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TECHNICAL NOTE

MASS-LUMPING NUMERICAL MODELS OF THREE-DIMENSIONAL HEAT CONDUCTION

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A variable mass-lumping numerical model (nodal domain integration) of three-dimensional heat conduction in an inhomogeneous continuum is developed. The domain is discretized by tetrahedron-shaped elements and the state variable is approximated by linear trial functions. The resulting model represents the Galerkin finite-element, subdomain intergration, and integrated finite-difference methods as special cases and accommodates both Dirichlet and Neumann boundary conditions similar to a Galerkin finite-element model. Consequently, a unified domain numerical model is developed that readily represents each of the abovementioned domain numerical methods and an infinity of finite-element mass-lumping schemes by the specification of a single constant model parameter. Application of the nodal domain integration model to linear heat conduction problems indicates that the degree of model mass lumping must vary to minimize the approximation error.

INTRODUCTION

Hromadka and Guymon [1–3] examined the finite-difference, subdomain integration, and Galerkin finite-element methods for the solution of partial differential equations in one- and two-dimensional problems. They combined these numerical approaches to obtain a single numerical statement that can represent any of the numerical methods by the specification of a single constant parameter η. In this note, the integrated finite-difference model with triangular elements [4] is extended to a three-dimensional model with tetrahedral elements.

Reduction of the Galerkin finite-element mass matrix to a diagonal mass-lumped matrix is a well-known technique [5]. However, it is important to note that the so-called mass-lumped diagonal matrix is analogous to the integrated finite-difference capacitance matrix developed by Spalding [6]. An infinity of mass weightings of element nodal contributions can be determined directly by introducing an improved linear trial function in the finite element, where the element-boundary trial function continuity requirements are relaxed, and then using the usual subdomain integration version of the weighted residual process. The fact that certain mass-lumping patterns may improve computational results [7] suggests that an overall domain numerical method may be developed with a variable mass matrix.

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GOVERNING EQUATIONS AND SET DEFINITIONS

A three-dimensional advection-diffusion process in an inhomogeneous anisotropic nondeformable medium without sources or sinks may be macroscopically described by *the nonlinear partial differential equation*

$$\frac{\partial}{\partial x}\left(K_x \frac{\partial T}{\partial x} - UT\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial T}{\partial y} - VT\right) + \frac{\partial}{\partial z}\left(K_z \frac{\partial T}{\partial z} - WT\right) = C\frac{\partial T}{\partial t} \quad (1)$$

where x, y, and z are spatial coordinates; t is time; $K_x = K_{xx}$, $K_y = K_{yy}$, and $K_z = K_{zz}$ are principal-axis values of conductivity (e.g., Fickian diffusivity or thermal conductivity); C is a capacitance coefficient; T is the state variable (e.g., temperature); and U, V, and W are x, y, z-axis advection components (e.g., fluid velocity). It is assumed that Eq. (1) describes the governing flow process in the nondeformable global domain of spatial definition Ω with global boundary Γ. In vector notation, Eq. (1) may be written as

$$\int_\Gamma \mathbf{q} \cdot \mathbf{d\Gamma} = \int_\Omega C \frac{\partial T}{\partial t}\, dV \quad (2)$$

where $\mathbf{d\Gamma}$ is the outward unit normal vector to surface Γ, $\|\mathbf{d\Gamma}\| = dA$, and

$$\mathbf{q} \equiv \left(K_x \frac{\partial T}{\partial x} - UT\right)\mathbf{i} + \left(K_y \frac{\partial T}{\partial y} - VT\right)\mathbf{j} + \left(K_z \frac{\partial T}{\partial z} - WT\right)\mathbf{k} \quad (3)$$

The numerical approximation of Eq. (3) requires a discretization of the problem domain Ω. The usual subdomain (control volume) and finite-element discretization patterns differ. However, by overlapping these two discretization patterns, a third discretization is developed that is composed of smaller nodal domains. For an n-nodal point distribution in Ω with associated subdomains R_j and boundaries B_j

$$\Omega \equiv \sum_{j=1}^{n} R_j \quad (4)$$

$$R_j \equiv \overline{R_j} = R_j \, U B_j \quad (5)$$

Combining Eq. (2) with Eqs. (4) and (5),

$$\int_\Gamma \mathbf{q} \cdot \mathbf{d\Gamma} = \int_{UB_j} \mathbf{q} \cdot \mathbf{d\Gamma} \quad \text{and} \quad \int_\Omega C \frac{\partial T}{\partial t}\, dV = \int_{UR_j} C \frac{\partial T}{\partial t}\, dV \quad (6)$$

A finite-element discretization of Ω is defined by

$$\Omega = U\Omega^e \quad (7)$$

where each finite element Ω^e has a boundary Γ^e where

$$\Omega^e \equiv \overline{\Omega^e} = \Omega^e U \Gamma^e \tag{8}$$

A set of nodal domains Ω_j^e can be defined for each finite element as the intersection with associated subdomains

$$\Omega_j^e \equiv R_j \cap \Omega^e \tag{9}$$

This set of nodal domains is defined for each finite element Ω^e by the index of element nodal numbers

$$\Omega^e = U\Omega_j^e \qquad j \in S^e \tag{10}$$

where S^e is the set of nodes assigned to Ω^e.

Expanding the transport intergral of Eq. (3) gives

$$\int_{\Gamma_j^e} \mathbf{q} \cdot \mathbf{d\Gamma} = \int_{\Gamma_j^e} \left(K_x \frac{\partial T}{\partial x} l_x + K_y \frac{\partial T}{\partial y} l_y + K_z \frac{\partial T}{\partial z} l_z - UTl_x - VTl_y - WTl_z \right) dA \qquad j \in S^e \tag{11}$$

where l_x, l_y, and l_z are the direction cosines of $\mathbf{d\Gamma}$, and dA is the differential surface area. Equation (11) can be written as

$$\int_{\Gamma_j^e} \mathbf{q} \cdot \mathbf{d\Gamma} = \int_{\Gamma_j^e \cap \Gamma^e} \left(K_x \frac{\partial T}{\partial x} l_x + K_x \frac{\partial T}{\partial y} l_y + K_x \frac{\partial T}{\partial y} l_z \right) dA - \int_{\Gamma_j^e \cap \Gamma^e} (UTl_x + VTl_y + WTl_z)\, dA + \int_{\Gamma_j^e - \Gamma_j^e \cap \Gamma^e} \mathbf{q} \cdot \mathbf{d\Gamma} \qquad j \in S^e \tag{12}$$

where Γ^e is the boundary of finite element Ω^e. The first integral in the expansion of Eq. (12) satisfies Neumann boundary conditions on Γ^e or preserves flux continuity (due to conduction processes) between finite elements Ω^e. In the global assemblage of $U\Omega^e$, the first integral in the expansion of Eq. (12) also satisfies Neumann boundary conditions on the discretized approximation of global boundary Γ by Γ^e. Using Eq. (12), the element matrix system is given by

$$\left\{ \int_{\Gamma_j^e - \Gamma_j^e \cap \Gamma^e} \mathbf{q} \cdot \mathbf{d\Gamma} - \int_{\Gamma_j^e \cap \Gamma^e} [UT\mathbf{i} + VT\mathbf{j} + WT\mathbf{k}] \cdot \mathbf{d\Gamma} - \int_{\Omega_j^e} C \frac{\partial T}{\partial t}\, dV \right\} = \{0\} \qquad j \in S^e \tag{13}$$

NUMERICAL SOLUTIONS

The state variable T is assumed to be approximated by a linear trial function T^e in each finite element Ω^e [5]. Therefore

$$T \simeq T^e = \Sigma L_j T_j^e \tag{14}$$

where the L_j are the usual tetrahedral volume local coordinates in Ω^e, and T_j^e are nodal point values of the trial function estimate T^e in Ω^e.

To simplify the various weighted residual domain model derivations, the following description variable is used:

$$\Phi \equiv \frac{\partial}{\partial x}\left(K_x \frac{\partial T}{\partial x} - UT\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial T}{\partial y} - VT\right) + \frac{\partial}{\partial z}\left(K_z \frac{\partial T}{\partial z} - WT\right) - C\frac{\partial T}{\partial t}$$

$$(x, y, z) \in \Omega \tag{15}$$

Galerkin Method of Weighted Residuals

In local element Ω^e,

$$\int_{\Omega^e} \Phi L_j \, dV \equiv 0 \tag{16}$$

generates a Galerkin finite-element matrix system for approximation of Eq. (1) on Ω^e. Equation (16) can be linearized by assuming all parameters quasi-constant during a small time step Δt. The x-direction terms of Eq. (16) are given by

$$\int_{\Omega^e} \left(K_x^e \frac{\partial^2 T^e}{\partial x^2} - U^e \frac{\partial T^e}{\partial x}\right) L_j \, dV = \int_{\Gamma^e} K_x^e \frac{\partial T^e}{\partial x} \, dA_x - \int_{\Omega^e} \left(K_x^e \frac{\partial T^e}{\partial x}\frac{\partial L_j}{\partial x} - U^e \frac{\partial T^e}{\partial x} L_j\right) dV \tag{17}$$

where the first integral satisfies Neumann-type boundary conditions on global boundary Γ or conduction flux continuity between Ω^e.

From Fig. 1, the shape function gradient in Eq. (17) is

$$\frac{\partial L_j}{\partial x} = \frac{\partial}{\partial x}\left(\frac{V_j}{V^e}\right) = \frac{1}{V^e}\frac{\partial V_j}{\partial x} = -\frac{1}{(h_j, x)} \tag{18}$$

Thus,

$$\frac{\partial L_1}{\partial x} V^e = -\frac{1}{(h_1, x)} (\tfrac{1}{3} h_1, x)(A_1, x) \tag{19}$$

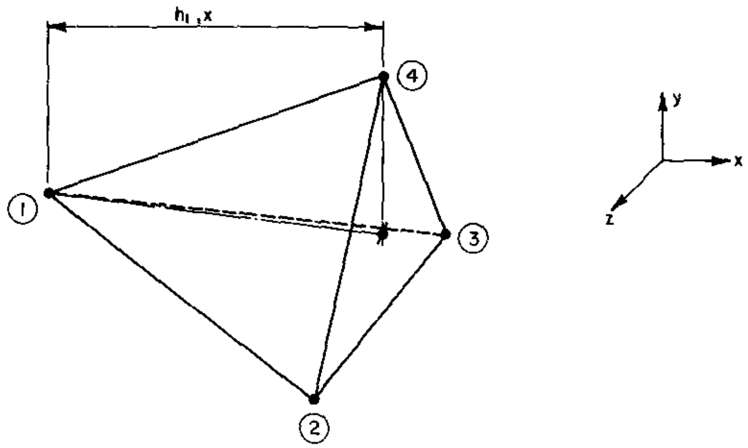

Fig. 1 Projection in the x direction of nodal point 1 onto the triangle face [2, 3, 4].

where (A_1, x) is the projection of the triangle face [2, 3, 4] onto the y, z coordinate plane. Simplifying Eq. (19) and substituting into Eq. (17) gives

$$\int_{\Omega^e} \left(K_x^e \frac{\partial^2 T^e}{\partial x^2} - U^e \frac{\partial T^e}{\partial x} \right) L_j \, dV = K_x^e \frac{\Sigma b_i T_i^e}{6V^e} \frac{(A_1, x)}{3} - U^e \frac{\Sigma b_i T_i^e}{6V^e} \frac{V^e}{4} \quad (20)$$

where V^e is an element volume and b_i are coordinate cofactors. The y, z direction terms are determined analogously. The time derivative term of Eq. (16) is modeled by

$$\int_{\Omega^e} C^e \frac{\partial T^e}{\partial t} L_j \, dV = C^e \int_{\Omega^e} L_i L_j \frac{\partial T_i^e}{\partial t} \, dV \quad (21)$$

Subdomain Integration

A cover of finite element Ω^e is given by the union of nodal domains Ω_j^e where $j \in S^e$. For a tetrahedral finite element, local nodel domain Ω_1^e in Ω^e is assumed to be defined by Fig. 2. The subdomain integration method solves Eq. (1) in Ω^e by

$$\int_{\Omega_j^e} \Phi \, dV = 0 \qquad j \in S^e \quad (22)$$

For the x-term transport components of Eq. (1),

$$\int_{\Omega_j^e} \left[\frac{\partial}{\partial x} \left(K_x^e \frac{\partial T^e}{\partial x} \right) - \frac{\partial}{\partial x} \left(U^e T^e \right) \right] dV = \dot{M}_j^e \qquad j \in S^e \quad (23)$$

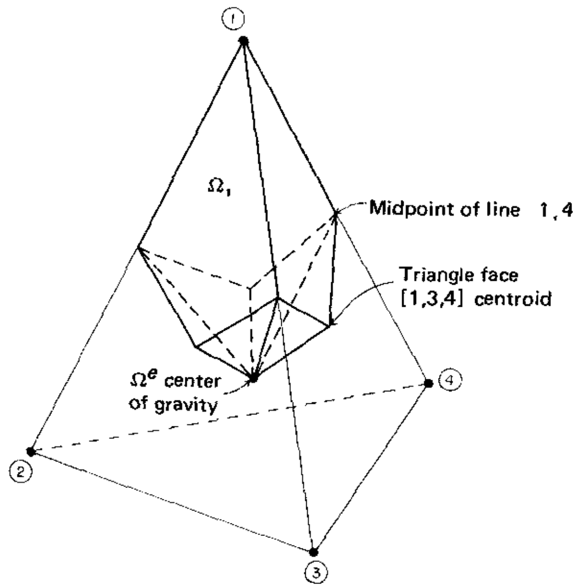

Fig. 2 Nodal domain Ω_1: geometric definition.

where $\dot{M}_j^e \equiv \int_{\Omega_j^e} C^e(\partial T^e/\partial t)\,dV$. Expanding Eq. (23) gives

$$\int_{\Gamma_j^e \cap \Gamma^e} K_x^e \frac{\partial T^e}{\partial x}\,dA_x + \int_{\Gamma_j^e - \Gamma_j^e \cap \Gamma^e} K_x^e \frac{\partial T^e}{\partial x}\,dA_x - \int_{\Omega_j^e} U^e \frac{\partial T^e}{\partial x}\,dV = \dot{M}_j^e \quad (24)$$

The first integral in Eq. (24) satisfies Neumann boundary conditions on Γ and conduction flux continuity between Ω^e, similar to the Galerkin formulation. From Figs. 1 and 2, the gradient terms of Eq. (24) are

$$K_x^e \frac{\partial T^e}{\partial x} \int_{\Gamma_j^e - \Gamma_j^e \cap \Gamma^e} dA_x - U^e \frac{\partial T^e}{\partial x} \int_{\Omega_j^e} dV = K_x^e \frac{\Sigma b_i T_i^e}{6V^e} \frac{(A_1, x)}{3} - U^e \frac{\Sigma b_i T_i^e}{6V^e} \frac{V^e}{4} \quad (25)$$

For the time derivative component of Eq. (24),

$$\dot{M}_j^e = \int_{\Omega_j^e} C^e \frac{\partial T^e}{\partial t}\,dV = C^e \frac{\partial}{\partial t} \int_{\Omega_j^e} T^e\,dV \qquad j \in S^e \quad (26)$$

Integrated Finite Difference

In this version of the subdomain integration method, it is assumed that

$$\int_{R_j} T^e \, dV = T_j^e \int_{R_j} dV \tag{27}$$

For a linear trial function T^e in each Ω^e, the transport terms of Eq. (1) evaluated on each B_j determine a conduction matrix identical to the Galerkin and subdomain integration approaches previously derived.

Nodal Domain Integration

The nodal domain integration numerical statement for solution of Eq. (1) on Ω^e is given in element matrix form for Ω^e by

$$\underset{\sim}{K}^e \underset{\sim}{T}^e + \underset{\sim}{P}^e(\eta)\dot{\underset{\sim}{T}}^e = \underset{\sim}{L}^e \tag{28}$$

where $\underset{\sim}{K}^e$ is the sum of element Ω^e conduction and convection matrices given (for the x term) by Eqs. (20) and (25), $\underset{\sim}{L}^e$ is a load vector of boundary conditions,

$$\underset{\sim}{P}^e(\eta) \equiv \frac{C^e V^e}{4(\eta + 3)} \begin{bmatrix} \eta & 1 & 1 & 1 \\ 1 & \eta & 1 & 1 \\ 1 & 1 & \eta & 1 \\ 1 & 1 & 1 & \eta \end{bmatrix} \tag{29}$$

and $\underset{\sim}{T}^e$, $\dot{\underset{\sim}{T}}^e$ are the vectors of the Ω^e nodal values and the time derivatives of the nodal values.

In Eq. (29), the Galerkin finite-element, subdomain integration, and integrated finite-difference numerical statemetns for a linear trial function in Ω^e are given by $\eta = (2, \frac{75}{23}, \infty)$, respectively.

SENSITIVITY OF DOMAIN MODELS TO DEGREE OF MASS LUMPING

To illustrate the sensitivity of the class of domain models to the factor η, two linear heat conduction problems (Figs. 3 and 4) are modeled to examine the approximation error for various values of mass lumping.

Using the mean relative error as the measurement, the finite-element mass matrix was varied by trial and error until a value of η was determined such that the time step advancement (Crank-Nicolson approach) resulted in the minimum error. Plots of optimum values from a typical simulation are given in Fig. 5. Both two- and three-dimensional solutions indicate that the integrated finite-difference approach reduces the mean relative error when the state variable gradient is severe within a finite element, and a subdomain integration analog best serves a milder variation of the state variable in a finite element.

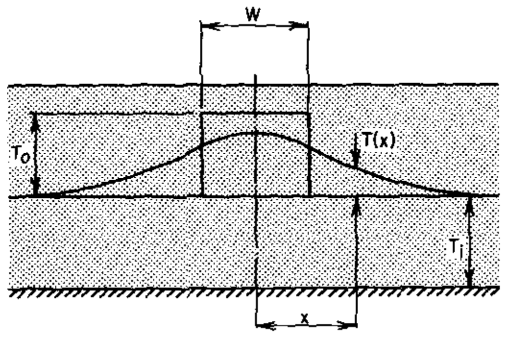

Fig. 3 Test problem 1. Thermal diffusion from a long heat source strip of width W that produces an instantaneous step change in temperature at T_0. Exact solution given by $T(x) = T_0$ (erf u_2 − erf u_1), where $u_1 = (x - W/2)/(4\alpha t)^{1/2}$ and $u_2 = (x + W/2)/(4\alpha t)^{1/2}$.

CONCLUSIONS

A nodal domain integration numerical model is derived to approximate a three-dimensional anisotropic heat conduction process in an inhomogeneous continuum. The model is found to represent the Galerkin finite-element, subdomain integration, and finite-difference methods as special cases. In addition, both Dirichlet and Neumann boundary conditions are accommodated as in a Galerkin finite-element numerical model. Application of the model to linear heat conduction problems indicates that the finite-element mass matrix must vary with time to provide an optimum numerical solution.

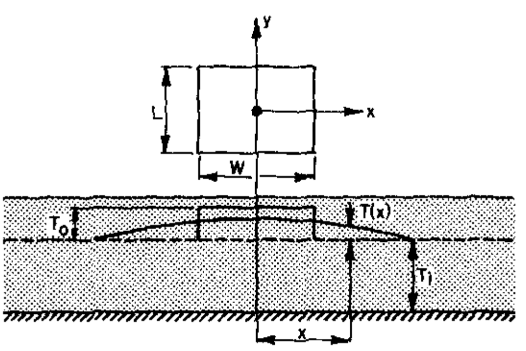

Fig. 4 Test problem 2. Thermal diffusion from a rectangular source that produces an instantaneous step change in temperature of T_0. Exact solution given by $T(x) = (T_0/4)$ (erf u_2 − erf u_1) (erf v_2 − erf v_1), where $u_1 = (x - W/2)/(4\alpha t)^{1/2}$, $u_2 = (x + W/2)/(4\alpha t)^{1/2}$, $v_1 = (y - L/2)/(4\alpha t)^{1/2}$, and $v_2 = (y + L)/(4\alpha t)^{1/2}$.

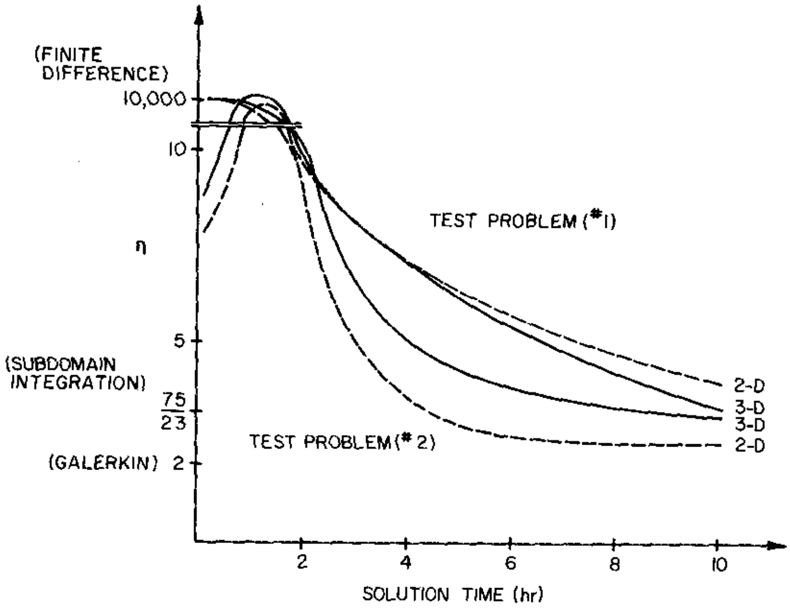

Fig. 5 Optimum mass weighting η-factors for two- and three-dimensional finite-element solution of test problems.

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