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A CONTROL-VOLUME FINITE ELEMENT METHOD FOR THE PREDICTION OF THREE-DIMENSIONAL DIFFUSION-TYPE PHENOMENA IN ANISOTROPIC MEDIA

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ABSTRACT

The formulation and testing of a control-volume finite element method (CVFEM) for the prediction of three-dimensional, linear and nonlinear, diffusion-type phenomena in anisotropic media in irregular calculation domains are presented and discussed in this paper. In this CVFEM, the calculation domain is discretized into four-node tetrahedral elements. Contiguous, non-overlapping, polyhedral control volumes are then associated with each node, and the governing differential equation is integrated over these control volumes. The dependent variable is interpolated linearly in each four-node tetrahedral element. Centroidal values of the diffusion coefficients are stored and assumed to prevail over the corresponding tetrahedral element. The source term is linearized, and nodal values of its coefficients are stored and assumed to prevail over the polyhedral sub-control volumes. Using these interpolation functions, the discretized equations, which are algebraic approximations to the integral conservation equations, are derived. The discretized equations, which in general, are nonlinear and coupled, are solved using an iterative procedure. The proposed CVFEM for the solution of anisotropic diffusion-type problems appears to be the first such method that is based on tetrahedral elements and vertex-centered polyhedral control volumes. These features make it particularly attractive for amalgamation with adaptive-grid schemes and applications to problems with complex irregular geometries, such those encountered in the general areas of drying, ground-water flows, conduction in composite materials, injection molding in heterogeneous porous media, and solidification. The proposed three-dimensional CVFEM and its computer implementation were tested using several steady conduction-type problems, for which analytical solutions were constructed using a special technique. In all cases, the agreement between the numerical and analytical solutions was excellent.

INTRODUCTION

Physical phenomena such as heat conduction, potential flow, mass diffusion, flows through porous media in the Darcy regime, electromagnetics and electrostatics, and lubrication flows are governed by equations that have the same general form, akin to that of the classical heat conduction or mass diffusion equations. In this sense, they can all be thought of as diffusion-type phenomena [Patankar (1980)]. Several naturally occurring materials, such as woods and soils, and also engineered materials, such as laminated metal sheets and composites, have properties that are intrinsically dependent on direction. Thus, it is important to account for anisotropy in the modeling of diffusion-type phenomena in such materials.

Elaborating a bit more on the points mentioned above, heat conduction processes in laminated metal sheets, commonly used in the construction of electric power transformers, and also in composites materials, now widely used in the aerospace industry, are anisotropic diffusion-type phenomena [Ozisik (1980); Ozisik and Shouman (1980); Bejan (1984)]. Volume-averaged approaches [Whitaker (1999)] to the modeling of heat and mass transfer in porous media, for example drying of wood or food stuff, ground water flow, and transport of solutes in ground, and modeling of wave propagation in biological tissues, often lead to anisotropic diffusion-type problems [Plumb and Spolek (1985); Ferguson (1995, 1998); Ferguson and Turner (1995, 1996); Kaviany (1995); Harrild and Henriquez (1997); Nield and Bejan (1999); Yang and Lee (1999); Delleur (1999); Lyuksyutov et al. (2001); Schwartz and Zhang (2003)]. Such problems typically involve complex geometries, are three-dimensional, and are governed by equations that cannot be solved analytically. Thus, though examples of analytical approaches to the solution of anisotropic diffusion-type problems are available in the literature [Poon and Chang (1978); Poon (1979); Ozisk (1980); Mikhailov and Ozisik (1981, 1984); Traianno et al. (997)], numerical methods are needed and used for solving the majority of the aforementioned problems.

Detailed descriptions of numerical methods for the solution of fluid flow and heat transfer problems are available in numerous textbooks and handbooks, for example, the works of Patankar (1980), Versteeg and Malalasekera (1995), Zienkiewicz and

Taylor (2000), Reddy and Gartling (2001), and Minkowycz et al. (2006). There are also many publications on numerical solutions of anisotropic diffusion-type problems. Examples of such publications include the contributions of Perre and Degiovanni (1990), Ozisik (1994), Rabbani (1994), Ferguson (1995, 1998), Ferguson and Turner (1995, 1996), Turner and Ferguson (1995a, 1995b), Murthy and Mathur (1998), Perre and Turner (1999), Jayantha and Turner (2003a, 2003b, 2005), and Truscott and Turner (2004). Some probabilistic methods have also been proposed for the solution of anisotropic heat conduction problems [Haji-Sheik and Sparrow (1967); Haji-Sheik (1988)].

The formulation and testing of a control-volume finite element method (CVFEM) for the prediction of three-dimensional, linear and nonlinear, diffusion-type phenomena in anisotropic media in irregular calculation domains are presented and discussed in this paper. CVFEMs combine key concepts from finite volume methods and finite element methods [Baliga and Patankar (1980); Baliga (1997); Baliga and Atabaki (2006)]. Thus, their formulations can be readily interpreted in terms of physically meaningful and relevant quantities such as fluxes, forces, and sources, and, if formulated correctly and consistently, they have the so-called conservative property [Patankar (1980)].

Publications on CVFEMs for the solution of anisotropic diffusion-type problems include the contributions of Ferguson (1995, 1998), Ferguson and Turner (1995, 1996), Turner and Ferguson (1995a, 1995b), Perre and Turner (1999), Jayantha and Turner (2003a, 2003b, 2005), and Truscott and Turner (2004), for example. Other finite-volume-based approaches to the solution of anisotropic diffusion-type problems in complex geometries have also been published, for example, in the works of Murthy and Mathur (1998) and Das et al. (2002). The CVFEM proposed in this paper adds to the repertoire of such methods. It appears to be the first such method in which four-node tetrahedral elements and node-centered (or vertex-based) polyhedral control volumes are used in the formulation. These features make it particularly attractive for the solution of problem with complex geometries, and also future amalgamation with adaptive-grid techniques [Minkowycz et al. (2006)].

NOMENCLATURE

a_j, a_n, a^o, b		Coefficients in general discretized equation; see Eq. (17)
A, B, C, D		Coefficients in interpolation functions
A^{nj}	[m^2]	Area of internal quadrilateral surfaces bounding sub-control-volumes within a tetrahedral element; see Figures 1 and 2 and also Eq. (12)
$\mathbf{J}$	[W/m^2]	General diffusion flux vector; given units apply for heat conduction problems
$\overline{\overline{K}}$	[W/m.K]	Thermal conductivity tensor; see Eq. (18), (19), and (24)
L_x, L_y, L_z	[m]	Extents of the calculation domain in the x, y, and z directions
S, dS	[m^2]	Surface area, and surface area element
S_ϕ	[W/m^3]	Volumetric source term associated with the general dependent variable ϕ; given units apply for heat conduction problems
T	[s]	Time
T	[^{o}C]	Temperature
V, dV	[m^3]	Volume, and differential volume element
x, y, z	[m]	Cartesian coordinates
X, Y, Z	[m]	Cartesian coordinates with origin at the centroid of the tetrahedral element

Greek symbols

$\overline{\overline{\Gamma}}_\phi$	[W/m.K]	General diffusion tensor; given units apply when it is interpreted as the thermal conductivity tensor
ρ	[kg/m^3]	Density
ϕ		General dependent variable; see Eq. (1)

MATHEMATICAL MODEL

Governing Equations: With reference to the Cartesian (x,y,z) coordinate system, unsteady, three-dimensional, anisotropic, diffusion-type problems are governed by differential equations that can be cast in the following general form [Patankar (1980); Osizik (1980); Kaviany (1995); Nield and Bejan (1999); Oosthuizen and Naylor (1999)]:

$$\frac{\partial}{\partial t}(\rho\phi) + div\mathbf{J} = S_\phi \tag{1}$$

$$\mathbf{J} = -\overline{\overline{\Gamma}}_\phi \overline{\nabla}\phi \tag{2}$$

Here, ϕ is a general specific (per unit mass) scalar dependent variable, ρ is the mass density, $\mathbf{J}$ is the diffusion flux vector, $\overline{\overline{\Gamma}}_\phi$ is the corresponding second-order tensor of diffusion coefficients, and S_ϕ is the appropriate volumetric (per unit volume) rate of generation or source term. Casting the governing equations into the form of Eq. (1) allows the development of general-purpose methodology and computer programs that can be used to solve a wide variety of the problems of interest, as was first proposed and pointed out in the seminal works of Spalding [Artemov et al. (2009)]. Each association of ϕ with a specific physical dependent variable of relevance to the problem of interest is accompanied by the corresponding specific meanings and expressions (or values) of $\overline{\overline{\Gamma}}_\phi$ and S_ϕ [Patankar (1980)].

It should also be noted that S_ϕ is meant primarily for modeling actual physical rates of internal generation or source terms. However, it can also be used as a catch-all term [Patankar (1980)]: whatever cannot conveniently be fitted into the other terms in Eqs. (1) and (2) can always be lumped in with S_ϕ.

This tensor, $\overline{\overline{\Gamma}}_\phi$, in general, has nine components, Γ_ϕ^{ij}, called generalized diffusion coefficients:

$$\overline{\overline{\Gamma}}_\phi = \begin{bmatrix} \Gamma_\phi^{11} & \Gamma_\phi^{12} & \Gamma_\phi^{13} \\ \Gamma_\phi^{21} & \Gamma_\phi^{22} & \Gamma_\phi^{23} \\ \Gamma_\phi^{31} & \Gamma_\phi^{32} & \Gamma_\phi^{33} \end{bmatrix} \tag{3}$$

It should be noted that the generalized diffusion tensor, $\overline{\overline{\Gamma}}_\phi$, is symmetric [Osizik (1980)]: thus, $\Gamma_\phi^{ij} = \Gamma_\phi^{ji}$.

In the case of anisotropic media that are being considered here, the components of the diffusion flux vector along the positive x, y, and z directions are given by the following expressions:

$$J_x = -(\Gamma_\phi^{11}\frac{\partial\phi}{\partial x} + \Gamma_\phi^{12}\frac{\partial\phi}{\partial y} + \Gamma_\phi^{13}\frac{\partial\phi}{\partial z})$$
$$J_y = -(\Gamma_\phi^{21}\frac{\partial\phi}{\partial x} + \Gamma_\phi^{22}\frac{\partial\phi}{\partial y} + \Gamma_\phi^{23}\frac{\partial\phi}{\partial z}) \quad (4)$$
$$J_z = -(\Gamma_\phi^{31}\frac{\partial\phi}{\partial x} + \Gamma_\phi^{32}\frac{\partial\phi}{\partial y} + \Gamma_\phi^{33}\frac{\partial\phi}{\partial z})$$

Therefore, for an anisotropic medium, the diffusion flux vector **J** at a point on a constant-ϕ surface is not necessarily normal to that surface.

Boundary Conditions: The boundary conditions are specific to each problem of interest. Typically, three kinds of boundary conditions are commonly encountered in the modeling of diffusion-type phenomena: 1) specified value of ϕ; 2) specified diffusion flux of ϕ, normal to the domain boundary, J_n. ; and 3) specification of flux via a reference value of the dependent variable far from the boundary, ϕ_{ref}, and a transfer coefficient, $\mathfrak{I}$, such that $J_{n,into\ domain} = \mathfrak{I}(\phi_{ref} - \phi_{boundary})$. Other boundary conditions, if encountered, can always be recast in the form of the aforementioned three conditions. For example, non-linear boundary conditions can be linearized and cast in a form akin to the third type, or a linear combination of all three types.

Initial Conditions: The initial conditions specify the distribution of the dependent variables, ϕ, at time t = 0. Again, the initial conditions are problem specific.

FORMULATION OF THE NUMERICAL METHOD

The proposed method belongs to the family of control-volume finite element methods (CVFEMs). Detailed discussions of CVFEMs are available in the works of Baliga (1997) and Baliga and Atabaki (2006). Thus, only some of the main aspects of the formulation of the proposed CVFEM for the solution of the anisotropic diffusion problems of interest here are succinctly presented in this section.

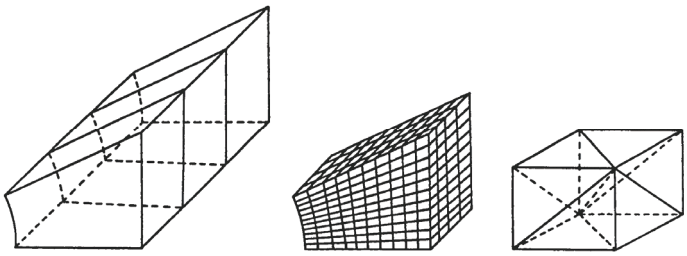

Figure 1 Three-step discretization of a calculation domain into tetrahedral elements: (a) division into slabs; (b) division of the slabs into eight-node brick elements; and (c) subdivision of the eight-node brick elements into four-node tetrahedral element.

Domain Discretization: The calculation domain is divided first into four-node tetrahedral elements; and then each node in the calculation domain is associated with contiguous, non-overlapping, polyhedral control volumes that fill the calculation domain. The proposed method is designed to work with complex geometries and unstructured grids. Here, however, for ease of presentation, the aforementioned discretization of three-dimensional calculation domains into four-node tetrahedral elements is illustrated in Figure 1 with respect to a relatively simple geometry and a three-step procedure. In the proposed CVFEM, the simple four-node tetrahedral element is preferred to brick or parallelepiped elements, because the latter introduce the complication of isoparametric transformations [Strang and Fix (1973); Baliga and Patankar (1980); LeDain-Muir and Baliga (1988)]. In the proposed CVFEM, curved boundary surfaces are approximated by piecewise-plane surfaces, and isoparametric transformations are not required.

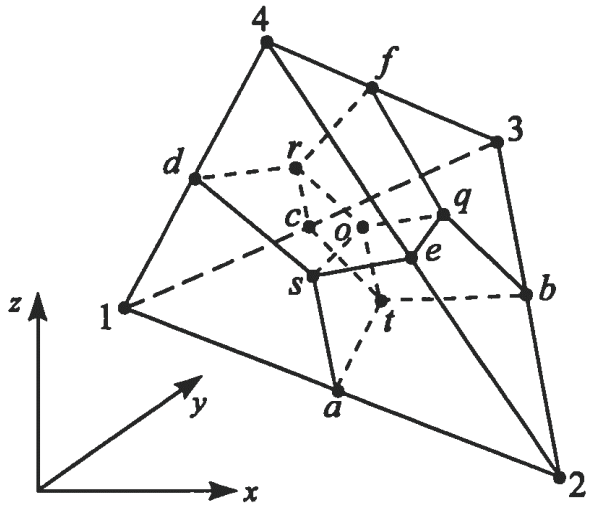

Figure 2 Division of a tetrahedral element into portions of polyhedral control volumes and related nomenclature.

Following the discretization of the calculation domain into four-node tetrahedral elements, each element is divided into four equal volumes, as illustrated in Figure 2. The procedure for this subdivision of the elements into the four equal volumes is the following: the centroid, *o*, of each tetrahedral element is first joined by straight lines to the centroids *q*, *r*, *s*, and *t* of the four triangular surfaces that make up the tetrahedron; then the centroid of each triangular surface is joined by straight lines to the midpoint of the corresponding sides. This procedure generates six plane quadrilateral surfaces within each tetrahedral element that divide it into four equal sub-control-volumes, V^1, V^2, V^3, and V^4, which are not necessarily similarly-shaped. Collectively, these surfaces create polyhedral control volumes associated with each node in the calculation domain and have the following desirable properties: they do not impose any restriction on the size or shape of the tetrahedral elements; they do not overlap; and, collectively, they fill the calculation domain completely.

Integral Conservation Equations: An integral formulation corresponding to Eqs (1) and (2) is obtained by applying the conservation principle for ϕ to a control volume, *V*, which is fixed in space:

$$\int_V \frac{\partial}{\partial t}(\rho\phi)dV + \int_{\partial V} \mathbf{J}.\mathbf{n}dS = \int_V S_\phi dV \tag{5}$$

Here, ∂V is the surface of the control volume V, and $\mathbf{n}$ is a unit outward normal to the differential area element dS. The resulting integral conservation equation, when applied to the polyhedral control volume surrounding node 1 of the tetrahedral element shown in Figure 2, can be cast in the following form:

$$\left[\begin{array}{l} \int_{1atcdsor} \frac{\partial}{\partial t}(\rho\phi)dV + \int_{atos} \mathbf{J}.\mathbf{n}dS + \int_{ctor} \mathbf{J}.\mathbf{n}dS + \\ \int_{dsor} \mathbf{J}.\mathbf{n}dS - \int_{1atcdsor} S_\phi dV \end{array}\right] + \left[\begin{array}{l}\text{Similar contributions from the other}\\ \text{elements associated with node 1}\end{array}\right] + \left[\text{Boundary contributions, if applicable}\right] = 0 \tag{6}$$

Interpolation Functions: Interpolation functions for the dependent variable, ϕ, the diffusion coefficients, Γ_ϕ^{ij}, the volumetric source term, S_ϕ, and the mass density, ρ, are required for the derivation of algebraic approximations to the integral conservation equations such as Eq. (6).

Within each tetrahedral element, the centroidal values of ρ and Γ_ϕ^{ij} are stored and assumed to prevail over the element. The source term is appropriately linearized, if required, and cast in the form:

$$S_\phi^i = S_c^i + S_p^i \phi^i \tag{7}$$

The coefficients in this equation, S_C^i and S_P^i, associated with the node i (i=1,2,3,4) are stored and assumed to prevail over the corresponding sub-control-volume, V^i, contained within the tetrahedral element.

In each four-node tetrahedral element, the scalar dependent variable, ϕ, is interpolated linearly, in terms of local, centroidal-based, Cartesian coordinates, X, Y, and Z:

$$\begin{array}{l} \phi = AX + BY + CZ + D \\ X = (x - x_o)\ ;\ Y = (y - y_o)\ ;\ Z = (z - z_o) \\ x_o = \left(\sum_{n=1}^{4} x_n \Big/ 4\right);\ y_o = \left(\sum_{n=1}^{4} y_n \Big/ 4\right);\ z_o = \left(\sum_{n=1}^{4} z_n \Big/ 4\right) \end{array} \tag{8}$$

The constants A, B, C, and D in this interpolation function can be uniquely determined in terms of the X, Y, and Z, coordinates of the four nodes of the tetrahedral element and their corresponding values of ϕ, and cast in the following forms:

$$\begin{array}{l} A = (A_1\phi_1 + A_2\phi_2 + A_3\phi_3 + A_4\phi_4)/Det \\ B = (B_1\phi_1 + B_2\phi_2 + B_3\phi_3 + B_4\phi_4)/Det \\ C = (C_1\phi_1 + C_2\phi_2 + C_3\phi_3 + C_4\phi_4)/Det \\ D = \phi_1 + (D_1\phi_1 + D_2\phi_2 + D_3\phi_3 + D_4\phi_4)/Det \end{array} \tag{9}$$

In various constant in this equation can be worked out using the following expressions:

$$\begin{array}{l} X_{ij} = (X_i - X_j)\ ;\ Y_{ij} = (Y_i - Y_j)\ ;\ Z_{ij} = (Z_i - Z_j) \\ Det = \{X_{14}(Y_{24}Z_{34} - Y_{34}Z_{24}) + Y_{14}(X_{34}Z_{24} - X_{24}Z_{34}) + \\ \qquad Z_{14}(X_{24}Y_{34} - X_{34}Y_{24})\} \\ A_1 = (Y_{24}Z_{34} - Y_{34}Z_{24})\ ;\ A_2 = (Y_{34}Z_{14} - Y_{14}Z_{34}) \\ A_3 = (Y_{14}Z_{24} - Y_{24}Z_{14})\ ;\ A_4 = -(A_1 + A_2 + A_3) \\ B_1 = (Z_{24}X_{34} - Z_{34}X_{24})\ ;\ B_2 = (Z_{34}X_{14} - Z_{14}X_{34}) \\ B_3 = (Z_{14}X_{24} - Z_{24}X_{14})\ ;\ B_4 = -(B_1 + B_2 + B_3) \\ C_1 = (X_{24}Y_{34} - X_{34}Y_{24})\ ;\ C_2 = (X_{34}Y_{14} - X_{14}Y_{34}) \\ C_3 = (X_{14}Y_{24} - X_{24}Y_{14})\ ;\ C_4 = -(C_1 + C_2 + C_3) \\ D_1 = -(A_1X_1 + B_1Y_1 + C_1Z_1)\ ;\ D_2 = -(A_2X_1 + B_2Y_1 + C_2Z_1) \\ D_3 = -(A_3X_1 + B_3Y_1 + C_3Z_1)\ ;\ D_4 = -(A_4X_1 + B_4Y_1 + C_4Z_1) \end{array} \tag{10}$$

Derivation of Discretized Equations: The discretized equations are obtained by first using the above-mentioned interpolation functions to derive algebraic approximations to the element contributions to integral conservation equation, similar to the first set of bracketed terms in Eq. (6), and then assembling these element contributions appropriately [Baliga and Patankar (1980); LeDain-Muir and Baliga (1986); Baliga (1997); Baliga and Atabaki (2006)].

Using Eqs. (4) and (8), the components of the diffusion flux vector, $\mathbf{J}$, can be approximated as follows:

$$\begin{array}{l} J_x = -(A\Gamma_\phi^{11} + B\Gamma_\phi^{12} + C\Gamma_\phi^{13}) \\ J_y = -(A\Gamma_\phi^{21} + B\Gamma_\phi^{22} + C\Gamma_\phi^{23}) \\ J_z = -(A\Gamma_\phi^{31} + B\Gamma_\phi^{32} + C\Gamma_\phi^{33}) \end{array} \tag{11}$$

With reference to the tetrahedral element 1234 shown in Figure 2, and the related notation, let A^{nj} be the area of one of the three interior quadrilateral surfaces bounding the sub-control-volume V_j associated with any node j (n = 1, 2, or 3; j = 1, 2, 3, or 4); and let $\mathbf{n}^{nj}$ denote the unit normal to A^n pointing out of the sub-control-volume V_j. Then the total rate of diffusion transport across surface A^{nj} in the direction of the unit normal $\mathbf{n}^{nj}$ can be approximated as follows:

$$\int_{A^{nj}} \mathbf{J}.\mathbf{n}^{nj} dS = -A^{nj} \left[\begin{array}{l} \left(A\Gamma_\phi^{11} + B\Gamma_\phi^{12} + C\Gamma_\phi^{13}\right)n_1^{nj} + \\ \left(A\Gamma_\phi^{21} + B\Gamma_\phi^{22} + C\Gamma_\phi^{23}\right)n_2^{nj} + \\ \left(A\Gamma_\phi^{31} + B\Gamma_\phi^{32} + C\Gamma_\phi^{33}\right)n_3^{nj} \end{array}\right] \tag{12}$$

Where n_1^{nj}, n_2^{nj}, and n_3^{nj} are the components of the unit vector $\mathbf{n}^{nj}$ in the x, y, and z directions, respectively. Using the expressions given in Eq. (10), and the expressions for the components of the unit normal $\mathbf{n}^{nj}$, along with the expression in Eq. (12), the algebraic approximations to the rates of diffusion transport across the three interior quadrilateral surfaces bounding the sub-control-volume V_j and flowing out of this volume can be cast in the following compact form:

$$\int_{A^{nj}} \mathbf{J}.\mathbf{n}^{nj}\, dS = -\sum_{k=1}^{4}\left(\sum_{l=1}^{3}\left(F_k^l E_l^{nj}\right)\right)\phi_k = \sum_{k=1}^{4} C_k^{nj}\phi_k$$

for k=1,2,3, and 4; and l=1,2, and 3; and

$$F_k^l = \left(A_k\Gamma_\phi^{l1} + B_k\Gamma_\phi^{l2} + B_k\Gamma_\phi^{l3}\right)/Det \qquad (13)$$

$$E_l^{nj} = A^{nj} n_l^{nj}$$

$$C_k^{nj} = -\sum_{l=1}^{3}\left(F_k^l E_l^{nj}\right)$$

Using a simple fully-implicit time-integration scheme for the unsteady term in Eq. (6), the following algebraic approximation is obtained for the element contribution to the unsteady term associated with node j:

$$\int_{V^j} \frac{\partial}{\partial t}(\rho\phi)\, dV = \frac{V_e}{4}\rho\frac{\phi_j^m - \phi_j^{m-1}}{\Delta t} \qquad (14)$$

In this equation, V_e is the volume of the tetrahedral element, and is given by $V_e = Det/6$. The values of ϕ_j at time levels m and (m-1) are denoted by ϕ_j^m and ϕ_j^{m-1}, respectively. The volume of any one of the four equal sub-control-volumes within the element is given by $V_j = V_e/4$. It should be noted in this context that higher-order time integration scheme could be incorporated relatively easily in this formulation, but that could entail putting some stability limits of the time step [Patankar (1980)].

The element contribution to the source term associated with the node j is approximated as follows:

$$\int_{V^j} S_\phi dV = \frac{V_e}{4}S_c^j + \frac{V_e}{4}S_p^j\phi_j \qquad (15)$$

Finally, the algebraic approximation to the full element contribution to the integral conservation equation for node 1 can be expressed compactly as follows:

$$\left[\int_{1atcdsor}\frac{\partial}{\partial t}(\rho\phi)dV + \int_{atos}\mathbf{J}.\mathbf{n}dS + \int_{ctor}\mathbf{J}.\mathbf{n}dS + \int_{dsor}\mathbf{J}.\mathbf{n}dS - \int_{1atcdsor}S_\phi dV\right] = C_1^1\phi_1^m + C_2^1\phi_2^m + C_3^1\phi_3^m + C_4^1\phi_4^m + Const^1 \qquad (16)$$

Similar algebraic approximations can be derived for the element contributions to the integral conservation equations associated with nodes 2, 3, and 4.

The algebraic approximations to the boundary contributions are derived in a similar manner. Guidance in this regard can be obtained from the derivations presented in Baliga and Patankar (1980), LeDain-Muir and Baliga (1986), and Baliga and Atabaki (2006).

The discretized equations can be cast in the following compact and general form:

$$a_j\phi_j^m = \sum_n a_n\phi_n^m + a_j^0\phi_j^{m-1} + b_j \qquad (17)$$

Solution of Discretized Equations: The discretized equations derived in the last section form a set of simultaneous algebraic equations that, in general, could be nonlinear. At each time step, the following simple successive-substitution sequential iterative variable adjustment (SIVA) procedure was used to solve these equations:

1. Guess all unknown values of ϕ in the calculation domain.
2. Calculate the coefficients in the linearized form of the discretized equations, using the currently available values of the dependent variables.
3. Sequentially solve the resulting sets of linear, or nominally linear, discretized equations.
4. Repeat steps 2 and 3 until convergence.

Step 3 in the above algorithm involves the sequential solution of sets of linear, or nominally linear, algebraic equations. In the proposed method, these equations were solved by a plane-by-plane iterative procedure. When the discretized equations associated with the nodes in any particular plane were being solved, the currently available values of the dependent variables at the nodes on neighboring planes were treated as known values. A line-by-line tri-diagonal-matrix-algorithm (TDMA) was used to solve the discretized equations in the plane of interest. Details of such methods are available in Patankar (1980) and Sebben and Baliga (1995). This procedure was repeated plane-by-plane until the entire calculation domain was covered. Such iterative sweeps, in alternating coordinate directions, were continued until convergence. In this work, the convergence criterion was that the absolute values of suitably normalized residuals of the discretized equations were all less than or equal to 10^{-6}.

The above-mentioned plane-by-plane-cum-line-by-line method for solving the linearized and decoupled sets of discretized equations is relatively simple and adequate for solving some test problems and also some simple demonstration problems. For practical applications that require large grids, however, incorporation of convergence acceleration techniques, such as algebraic multigrid methods [Briggs (1987)], or some other efficient iterative solution methods such as the bi-conjugate gradient stabilized (BI-CGSTAB) method [Van der Vorst (1992)], is highly desirable and recommended.

RESULTS AND DISCUSSION

The testing of the proposed three-dimensional CVFEM and its computer implementation was done by using steady conduction-type problems, for which analytical solutions were constructed using a special technique proposed by Patankar (1980). This technique consists of the following steps: 1) choose a calculation domain, regular or irregular; 2) propose a reasonable distribution of temperature as a solution; 3) prescribe boundary conditions using the values of the prescribed temperature distribution on the boundaries; and 4) substitute the proposed temperature distribution in the governing equation, and determine the volumetric source term that would ensure that the proposed temperature distribution is indeed a solution. This technique works when the solution to the governing equations (with the calculated source term) and the proposed boundary conditions is unique. Once the aforementioned steps are completed, the proposed numerical method is used to solve the problem (compute the temperature) with the prescribed calculation domain, boundary conditions, and the calculated source terms as inputs.

In the proposed test problems, the focus was only on steady-state problems. Thus, the governing equation for the test problems was the following:

$$\nabla.\left(\overline{\overline{K}}\nabla T\right)+S=0 \tag{18}$$

In this equation, $\overline{\overline{K}}$ is the conductivity tensor:

$$\overline{\overline{K}}=\begin{bmatrix} k^{11} & k^{12} & k^{13} \\ k^{21} & k^{22} & k^{23} \\ k^{13} & k^{23} & k^{33} \end{bmatrix} \tag{19}$$

In the test problems, the components of the conductivity tensor given in Eq. (19) are assumed to be constant. Thus, with respect to a Cartesian coordinate system, and keeping in mind that the conductivity tensor is symmetric [Ozisik (1980)], Eqs. (18) and (19) can be combined and rewritten as follows:

$$\begin{aligned} &k^{11}\frac{\partial^2 T}{\partial x^2}+k^{22}\frac{\partial^2 T}{\partial y^2}+k^{33}\frac{\partial^2 T}{\partial z^2}+ \\ &2\left(k^{12}\frac{\partial^2 T}{\partial x\partial y}+k^{13}\frac{\partial^2 T}{\partial x\partial z}+k^{23}\frac{\partial^2 T}{\partial y\partial z}\right)+S=0 \end{aligned} \tag{20}$$

To ensure the testing of all aspects of the proposed CVFEM, the following three different temperature distributions (one linear, and two non-linear) and three different conductivity tensors (isotropic, orthotropic, and anisotropic) were considered:

1. Linear temperature distribution (LTD)

$$T=A\left(X/L_x\right)+B\left(Y/L_y\right)+C\left(Z/L_z\right)+D \tag{21}$$

2. Non-linear temperature distribution, Type 1

$$T=A\left(1-\frac{X}{L_x}\right)^2+B\left(1-\frac{Y}{L_y}\right)^2+C\left(1-\frac{Z}{L_z}\right)^2 \tag{22}$$

3. Non-linear temperature distribution, Type 2

$$T=A\left(1-\frac{X}{L_x}\right)\left(1-\frac{Y}{L_y}\right)\left(1-\frac{Z}{L_z}\right) \tag{23}$$

The conductivity tensors for the isotropic, orthotropic, and anisotropic cases were set to the following values:

$$\begin{aligned} \overline{\overline{K}}_{isot.}&=\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \\ \overline{\overline{K}}_{Orthot.}&=\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1.05 & 0 \\ 0 & 0 & 1.1 \end{pmatrix} \\ \overline{\overline{K}}_{Anisot.}&=\begin{pmatrix} 1 & 0.05 & 0.1 \\ 0.05 & 1.05 & 0.05 \\ 0.1 & 0.05 & 1.01 \end{pmatrix} \end{aligned} \tag{24}$$

The proposed CVFEM and its computer implementation were used to solve the proposed test problems with cubical domains and three different uniform grids, with the following number of nodes in the *x*, *y*, and *z* directions, arranged in a line-by-line pattern: 6x6x6 nodes; 11x11x11 nodes; 21x21x21 nodes, and 31x31x31 nodes. In all cases, the overall iterations of the aforementioned SIVA solution procedure were continued until all normalized residues were less than 10^{-12}.

In all cases, excellent numerical results were obtained. With the three-dimensional linear temperature distribution, Eq. (21), the numerical solutions matched the exact solution perfectly (within round-off precision), for the coarsest to the finest grids. These results were expected, as the proposed CVFEM is formally second-order accurate [Baliga and Patankar (1980); Baliga (1997)] for the solutions of such problems. For the cases with the nonlinear temperature distributions, Eqs. (22) and (23), the numerical results were also excellent, with relative differences between the numerical and exact solutions all less than 10^{-10} for the finest grid (31x31x31 nodes).

Details of the numerical results are not given here (either in tabular or graphical forms) as they matched the aforementioned analytical solutions to almost machine precision in all cases. It should also be noted that in the test problems described above, the convergence of the above-mentioned SIVA iterative solution procedure was achieved (with all normalized residues less than 10^{-12}) without any difficulties, even with the relatively simple plane-by-plane-cum-line-by-line technique that was used to solve the sets of linear, or nominally linear, discretized equations in Step 3 of this procedure. No details of the rate of convergence of

the SIVA procedure are provided here, as the emphasis in this work was on the formulation of the proposed CVFEM, rather than optimization of the solver or enhancements of its rate of convergence using multigrid or bi-conjugate gradient methods [Briggs (1987); Van der Vorst (1992)].

CONCLUSION

The formulation and testing a control-volume finite element method (CVFEM) for the prediction of three-dimensional, linear and nonlinear, diffusion-type phenomena in anisotropic media in irregular calculation domains were presented and discussed in this paper. The proposed CVFEM adds to the repertoire of numerical methods available in the published literature for the solution of three-dimensional anisotropic diffusion-type problems. It appears to be the first such method in which four-node tetrahedral elements and node-centered (or vertex-based) polyhedral control volumes are used in the formulation. These features make it particularly attractive for the solution of problem with complex geometries, and also future amalgamation with adaptive-grid techniques [Minkowycz et al. (2006)].

The proposed three-dimensional CVFEM and its computer implementation were tested using several steady conduction-type problems, for which analytical solutions were constructed using a special technique proposed by Patankar (1980). In all cases, the agreement between the numerical and analytical solutions was excellent.

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