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Five-Point Form of the Nodal Diffusion Method and Comparison with Finite-Difference*

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Five-Point Form of the Nodal Diffusion Method and Comparison with Finite Difference

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Nodal Methods have been derived, implemented and numerically tested for several problems in physics and engineering. In the field of nuclear engineering, many nodal formalisms have been used for the neutron diffusion equation,[1,2] all yielding results which were far more computationally efficient than conventional Finite Difference (FD) and Finite Element (FE) methods. However, not much effort has been devoted to theoretically comparing nodal and FD methods in order to explain the very high accuracy of the former. In this Summary we outline the derivation of a simple five-point form for the lowest order nodal method and compare it to the traditional five-point, edge-centered FD scheme.[3,4] The effect of the observed differences on the accuracy of the respective methods is established by considering a simple test problem. It must be emphasized that the nodal five-point scheme derived here is mathematically equivalent to previously derived lowest order nodal methods.[5,6]

The first step in the derivation[7] is to divide the domain of the problem into M two-dimensional (for simplicity) "nodes", i.e., Cartesian rectangles of the form $[-a_m, +a_m] \times [-b_m, +b_m]$, with constant material properties in each node. The steady-state monoenergetic, external source diffusion equation is averaged over the area of each node, to obtain a nodal conservation equation relating the transverse-averaged net currents, J, on node surfaces to the node-averaged flux, $\bar{\bar{\phi}}_m$,

$$\frac{1}{2a_m}[J^x_{+m} - J^x_{-m}] + \frac{1}{2b_m}[J^y_{+m} - J^y_{-m}] + \sigma_m \bar{\bar{\phi}}_m = \bar{\bar{S}}_m, \qquad (1)$$

where $J^u_{\pm m} \equiv -[D_m d\bar{\phi}^v/du]_{u=\pm s_m}$, $u \equiv x$ *or* y, $v \equiv y$ *or* x and $s \equiv a$ *or* b; σ_m and D_m are the macroscopic removal cross section and the diffusion coefficient in node m, respectively,

S_m is the mth node-averaged external source defined in analogy to ϕ_m and ϕ^v is the v-averaged u-dependent flux. Next, the diffusion equation is transverse-averaged once with respect to x and once with respect to y. The two resulting ODE's can be solved exactly using a complementary function and a particular integral, which introduces two integration constants in each dimension and requires the only approximation in the whole process,[7] namely, expanding the external source and the leakage terms in a local series truncated at the lowest order. The integration constants can be eliminated in favor of the transverse-averaged flux evaluated on node surfaces which serve as the variable unknowns here. By assigning only one transverse-averaged flux to each surface, the continuity of the flux across node boundaries is automatically satisfied; continuity of the net current is discussed later.

Two processes can be performed on the resulting in-node solutions, $\bar{\phi}^x(y)$ and $\bar{\phi}^y(x)$: (1) they can be differentiated with respect to y and x, respectively, to obtain relations between the transverse-averaged, surface-evaluated currents, fluxes and source-leakage expansion coefficients. (2) They can be integrated over a node with respect to the independent variable to yield expressions for the node-averaged flux in terms of the transverse-averaged, surface-evaluated currents and source-leakage expansion coefficients. These two equations can be used to eliminate the source-leakage coefficients and obtain a weighted difference relation:

$$\bar{\phi}_m = \frac{1}{2}\left(\bar{\phi}^y_{+m} + \bar{\phi}^y_{-m}\right) + \left[\frac{1-\rho^x_m}{2\sigma_m a_m \rho^x_m}\right]\left(J^x_{+m} - J^x_{-m}\right), \tag{2}$$

where $\rho^x_m \equiv [\tanh(\gamma_m a_m)]/\gamma_m a_m$, $\gamma^2_m \equiv \sigma_m/D_m$; an equation analogous to Eq. (2) in the x-averaged variables can easily be obtained. Equation (2) is a weighted difference relation because it relates the variable unknowns in only one direction to the node-averaged flux. The five-point form of the nodal method follows immediately from substituting Eq. (2) and its x-averaged analogue in Eq. (1) to obtain,

$$\frac{\rho^x_m}{2(1-\rho^x_m)}\left(\bar{\phi}^y_{+m} - 2\bar{\bar{\phi}}_m + \bar{\phi}^y_{-m}\right) + \frac{\rho^y_m}{2(1-\rho^y_m)}\left(\bar{\phi}^x_{+m} - 2\bar{\bar{\phi}}_m + \bar{\phi}^x_{-m}\right)$$

$$-\bar{\bar{\phi}}_m = -\bar{\bar{S}}_m/\sigma_m. \tag{3}$$

This is a generalization of the result presented in Ref. 7.

A necessary condition for a well-posed algebraic problem is that the number of equations equals the number of variable unknowns. Thus, for a retangular mesh with I(J)nodes in the $x-(y-)$ direction, there are I×J $\bar{\phi}$-variables, (I+1)×J $\bar{\phi}^y$-variables and (J+1)×I $\bar{\phi}^x$-variables. Equation (3) represents a set of I×J equations; in addition, the global boundary conditions on $y(x)$ = constant surfaces supply 2I(2J) equations. The deficit in the number of equations is closed by imposing (I-1)×J and (J-1)×I net current continuity conditions on x=constant and y=constant internal surfaces, respectively.

There are three essential differences between the nodal and edge-centered FD five-point schemes.[3,4] First, the unknowns in FD are point quantities representing the flux at specified mesh points, while in the nodal method they represent averages over node surfaces or areas. Thus, the FD analogue of Eq. (3) covers four adjacent cells, while for nodal it is valid within one cell. Second, the spatial weights appearing in the discrete representation of the second derivatives in Eq. (3) involve hyperbolic functions unlike the algebraic type weights in FD. Third, in FD the net current is not required to be continuous across node boundaries: for an I×J rectangular mesh there are (I+1)×(J+1) unknowns; the FD analogue of Eq. (3) is required to hold at <u>each</u> interior mesh point thus producing (I-1)×(J-1) equations plus 2I and 2J global boundary conditions.

In order to illustrate the effect of these differences on the accuracy we applied the two methods to solving a simple test problem: A square region of dimension 1 cm with vacuum boundary conditions on all sides, and uniform removal cross section, $\sigma = 1\text{cm}^{-1}$; quadrant I had a unit source and D = 400, 100, 100, 25 cm for quadrants I, II, III, and IV, respectively, where II and III are diagonally opposite. The solution obtained on different meshes was used to calculate quadrant-averaged fluxes as shown in Table I. Infinitesimal mesh value for each quantity was obtained by h^2-extrapolation of the two finest mesh results for each method; the FD and nodal extrapolated values differ by less than 1/2%. Based on the number of discrete variables solved in each method, the I×I nodal calculation

should be compared with 2I×2I FD calculation. In quadrant I the nodal method is about ten times more accurate, while in II it is three times more accurate and in IV it is twice as accurate as FD for the coarse meshes.

We have reduced the final equations for the two-dimensional lowest order nodal diffusion method to a simple five-point scheme comparable in structure to the traditional FD edge-centered method. The nodal method, which is mathematically equivalent to previously derived nodal diffusion methods, has been shown to be far more accurate than the FD method for a test problem with large flux gradients. The high accuracy of the nodal method results from the hyperbolic-type spatial weights, and imposing the continuity of the current across node boundaries. The relative importance of these two effects is currently under investigation. This may suggest a simple modification of conventional FD methods and codes that would significantly enhance their accuracy.

Table I

Comparison of the quadrant-averaged fluxes and percent errors calculated by the nodal and finite-difference methods for the test problem described in the text. The h^2-extrapolated values were obtained from the two finest meshes for each method. The errors for each method were calculated relative to that method's extrapolated fluxes, i.e., $\epsilon \equiv 100 \times (\phi^{\mu}/\phi^{\mu}_{ex} - 1)$, $\mu \equiv$ nodal, or FD.

	Quadrant I average flux (% error)	Quadrant II average flux (% error)	Quadrant IV average flux (% error)
Nodal (4x4)	.190160e-2(1.0)	.232634e-3(-7.0)	.949671e-4(14.)
(8x8)	.189161e-2(.49)	.242931e-3(-2.9)	.872587e-4(4.9)
(16x16)	.188534e-2(.16)	.248030e-3(-.87)	.842979e-4(1.4)
(20x20)	.188425e-2(.10)	.248817e-3(-.56)	.838918e-4(.87)
h^2-extrapolated	.188231e-2	.250216e-3	.831698e-4
FD (4x4)	.110662e-2(-41)	.388849e-3(55)	.162222e-3(95)
(8x8)	.158018e-2(-16)	.315226e-3(25)	.104877e-3(26)
(16x16)	.178744e-2(-4.9)	.272290e-3(8.4)	.890755e-4(7.0)
(32x32)	.185623e-2(-1.2)	.256530e-3(2.1)	.846857e-4(1.7)
h^2-extrapolated	.187916e-2	.251277e-3	.832224e-4

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