i-1, j, k) can be given for uniform nodal spacing by

$$T_{i+1,j,k} = T_{i,j,k} + \left.\frac{\partial T}{\partial u_1}\right|_{i,j,k}(\Delta u_1) + \left.\frac{\partial^2 T}{\partial u_1^2}\right|_{i,j,k}\frac{(\Delta u_1)^2}{2} + \ldots \quad (9)$$

and

$$T_{i-1,j,k} = T_{i,j,k} - \left.\frac{\partial T}{\partial u_1}\right|_{i,j,k}(\Delta u_1) + \left.\frac{\partial^2 T}{\partial u_1^2}\right|_{i,j,k}\frac{(\Delta u_1)^2}{2} - \ldots \quad (10)$$

Subtracting (10) from (9) yields

$$\left.\frac{\partial T}{\partial u_1}\right|_{i,j,k} = \frac{T_{i+1,j,k} - T_{i-1,j,k}}{2\,\Delta u_1} + O[(\Delta u_1)^3] \quad (11)$$

An expression for the second derivative can be obtained by adding the two equations (9) and (10). This gives

$$\left.\frac{\partial^2 T}{\partial u_1^2}\right|_{i,j,k} = \frac{T_{i+1,j,k} + T_{i-1,j,k} - 2T_{i,j,k}}{(\Delta u_1)^2} + O[(\Delta u_1)^4] \quad (12)$$

Neglecting terms of order Δu_1^3 and higher, equations (11) and (12) can be used in equation (8) as approximations to the differentials appearing there. This substitution yields the result

$$\frac{\partial}{\partial u_1}\left[\frac{\lambda\sqrt{g}}{g_1}\frac{\partial T}{\partial u_1}\right] \approx \left.\left[\frac{\lambda\sqrt{g}}{g_1}\right]\right|_{i,j,k}\left\{\frac{T_{i+1,j,k} + T_{i-1,j,k} - 2T_{i,j,k}}{(\Delta u_1)^2}\right\}$$
$$+\left.\left[\frac{\partial}{\partial u_1}\left[\frac{\lambda\sqrt{g}}{g_1}\right]\right]\right|_{i,j,k}\left\{\frac{T_{i+1,j,k} - T_{i-1,j,k}}{2\Delta u_1}\right\} \quad (13)$$

Again, similar expressions can be obtained for the other two directions by a systematic rotation of the subscripts in equation (13).

The fourth term of equation (1) can be approximated by its evaluation at the location of interest (i,j,k) for the nodal equation. Thus the equality is assumed

$$P\sqrt{g} = [P\sqrt{g}]_{i,j,k} \quad (14)$$

The final term of equation (1) involves a time derivative of the quantity ($\sqrt{g}\,\rho\,C_p\,T$). A central difference or forward difference approximation here requires an input of temperatures taken from a time-plane in the future, whose values are not known. Moreover, these are not of concern in the solution of the current time plane temperatures. Therefore, unless a fully implicit solution with respect to time is attempted (and this is not practical with present computational facilities) the best approximation to time derivatives must take the form of a backward difference quotient. Thus the approximation is

$$\frac{\partial}{\partial t}(\sqrt{g}\,\rho\,C_p\,T) \approx \sqrt{g}\left[\frac{(\rho\,C_p\,T)_{i,j,k} - (\rho\,C_p\,T)^{o}_{i,j,k}}{\Delta t}\right] \quad (15)$$

where the superscript (o) is used to indicate that the information required for evaluation be taken from the 'old' (most recent) time plane.

Reforming equation (1) using approximations (13), (14), and (15), and combining coefficients of common nodal temperatures yields the final result

$$\left.\left[\frac{\lambda_1\sqrt{g}}{g_1\,\Delta u_1^2} - \frac{1}{2\Delta u_1}\frac{\partial}{\partial u_1}\left(\frac{\lambda_1\sqrt{g}}{g_1}\right)\right]\right|_{i,j,k} T_{i-1,j,k}$$
$$+\left.\left[\frac{\lambda_2\sqrt{g}}{g_2\,\Delta u_2^2} - \frac{1}{2\Delta u_2}\frac{\partial}{\partial u_2}\left(\frac{\lambda_2\sqrt{g}}{g_2}\right)\right]\right|_{i,j,k} T_{i,j-1,k}$$
$$+\left.\left[\frac{\lambda_3\sqrt{g}}{g_3\,\Delta u_3^2} - \frac{1}{2\Delta u_3}\frac{\partial}{\partial u_3}\left(\frac{\lambda_3\sqrt{g}}{g_3}\right)\right]\right|_{i,j,k} T_{i,j,k-1}$$
$$+\left.\left[\frac{\lambda_3\sqrt{g}}{g_3\,\Delta u_3^2} + \frac{1}{2\Delta u_3}\frac{\partial}{\partial u_3}\left(\frac{\lambda_3\sqrt{g}}{g_3}\right)\right]\right|_{i,j,k} T_{i,j,k+1}$$
$$+\left.\left[\frac{\lambda_2\sqrt{g}}{g_2\,\Delta u_2^2} + \frac{1}{2\Delta u_2}\frac{\partial}{\partial u_2}\left(\frac{\lambda_2\sqrt{g}}{g_2}\right)\right]\right|_{i,j,k} T_{i,j+1,k}$$

$$+ \left[\frac{\lambda_1 \sqrt{g}}{g_1 \Delta u_1^2} + \frac{1}{2\Delta u_1} \frac{\partial}{\partial u_1} \left(\frac{\lambda_1 \sqrt{g}}{g_1}\right)\right]\Bigg|_{i,j,k} T_{i+1,j,k}$$

$$- \left[2\left[\frac{\lambda_1 \sqrt{g}}{g_1 \Delta u_1^2} + \frac{\lambda_2 \sqrt{g}}{g_2 \Delta u_2^2} + \frac{\lambda_3 \sqrt{g}}{g_3 \Delta u_3^2}\right]\Bigg|_{i,j,k} + \left(\frac{\sqrt{g}\,\rho\, C_p}{\Delta t}\right)\right]\Bigg|_{i,j,k} T_{i,j,k}$$

$$+ \left[P \sqrt{g} + \left(\frac{\sqrt{g}\,\rho\, C_p}{\Delta t}\right) T^o\right]\Bigg|_{i,j,k} = 0 \qquad (16)$$

A comparison of equation (16) with equation (4)

$$C_1 T_{i-1,j,k} + C_2 T_{i+1,j,k} + C_3 T_{i,j-1,k}$$

$$C_4 T_{i,j+1,k} + C_5 T_{i,j,k-1} + C_6 T_{i,j,k+1}$$

$$C_s T_{i,j,k} + D = 0 \qquad (4)$$

leads to the definitions

$$C_{1,2} = \left[\frac{\lambda_1 \sqrt{g}}{g_1 (\Delta u_1^2)} \mp \frac{1}{2\Delta u_1} \frac{\partial}{\partial u_1} \left(\frac{\lambda_1 \sqrt{g}}{g_1}\right)\right]_{i,j,k}$$

$$C_{3,4} = \left[\frac{\lambda_2 \sqrt{g}}{g_2 (\Delta u_2^2)} \mp \frac{1}{2\Delta u_2} \frac{\partial}{\partial u_2} \left(\frac{\lambda_2 \sqrt{g}}{g_2}\right)\right]_{i,j,k}$$

$$C_{5,6} = \left[\frac{\lambda_3 \sqrt{g}}{g_3 (\Delta u_3^2)} \mp \frac{1}{2\Delta u_3} \frac{\partial}{\partial u_3} \left(\frac{\lambda_3 \sqrt{g}}{g_3}\right)\right]_{i,j,k} \qquad (17)$$

$$C_s = -\left[\sum_{n=1}^{6} C_n + \left(\frac{\sqrt{g}\,\rho\, C_p}{\Delta t}\right)\right]_{i,j,k}$$

and

$$D = \left[P \sqrt{g} + \frac{\sqrt{g}\,\rho\, C_p}{\Delta t} T^o\right]_{i,j,k}$$

as the finite difference coefficients required for each nodal location of the discretized spatial domain. Equation (4) with the coefficients (17) can be easily used for finite difference modelling of heat conduction and other field problems in any orthogonal curvilinear coordinate system.

Applications

1. As a first example of the application of the general expressions for the finite difference coefficients (17), the circular cylinder coordinate system will be considered. Assigning the coordinate directions as

$$u_1 = r, \quad u_2 = \phi, \quad u_3 = z \qquad (18)$$

the metric coefficients can be easily determined to be

$$g_1 = 1, \quad g_2 = r^2, \quad g_3 = 1, \qquad \sqrt{g} = r \qquad (19)$$

Considering the case of uniform, isotropic thermal properties, the finite difference coefficients are obtained by direct application of equation (17) and division by λr_i, where r_i is the radial coordinate at the central node. These are

$$C_{1,2} = \frac{1}{(\Delta r)^2} \left[1 \mp \frac{\Delta r}{2 r_i}\right]$$

$$C_{3,4} = \frac{1}{(r_i\, \Delta\phi)^2}$$

$$C_{5,6} = \frac{1}{(\Delta z)^2} \qquad (20)$$

$$C_s = -\left\{\sum_{n=1}^{6} C_n + \frac{1}{\alpha \Delta t}\right\}$$

and

$$D = \frac{P}{\lambda} + \frac{T^o}{\alpha \Delta t}$$

The determination of the above coefficients (20) is extremely simple using the relations (17) and can be compared with the relatively laborious procedure required when using the conventional approach[10]. The advantages of using the generalized expressions (17) becomes immediately apparent.

2. As a second example of the application of the general expressions for the finite difference coefficients (17), the oblate spheroidal coordinate system will be considered. The transformation equations are[2]

$$x = a \cosh\eta \sin\theta \cos\psi$$

$$y = a \cosh\eta \sin\theta \sin\psi \qquad (21)$$

$$z = a \sinh\eta \cos\theta$$

where the assignment has been made that

$$u_1 = \eta, \quad u_2 = \theta, \quad u_3 = \psi \qquad (22)$$

The coordinate system is illustrated in Figure 3.

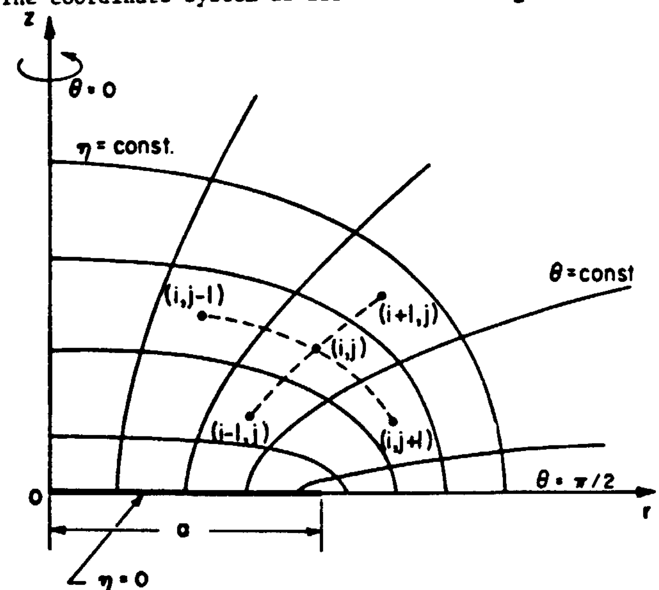

Fig. 3 Oblate Spheroidal Coordinate System

It is an easy task using the transformation equations (21) to show that the metric coefficients are given by

$$g_\eta = g_\theta = a^2 (\cosh^2\eta - \sin^2\theta)$$

$$g_\psi = a^2 \cosh^2\eta \sin^2\theta \qquad (23)$$

with

$$\sqrt{g} = a^3 (\cosh^2\eta - \sin^2\theta) \cosh\eta \sin\theta$$

The special case of uniform, isotropic thermal properties will be considered here. Using the metric coefficients (23) in the expressions for the general finite difference coefficients (17) and performing the indicated operations yields the result

$$C_{1,2} = \{\frac{1}{\Delta\eta^2} \mp \frac{\tanh\eta_i}{2\Delta\eta}\}$$

$$C_{3,4} = \{\frac{1}{\Delta\theta^2} \mp \frac{\cot\theta_j}{2\Delta\theta}\}$$

$$C_{5,6} = \frac{(\cosh^2\eta_i - \sin^2\theta_j)}{\Delta\psi^2 \cosh^2\eta_i \sin^2\theta_j} \qquad (24)$$

$$C_s = -\{\sum_{n=1}^{6} C_n + \frac{\cosh^2\eta_i - \sin^2\theta_j}{\Delta Fo}\}$$

and $$D = (\cosh^2\eta_i - \sin^2\theta_j)\{\frac{P_{i,j,k}\, a^2}{\lambda} + \frac{T^o_{i,j,k}}{\Delta F_o}\}$$

In the above, division of each coefficient by ($a\lambda \cosh\eta_i \sin\theta_j$) has been performed and the definition of a Fourier modulus ($Fo \equiv \alpha t/a^2$) has been introduced. The results (24) of applying the general expressions derived herein indicate the ease with which finite difference analyses can be performed on any system provided there is a compatible orthogonal curvilinear coordinate system. The expressions given for oblate spheroidal coordinates (24) have been successfully applied for axi-symmetric steady state heat transfer with no internal heat generation[11]. In addition, a complete transient solution[12] (axi-symmetric, no heat generation) has been successfully computed describing the heat flow from a thin circular ... to a half-space, using the above expressions. ...e not discussed here, boundary conditions can be handled in the usual fashion provided the relevant approximations are made in the curvilinear frame rather than the cartesian one from which it was derived.

Discussion and Conclusions

A set of generalized expressions has been derived for determination of the coefficients required for finite difference modelling of the heat conduction equation or other potential field governing differential equation. The coefficient definition generalization is such that the coefficients may be applied to any orthogonal curvilinear coordinate system for which the metric coefficients are known. The expressions derived can easily be shown to yield the known values for the three conventional coordinate systems.

This development significantly extends the analytical capability of the finite difference method in that many highly complex problems can now be handled with relative ease. This is best illustrated by the second example cited earlier where oblate spheroidal coordinates were employed in the analysis.

An additional advantage may also be available in certain problems where the field is expected to be predominantly uni-directional in the curvilinear system, while highly two- or three-dimensional in either of the three conventional systems. For these problems, considerable computational economy can be achieved since a fine mesh in the predominant flow direction can be used to 'pick up' the gradients there while a coarser mesh may be adequate to account for the two- or three-dimensional perturbations from this one-dimensional predominance. Were a conventional system used for such a problem, fine numerical detail would be required in all three principal directions resulting in substantially increased computational labor and cost.

Physical considerations also suggest an apparent advantage available through the use of curvilinear finite differencing. For problem geometries compatible with a curvilinear net, the conformal transformation generating the net is such that even for uniform increments in each coordinate direction, a finer mesh (in terms of physical size) is generated near the discontinuities which themselves initially suggested the transformation of coordinates. This has the effect of automatically generating a variable mesh size with fine and coarse subdivisions located as required. This inherent behavior is a substantial advantage to finite differencing in the most appropriate coordinate system. The expressions developed in this work allow flexibility in this choice of coordinate frame.

Finally a secondary advantage of the generality of the derived coefficients is that a program can be developed in which the finite difference coefficients appear as statement function definitions. In this way, problem geometry can be altered (within the realm of orthogonal curvilinear systems) with minimal change to the bulk of the solution program. This programming flexibility can be directly reflected in the analysis flexibility of the investigator.

Acknowledgements

The authors acknowledge the National Research Council of Canada for their financial support of this research. One of the authors (G.E.S.) acknowledges the financial support of the Communications Research Center, Ottawa, Canada.

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