Final Report

IMPROVED DETERMINISTIC CALCULATIONAL METHODS
FOR IRREGULARLY SHAPED SHIELDS

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EXECUTIVE SUMMARY

The work done under the Department of Energy Grant No. DE-FG07-88ER12818, "Improved Deterministic Calculational Methods for Irregularly Shaped Shields" was completed on November 30, 1990. The research done under the grant included the development of the first deterministic neutron and radiation transport methods for irregularly shaped geometries. Three methods were developed by first introducing boundary-fitted-coordinate transformations for the transport equation, and then deriving compatible methods for the accurate and efficient numerical solution of the transformed transport equation. The first of these three was an S_N method, developed principally as a reference against which to compare the other two methods, whose developments were the main objectives. The other two methods were a constant-constant nodal transport method and a linear-linear nodal transport method.

This final report summarizes the development, testing and evaluation of our boundary-fitted-coordinate S_N method and of our boundary-fitted-coordinate nodal methods for neutron and radiation transport. The results obtained show that for given accuracy requirements the constant-constant nodal method is computationally the most efficient of the three numerical transport methods developed for irregularly shaped shields. More generally, they show that the use of boundary-fitted-coordinate transformations in conjunction with the compatible nodal transport methods we have developed comprises a practical approach to the deterministic calculation of neutron and radiation transport in irregular geometries. Thus these new nodal methods provide efficient techniques for practical deterministic calculations of particle transport in irregular geometries, as alternatives to costly Monte Carlo methods which traditionally have been required for such computations.

IMPROVED DETERMINISTIC CALCULATIONAL METHODS FOR IRREGULARLY SHAPED SHIELDS

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ABSTRACT

A new discrete nodal transport method has been developed for general two-dimensional curvilinear geometry by using a boundary-fitted coordinate transformation from the general 'physical' coordinates to square 'computational' coordinates. The metrics which appear in the transformed transport equation are expanded using a simple polynomial function, and the angular divergence term is treated in the same way it is treated in S_N methods for curved geometries. Because the metrics of the transformation depend upon the computational coordinates, the technical details of the formal development of the nodal method differ from those of ordinary nodal methods for rectangular geometry. However, the computational process in the transformed rectangular coordinate system is very similar to that used in conventional discrete nodal transport methods. A discrete S_N method also has been developed to solve the boundary-fitted coordinate transformed transport equation. Simple test problems for non-simple geometries were solved using the zeroth-order (constant-constant) nodal method, the first-order (linear-linear) nodal method, and the S_N method for the same physical and computational grids. The results for the test problems studied showed that, for most performance criteria, the computational efficiency of the zeroth-order nodal method was the highest of the three methods.

INTRODUCTION

Various nodal methods for solving the direction-discretized transport equation(1-8), collectively referred to here as discrete nodal transport methods (DNIM's), have been shown, since they first were developed in the late 70s, to be superior in computational efficiency to the conventional discrete S_H method. Although zeroth- and first-order multidimensional DNIM's have been developed and applied to fuel assembly, shielding, and well-logging problems, their development has been limited for the most part to Cartesian geometry(1-5) with some extensions to cylindrical geometry(6-8), even though most practical problems arise in the contexts of far more complicated geometric configurations.

Recognizing the practical importance of accommodating more complicated geometries, especially in realistic radiation shielding problems, nodal methods and S_H methods have been developed to solve such problems in conjunction with boundary-fitted coordinate transformations. Their development, implementation, testing and initial evaluation is reported here. The coordinate transformations, from the general curvilinear geometry 'physical grid' to the square Cartesian geometry 'computational grid' -- or more precisely the inverse transformations -- are made via recently developed elliptic grid generation techniques (9-13). Such techniques have been used in conjunction with finite-difference solutions to the neutron diffusion equation(14); but that application is similar to, and in many ways simpler than, the applications to fluid mechanics, where boundary-fitted coordinate transformations have been used extensively in conjunction with finite difference solutions to the transformed fluids equations. The situation here is more complicated for two important reasons. The first is because the problems being solved are not simple diffusion or continuum flow problems; rather, they are radiation

transport problems that require the inclusion of the direction vectors of the particles which adds significant complexities. The second is because, in the interest of computational efficiency, the transformed transport equations are being solved by nodal methods rather than only by a simple finite difference or S_N method (although an S_N method also is developed for comparison purposes); hence, the complications that arise from the space dependence of the transformation metrics must be addressed in the formulations of the nodal methods. The transformed transport equations are general curvilinear geometry transport equations in the transformed or computational spatial variables (ξ, η) . Hence, the spatial divergence terms include spatial differential operators with space-dependent coefficients (the metrics of the transformations), and there also are angular divergence terms in the transformed equations. Thus, there are two points which make the problem complicated in a general curved geometry. One is the metrics that exist in the spatial divergence term; the other is the angular divergence term. In the nodal methods, we expand the metrics using Legendre polynomials, and we treat the angular divergence term using the angular redistribution coefficients utilized in S_N methods. In the S_N method the metrics simply are treated as they are in S_N methods for cylindrical and spherical geometries. The transformed transport equation is solved on the computational grid using one or more of these three methods: the constant-constant (C-C) nodal method (i.e., the discrete nodal method with constant node-surface and constant node-interior spatial expansions of the discretized angular flux), the linear-linear (L-L) nodal method, and the diamond-difference S_N method.

After reviewing the orthogonal boundary-fitted coordinate transformation used in the next section, the development of the nodal methods is summarized in the third section. The results of the application of the three methods to two

test problems are presented and discussed in the next-to-last section, and the conclusions are presented in the final section.

THE BOUNDARY-FITTED COORDINATE TRANSFORMATION

Many numerical grid generation techniques have been developed in recent years; however, because practical radiation transport problems usually involve bounded geometries, elliptic grid generation techniques seem particularly appropriate for them. The previously developed elliptic grid generation technique⁽¹²⁾ that we have used begins from a set of two coupled elliptic partial differential equations for the computational coordinates ξ and η written in terms of the physical coordinates x and y

$$\xi_{xx} + \xi_{yy} = P(\xi, \eta); \quad \eta_{xx} + \eta_{yy} = Q(\xi, \eta) \quad (1)$$

where the subscripts indicate differentiation with respect to these subscripts, and $P(\xi, \eta)$ and $Q(\xi, \eta)$ are control functions which can be specified to control the concentration of the grid in various physical regions. Since the computational grid (ξ, η) actually is fixed first as a simple square grid and the structure of the physical grid (x, y) actually is calculated, the dependent and independent variables in these equations must be interchanged so that $x(\xi, \eta)$ and $y(\xi, \eta)$ can be determined. The result is⁽¹²⁾

$$\begin{aligned} \alpha x_{\xi\xi} - 2\beta x_{\xi\eta} + \gamma x_{\eta\eta} &= -J^2(x_{\xi}P + x_{\eta}Q) \\ \alpha y_{\xi\xi} - 2\beta y_{\xi\eta} + \gamma y_{\eta\eta} &= -J^2(y_{\xi}P + y_{\eta}Q) \end{aligned} \quad (2)$$

where

$$\begin{aligned} \alpha &= (x_{\eta})^2 + (y_{\eta})^2, & \beta &= x_{\xi}x_{\eta} + y_{\xi}y_{\eta}, \\ \gamma &= (x_{\xi})^2 + (y_{\xi})^2, & J &= x_{\xi}y_{\eta} - y_{\xi}x_{\eta}. \end{aligned} \quad (3)$$

This set of two coupled nonlinear elliptic partial differential equations is solved numerically for the boundary-fitted coordinates $x(\xi, \eta)$ and $y(\xi, \eta)$ in physical space for a specific set of control functions $P(x, y)$ and $Q(x, y)$ and specific boundary conditions that associate segments of the boundary of the physical domain with some or all the sides of the square computational domain. For certain choices of $P(x, y)$ and $Q(x, y)$, general elliptic grid generation transformations become orthogonal mappings. The use of such orthogonal mappings is convenient in radiation transport problems for two reasons. The first is that in this case, because certain rearranged combinations of the metrics which appear in the transformed transport equation depend upon only one of the transformed coordinates, it is possible to expand these quantities and develop various order self-consistent nodal methods. The second reason is that the most common transport boundary conditions such as specified incoming angular fluxes are most easily applied in the context of orthogonal transformations. Hence, we restrict the boundary-fitted coordinate transformations used here to the subclass that are orthogonal mappings⁽¹³⁾. This is done by restricting the control functions to satisfy $P(x, y) = (\alpha\gamma)^{-1/2} (\partial/\partial\xi)(f)$ and $Q(x, y) = (\alpha\gamma)^{-1/2} (\partial/\partial\eta)(1/f)$ where $f(x, y)$ is called the distortion function. Under these conditions, Eqs. (2) become

$$(fx_\xi)_\xi + \left(\frac{1}{f} x_\eta\right)_\eta = 0; \quad (fy_\xi)_\xi + \left(\frac{1}{f} y_\eta\right)_\eta = 0; \quad f = (\alpha/\gamma)^{1/2} \quad (4)$$

Since an accurate representation of the boundary conditions usually is important in transport problems, retaining the flexibility of specifying the grid point distribution along the boundaries is desirable. Hence the "weak constraint" method⁽¹³⁾ of solving Eqs. (4) was used. This method permits the complete specification of all the "boundary values" for $x(\xi, \eta)$ and $y(\xi, \eta)$ on

the (ξ, η) grid boundary. Then the distortion function $f(x, y)$ is determined along with a self-consistent solution to Eqs. (4). Thus, after complete specification of the boundary conditions, these equations were solved numerically via a finite difference method by iterating on the function $f(x, y)$ from an initial guess to determine the coordinate points $(x(\xi, \eta), y(\xi, \eta))$ in the physical plane which correspond to those in the computational plane (ξ, η) at which the angular flux values, etc. are to be determined. Then the transport equation, transformed from physical spatial coordinates (x, y) to computational spatial coordinates (ξ, η) , was solved via the C-C nodal method, the L-L nodal method or the S_N method, and the angular flux calculated for a point or region indexed by (ξ_i, η_j) in the computational domain was plotted or tabulated (assigned) at the point or region corresponding to $(x(\xi_i, \eta_j), y(\xi_i, \eta_j))$ in the physical domain.

THE NODAL METHOD

The direction-discretized transport equation, for a one-group, two-dimensional problem with two curvilinear coordinates, after transformation from the physical (x, y) coordinates in a complicated physical domain to computational coordinates (ξ, η) in a square domain, becomes

$$\frac{1}{(x_\xi^2 + y_\xi^2)^{1/2} (x_\eta^2 + y_\eta^2)^{1/2}} \left[\mu \frac{\partial}{\partial \xi} ((x_\eta^2 + y_\eta^2)^{1/2} N) + \nu \frac{\partial}{\partial \eta} ((x_\xi^2 + y_\xi^2)^{1/2} N) + \right. \\ \left. \frac{\partial}{\partial \omega} \left\{ \left(\mu \frac{\partial (x_\xi^2 + y_\xi^2)^{1/2}}{\partial \eta} - \nu \frac{\partial (x_\eta^2 + y_\eta^2)^{1/2}}{\partial \xi} \right) N \right\} \right] + \sigma N(\xi, \eta) = S \quad (5)$$

(Since η is used traditionally both for a computational coordinate and a direction cosine, ν has been used for the latter here.) The detailed development of Eq. (5), the two-dimensional transport equation in general

curvilinear coordinates, needed here to accommodate general boundary-fitted coordinate transformations is given in the appendix which very closely follows Ref. 15, adding to that work only its explicit completion for the general two-dimensional case.

The development of the nodal methods begins by decomposing the square computational domain into computational volume elements. Equation (5) is then transformed from global computational coordinates (ξ, η) to local coordinates (ξ', η') , $-1 \leq \xi', \eta' \leq +1$, using the simple transformations

$$\xi = (\Delta\xi/2) \xi' + \xi_I; \quad \eta = (\Delta\eta/2) \eta' + \eta_J, \quad (6)$$

where

$$\begin{aligned} \xi_I &= (\xi_{i+1} + \xi_i)/2; & \Delta\xi &= \xi_{i+1} - \xi_i \\ \eta_J &= (\eta_{j+1} + \eta_j)/2; & \Delta\eta &= \eta_{j+1} - \eta_j \end{aligned} \quad (7)$$

The transport equation in these local coordinates (ξ', η') then is multiplied by $\Delta\xi\Delta\eta$ yielding

$$\begin{aligned} \mu \frac{\partial}{\partial \xi'} \{ (x_\eta^2 + y_\eta^2)^{1/2} \Delta\eta N \} + \nu \frac{\partial}{\partial \eta'} \{ (x_\xi^2 + y_\xi^2)^{1/2} \Delta\xi N \} + \frac{\partial}{\partial \bar{\omega}} \{ (\mu \frac{\partial (x_\xi^2 + y_\xi^2)^{1/2} \Delta\xi}{\partial \eta'} - \\ \nu \frac{\partial (x_\eta^2 + y_\eta^2)^{1/2} \Delta\eta}{\partial \xi'}) N \} + \frac{1}{2} (\sigma N - S) ((x_\xi^2 + y_\xi^2)(x_\eta^2 + y_\eta^2))^{1/2} \Delta\xi \Delta\eta = 0 \end{aligned} \quad (8)$$

where the denominator in Eq. (5) also has been cleared. Next, the direction vector Ω (or angle cosines μ and ν) is discretized, and the angular divergence -- the third term in Eq. (8) -- is treated using the angular redistribution approach normally employed in the S_N method⁽¹⁶⁾. The quantities $(x_\eta^2 + y_\eta^2)^{1/2} \Delta\eta$ and $(x_\xi^2 + y_\xi^2)^{1/2} \Delta\xi$ -- incorrectly written in Ref. 17 in which $\Delta\eta$ and $\Delta\xi$ were inadvertently interchanged -- are expanded within each computational element

using Legendre polynomials of the single variable ξ' or η' upon which each respectively depends. These expansions are then truncated at first order, and with a and b defined as the zeroth and first coefficients in the Legendre expansion of the first of these quantities and c and d as the zeroth and first coefficients in the expansion of the second quantity, Eq. (8) becomes

$$\begin{aligned} \mu_{m,\ell} \frac{\partial}{\partial \xi} ((a+b\xi)N) + \nu_{m,\ell} \frac{\partial}{\partial \eta} ((c+d\eta)N) + \frac{\Delta A_i}{2W} (\alpha_{m+1/2} N_{m+1/2} - \alpha_{m-1/2} N_{m-1/2}) \\ + \frac{\Delta B_j}{2W} (\beta_{\ell+1/2} N_{\ell+1/2} - \beta_{\ell-1/2} N_{\ell-1/2}) + \frac{1}{2} (\sigma N - S)(a+b\xi)(c+d\eta) = 0 \end{aligned} \quad (9)$$

where the primes ($'$) on ξ' and η' have been dropped so that ξ and η henceforth represent the local spatial computational coordinates, and the additional symbols introduced have the standard definitions used for them in the development of the S_N method for curved geometries

$W = W_{m,\ell}$: The area element on the unit directional sphere associated with direction vector $\Omega_{m,\ell}$.

$\alpha_{m-1/2}$: The angular redistribution coefficient in the i -direction at the inner edge of the angular mesh denoted by $W_{m,\ell}$.

$\beta_{\ell-1/2}$: The angular redistribution coefficient in the j -direction at the inner edge of the angular mesh denoted by $W_{m,\ell}$.

ΔA_i : $A_{i+1} - A_i$.

A_i : The area element of the i surface of a spatial computational element.

ΔB_j : $B_{j+1} - B_j$.

B_j : The area element of the j surface of a spatial computational element.

The zeroth-order (C-C) and first-order (L-L) nodal methods are developed directly from Eq. (9) by obtaining expressions for the zeroth and first

transverse moments of the outgoing angular fluxes on the surfaces of the computational elements. This is done by first transverse integrating Eq. (9) in one direction (e.g., the η -direction) within a computational element to obtain a one-dimensional transport equation, formally solving the resulting ξ -dependent equation analytically, and taking the limit as $\xi \rightarrow +1$ to arrive at the following expression for the outgoing angular flux on the right boundary of the square element in the computational plane

$$N_R = N_0^\eta(\xi=+1) = L^\xi \left[\frac{1}{2}(a+b\xi)(c+d\eta)S_0^\eta(\xi) - \frac{\Delta\mu}{2W}(\alpha_{m+1/2}N_{0,m+1/2}^\eta(\xi) - \alpha_{m-1/2}N_{0,m-1/2}^\eta(\xi)) - \frac{\Delta\nu}{2W}(\beta_{\ell+1/2}N_{0,\ell+1/2}^\eta(\xi) - \beta_{\ell-1/2}N_{0,\ell-1/2}^\eta(\xi)) - \frac{\nu_{m,\ell}}{2} \left[(c+d\eta)N(\xi,\eta) \right]_{\eta=-1}^{\eta=+1} - \frac{\sigma}{4} d(a+b\xi)N_1^\eta(\xi) \right] + L_0^\xi N_0^\eta(\xi=-1),$$

$$\mu_{m,\ell}, \nu_{m,\ell} > 0 \quad (10)$$

Here $2N_0^\eta(\xi)$ is the zeroth spatial Legendre moment in the η direction, within the computational element, of the flux in the direction $(\mu_{m,\ell}, \nu_{m,\ell})$. The same quantity is indicated at the boundaries of $(\Delta\mu_{m,\ell}, \Delta\nu_{m,\ell})$ by the additional subscripts $m \pm 1/2$ or $\ell \pm 1/2$. The integral operator L^ξ and the constant coefficient L_0^ξ in Eq. (10) are given by

$$L^\xi = \int_{-1}^{+1} d\xi' \frac{\exp\left\{-\int_{\xi'}^1 \left[\frac{\sigma c}{2\mu} + \frac{b}{(a+b\xi')}\right] d\xi''\right\}}{\mu(a+b\xi)} \quad (11-a)$$

and

$$L_0^\xi = \exp\left\{-\int_{-1}^{+1} \left[\frac{\sigma c}{2\mu} + \frac{b}{(a+b\xi)}\right] d\xi\right\} \quad (11-b)$$

To obtain the equation for the first spatial Legendre moment $N_1^\eta(\xi)$ of the outgoing surface angular flux, the linear moment of Eq. (9) is taken in the η

direction, the one-dimensional equation thus generated is solved, and the result is evaluated at $\xi = +1$ yielding

$$\begin{aligned} \theta_R = \bar{N}_1^\eta(\xi=+1) = L^\xi \left[\frac{1}{2}(a+b\xi)(c+d\eta)\bar{S}_1^\eta(\xi) - \frac{\Delta\lambda}{2W}i(\alpha_{m+1/2}\bar{N}_{1,m+1/2}^\eta(\xi) - \right. \\ \left. \alpha_{m-1/2}\bar{N}_{1,m-1/2}^\eta(\xi)) - \frac{\Delta B}{2W}j(\beta_{\ell+1/2}\bar{N}_{1,\ell+1/2}^\eta(\xi) - \beta_{\ell-1/2}\bar{N}_{1,\ell-1/2}^\eta(\xi)) \right. \\ \left. - \nu_{m,\ell} \left[\eta(c+d\eta)N(\xi,\eta) \right]_{\eta=-1}^{\eta=+1} + \nu_{m,\ell}(2c\bar{N}_0^\eta(\xi) + d\bar{N}_1^\eta(\xi)) - \frac{\sigma}{2}d(a+b\xi)\bar{N}_2^\eta(\xi) \right] \\ + L_0^\xi \bar{N}_1^\eta(\xi=-1), \end{aligned} \quad \mu_{m,\ell}, \nu_{m,\ell} > 0 \quad (12)$$

Here $\bar{N}_2^\eta(\xi)$ which arises from the combination of the first transverse Legendre moment with the linear term in the expansion of $(x_\xi^2 + y_\xi^2)^{1/2} \Delta\xi$, is the simple η^2 moment, not the second Legendre moment. These expressions, Eqs. (10) and (12), are formal analytical solutions for the zeroth and first η -moments of the outgoing angular fluxes at the right boundary of the computational element. Procedures similar to these, carried out on the ξ -integrated η -dependent equations, yield analogous expressions for $N_T = \bar{N}_0^\xi(\eta = +1)$ and $\theta_T = \bar{N}_1^\xi(\eta = +1)$. These are

$$\begin{aligned} N_T = \bar{N}_0^\xi(\eta=+1) = L^\eta \left[\frac{1}{2}(a+b\xi)(c+d\eta)\bar{S}_0^\xi(\eta) - \frac{\Delta\lambda}{2W}i(\alpha_{m+1/2}\bar{N}_{0,m+1/2}^\xi(\eta) - \right. \\ \left. \alpha_{m-1/2}\bar{N}_{0,m-1/2}^\xi(\eta)) - \frac{\Delta B}{2W}j(\beta_{\ell+1/2}\bar{N}_{0,\ell+1/2}^\xi(\eta) - \beta_{\ell-1/2}\bar{N}_{0,\ell-1/2}^\xi(\eta)) \right. \\ \left. - \frac{\mu_{m,\ell}}{2} \left[(a+b\xi)N(\xi,\eta) \right]_{\xi=-1}^{\xi=+1} - \frac{\sigma}{4}b(c+d\eta)\bar{N}_1^\xi(\eta) \right] + L_0^\eta \bar{N}_0^\xi(\eta=-1), \end{aligned} \quad \mu_{m,\ell}, \nu_{m,\ell} > 0 \quad (13)$$

and

$$\begin{aligned}
\theta_T = \bar{N}_1^\xi(\eta=+1) = L^\eta & \left[\frac{1}{2}(a+b\xi)(c+d\eta)\bar{S}_1^\xi(\eta) - \frac{\Delta A}{2W}i(a_{m+1/2}\bar{N}_{1,m+1/2}^\xi(\eta) - \right. \\
& a_{m-1/2}\bar{N}_{1,m-1/2}^\xi(\eta)) - \frac{\Delta B}{2W}j(\beta_{\ell+1/2}\bar{N}_{1,\ell+1/2}^\xi(\eta) - \beta_{\ell-1/2}\bar{N}_{1,\ell-1/2}^\xi(\eta)) \\
& - \mu_{m,\ell} \left[\xi(a+b\xi)N(\xi,\eta) \right]_{\xi=-1}^{\xi=+1} + \mu_{m,\ell}(2a\bar{N}_0^\xi(\eta) + b\bar{N}_1^\xi(\eta)) - \frac{\sigma}{2} b(c+d\eta)\bar{N}_2^\xi(\eta) \Big] \\
& + L_0^\eta \bar{N}_1^\xi(\eta=-1), \quad \mu_{m,\ell}, \nu_{m,\ell} > 0 \quad (14)
\end{aligned}$$

where the integral operator L^η and the constant L_0^η are given by

$$L^\eta = \int_{-1}^{+1} d\eta' \frac{\exp\{-\int_{\eta'}^1 [\frac{\sigma a}{2\nu} + \frac{d}{(c+d\eta')}] d\eta''\}}{\nu (c+d\eta)} \quad (15-a)$$

$$L_0^\eta = \exp\left\{-\int_{-1}^{+1} \left[\frac{\sigma a}{2\nu} + \frac{d}{(c+d\eta)}\right] d\eta\right\} \quad (15-b)$$

The integrals, that arise as a result of the two integral operators L^ξ and L^η in these expressions, are evaluated by expanding the spatial variations of the node transverse-surface fluxes $N(\xi, \pm 1)$ and $N(\pm 1, \eta)$ and the node-interior flux in Legendre polynomials through first order in ξ and η . For example,

$$N(1, \eta) = N_R + (3/2)\theta_R\eta + \dots \quad (16-a)$$

$$N(\xi, 1) = N_T + (3/2)\theta_T\xi + \dots \quad (16-b)$$

and

$$N(\xi, \eta) = (1/4)\bar{N}_{00} + (3/4)\bar{N}_{10}\xi + (3/4)\bar{N}_{01}\eta + (9/4)\bar{N}_{11}\xi\eta + \dots \quad (16-c)$$

or

$$2\bar{N}_0^\eta(\xi) = (1/2)\bar{N}_{00} + (3/2)\bar{N}_{10}\xi + \dots \quad (16-d)$$

$$\bar{N}_1^\eta(\xi) = (1/2)\bar{N}_{01} + (3/2)\bar{N}_{11}\xi + \dots \quad (16-e)$$

and

$$\bar{N}_2^\eta(\xi) = (1/6)\bar{N}_{00} + (1/2)\bar{N}_{10}\xi + \dots \quad (16-f)$$

also is used. The double moments $\bar{N}_{00}$, $\bar{N}_{10}$, $\bar{N}_{01}$ are obtained from the balance equation Eq. (9), by taking the corresponding moments. The double linear moment $\bar{N}_{11}$ is neglected since it is second order.

The double zeroth moment equation is obtained by integrating Eq. (9) over the computational element in both the ξ and η directions which gives

$$\begin{aligned} & \mu\{(a+b)N_R - (a-b)N_L\} + \nu\{(c+d)N_T - (c-d)N_B\} + \frac{\Delta\lambda}{2W}i(\alpha_{m+1/2}\bar{N}_{00,m+1/2} - \\ & \alpha_{m-1/2}\bar{N}_{00,m-1/2}) + \frac{\Delta B}{2W}j(\beta_{\ell+1/2}\bar{N}_{00,\ell+1/2} - \beta_{\ell-1/2}\bar{N}_{00,\ell-1/2}) + \\ & \sigma(ac\bar{N}_{00} + bc\bar{N}_{10} + ad\bar{N}_{01})/4 = (ac\bar{S}_{00} + bc\bar{S}_{10} + ad\bar{S}_{01})/4 \end{aligned} \quad (17)$$

The first ξ -moment zeroth η -moment equation is obtained by multiplying Eq. (9) by ξ and again integrating over the computational element in both directions which yields

$$\begin{aligned} & \mu\{2(a+b)N_R + 2(a-b)N_L - a\bar{N}_{00} - b\bar{N}_{10}\} + \nu\{(c+d)\theta_T - (c-d)\theta_B\} \\ & + \frac{\Delta\lambda}{2W}i(\alpha_{m+1/2}\bar{N}_{10,m+1/2} - \alpha_{m-1/2}\bar{N}_{10,m-1/2}) + \frac{\Delta B}{2W}j(\beta_{\ell+1/2}\bar{N}_{10,\ell+1/2} \\ & - \beta_{\ell-1/2}\bar{N}_{10,\ell-1/2}) - \sigma(bc\bar{N}_{00} + 3ac\bar{N}_{10} + 2bd\bar{N}_{01})/6 = \\ & (bc\bar{S}_{00} + 3ac\bar{S}_{10} + 2bd\bar{S}_{01})/6 \end{aligned} \quad (18)$$

Finally, the zeroth ξ -moment first η -moment equation is obtained by multiplying Eq. (9) by η and integrating over the element which gives

$$\begin{aligned} & \mu\{(a+b)\theta_R - (a-b)\theta_L\} + \nu\{2(c+d)N_T + 2(c-d)N_B - c\bar{N}_{00} - d\bar{N}_{01}\} \\ & + \frac{\Delta\lambda}{2W}i(\alpha_{m+1/2}\bar{N}_{01,m+1/2} - \alpha_{m-1/2}\bar{N}_{01,m-1/2}) + \frac{\Delta b}{2W}j(\beta_{\ell+1/2}\bar{N}_{01,\ell+1/2} \\ & - \beta_{\ell-1/2}\bar{N}_{01,\ell-1/2}) - \sigma(ad\bar{N}_{00} + 3ac\bar{N}_{01} + 2bd\bar{N}_{10})/6 = \\ & (ad\bar{S}_{00} + 3ac\bar{S}_{01} + 2bd\bar{S}_{10})/6 \end{aligned} \quad (19)$$

These three balance equations are used with the surface flux moment equations, Eqs. (10), (12), (13) and (14), which together yield a closed system of equations.

In the C-C DNTM, we keep the constant terms in the surface and interior flux expansions in Eq. (16). For the three unknowns N_R , N_T and $\bar{N}_{00}$, we use respectively the expressions for the zeroth moments of the outgoing surface fluxes, Eqs. (10) and (13), and the double zeroth moment of the balance equation, Eq. (17). In the L-L DNTM, we keep the constant and linear terms in the surface and interior flux expansions in Eq. (16). For the seven unknowns N_R , N_T , θ_R , θ_T , $\bar{N}_{00}$, $\bar{N}_{10}$ and $\bar{N}_{01}$, we use the expressions for the zeroth and first moments of the outgoing surface fluxes, Eqs. (10), (13), (12) and (14), and the three double moment balance equations, Eqs. (17), (18) and (19). We employ the method used in TWOTRAN(16) to estimate the unknown interior flux moments at the outer edge of the angular mesh. That is, to initialize the angular sweep we set the interior moments of the flux at the first discretized angle equal to those at the inner edge of the first discretized angular mesh cell. After that, the diamond difference approximation is used to estimate the values at the outer edge of an angular mesh cell in terms of the values at the

center and inner edge of that cell.

The solution algorithm is similar to that used in Cartesian geometry nodal methods except that for certain physical geometries iterations must be performed because we must use initial guesses for the 'incoming' angular fluxes at an internal 'boundary', rather than known boundary values for true incoming angular fluxes at an exterior boundary.

The detailed development of the S_N method for solving Eq. (5), the boundary-fitted coordinate transformed transport equation, will be omitted because it is analogous to that used for spherical geometry⁽¹⁶⁾ in which there also are two curved coordinates.

RESULTS AND DISCUSSION

In order to validate the boundary-fitted coordinate nodal methods, they were applied to special-case test problems in conventional right circular cylindrical geometry⁽⁸⁾ prior to the applications to problems in more complicated geometries reported here. Those studies⁽⁸⁾ established that the metrics could be treated in the nodal methods as they are treated here and that the angular divergence term could be adequately approximated in the nodal methods via an angular redistribution term, as it is approximated in S_N methods. They also demonstrated that the computational efficiency of the C-C nodal method was greater than those of the S_N method and the L-L nodal method for cylindrical geometry, at least for the test problems studied. This is in contrast to conclusions made for an earlier cylindrical geometry C-C nodal method⁽⁶⁾, in which the angular divergence term was treated via a transverse integration procedure analogously to the way the spatial derivatives are treated in nodal transport methods. There, the authors concluded that the C-C nodal method was less efficient than the S_N method because the nodal-method-

like treatment of the angular divergence term resulted in the need to solve nodal equations for two-dimensional cylindrical geometry that require computational effort which is comparable to that required for three-dimensional Cartesian geometry nodal equations⁽⁶⁾. Hence, the approach used here to treat the angular divergence term in the boundary-fitted coordinate transformed transport equation not only worked for the cylindrical geometry transport equation, but it also was more efficient than that clearly more elegant but less practical alternative.

The first problem solved that was not a 'conventional geometry' special case was one made up of two cylinders, the smaller one located eccentrically inside the larger one. This problem involves two curvilinear coordinates and is meant to be an extreme idealization of the salient features of the problem of shielding an eccentrically located cylindrical shell radiation source. Although it is not cylindrically symmetric, there is left-right symmetry; hence, the problem was solved using half the physical domain with a reflective boundary condition at the plane of symmetry. The boundary-fitted coordinate grid on the physical domain for an 80x80 'radial'(I)-'angular'(J) grid is shown in Fig. 1 for the region exterior to the inner cylinder. The corresponding computational grid, from which it was generated, of course is a simple 80x80 square grid. None of the coarser boundary-fitted coordinate grids used in the studies reported here was generated directly; rather, they were derived from the 80x80 grid by successively combining two or four cells into one to obtain the next coarser grid. This was done by connecting the four resulting cell corner points on the new coarser grid by straight lines for grid illustration purposes, but by preserving cell volume and cell surface area for computational purposes. The one-energy-group problem was solved in the S-2 approximation with $\mu_1 = -\mu_2 = \nu_1 = -\nu_2 = -0.577350269$ and equal weights $w = \pi/2$. The

radii of the two cylinders were 14 cm and 4 cm, and the center of the latter was 6 cm below the center of the former. The cross sections in the outer region were $\Sigma_a = 1.00 \text{ cm}^{-1}$ and $\Sigma_s = 0.25 \text{ cm}^{-1}$. The inner cylinder was comprised of a 'perfect absorber' (all particles that enter are absorbed). A unit (per cm) half-range isotropic (outward-directed) source was located on the circumference of the inner cylinder.

Some of the results for this test problem are summarized in Table 1 in which the computer leakages from the outer cylinder are compared. Since both Cartesian geometry and cylindrical geometry approximations to a problem like this have errors that are difficult to quantify, the reference solution for the leakage was obtained from an h-squared extrapolation of the 40x40 and 80x80 S_N computed values. Although this might bias the comparison a little in favor of the S_N method, that bias is very small since the h-squared extrapolation of the 20x20 and 40x40 values computed by the C-C nodal method was only about 0.002 (0.25 percent) lower. Notwithstanding some small error in the reference value, it is clear from Table 1 that the C-C DNTM satisfies a given error criterion on the leakage in less iteration time than either the S_N method or the L-L DNTM. For example, the 20x20 C-C nodal calculation (2.45 sec) leads to an error (-2.54 percent) between those that result in the 40x40 S_N calculation (5.67 sec, -4.69 percent) and the 80x80 S_N calculation (24.42 sec, -1.20 percent); and the error in the 40x40 C-C nodal calculation (10.16 sec, -0.65 percent) is less than that in the 80x80 S_N calculation (24.42 sec, -1.20 percent). At the other extreme, for looser error criteria, the 5x5 C-C nodal calculation (0.16 sec, 15.38 percent) leads to a smaller error than the 20x20 S_N calculation (1.71 sec, -17.86 percent) in considerably less time. The leakage calculated using the L-L nodal method on the 10x10 and 20x20 meshes for this problem were only slightly more accurate than those obtained using the C-C nodal method on the

same meshes and the computation times were very dramatically larger. This is because it is necessary to invert a 7×7 matrix to calculate the outgoing angular fluxes from each node in the present L-L nodal method formulation. Methods of circumventing this problem are being explored. However, if a significant improvement in the accuracy of the L-L DNTM over that of the C-C DNTM cannot be demonstrated for other test problems, there is little practical motivation to doing this. The error in the leakage in the 5×5 L-L DNTM calculation is larger than that in the 5×5 C-C DNTM calculation; however, this may be due to the fact that on such a coarse mesh the L-L DNTM yields a negative flux in some nodes whereas the C-C DNTM does not.

Additional results for this first test problem are shown in Figs. 2-5. Calculations were done for this problem using the C-C nodal and S_N methods on a sequence of grids in which the spatial 'angular' mesh (J) was fixed at 40. This was done because, as one would expect, the spatial flux distributions are less sensitive to grid refinement in this direction than in the 'radial' direction. The 'radial' traverses, along the $j = 39$ mesh boxes of a $J = 40$ mesh (i.e., a little to the right of vertically upward), of the angular fluxes at the outer surfaces of the computational elements in the direction to the left of the outward normal at the element surface, computed on three S_N grids (40×40 , 80×40 , 120×40) and on three C-C nodal grids (20×40 , 40×40 , 80×40) are shown in Fig. 1. The 40×40 S_N results oscillate fairly dramatically over the outer two-thirds of the radial mesh and the distribution near the surface, even if smoothed, would be in substantial error. As the 'radial' mesh is refined to 80 and 120, these S_N angular fluxes become more accurate, but the oscillations, although less severe, are still significant. Conversely, the angular fluxes that result from the 40×40 and 80×40 C-C nodal calculations are smooth and appear to be quite accurate, agreeing reasonably well with the 120×40 S_N

results except, of course, that they do not exhibit the erroneous oscillations that plague the S_N method on these 'insufficiently fine' S_N meshes. Moreover, even the 20x40 C-C nodal results appear to be quite accurate in addition to being smooth. Finally, the spatial distributions of the angular flux that result from the C-C nodal calculations appear to be converging smoothly and quickly as a function of the 'radial' (I) mesh. Although those that result from the S_N calculations also appear to be converging, due to the oscillations it is not clear how smooth or rapid this convergence is. The 'radial' transverses along the same mesh boxes of the total scalar fluxes resulting from the same six computations are shown in Fig. 3. They have similar characteristics to those of the angular fluxes that were just discussed.

Finally, the angular fluxes at the surface of the outer cylinder in the direction to the left of the outward normal, and the outgoing fluxes at this surface (which also are the total scalar fluxes there) that resulted from the three S_N calculations and from the three C-C nodal calculations are shown in Figs. 4 and 5. The fluxes are plotted in both figures as functions of position along the circumference of the outer cylinder starting from the bottom (i.e., as functions of the 'angular' (J) mesh). Naturally, the fluxes decrease as the top of the cylinder is approached since the optical distance from the source is maximum there. Just as in the two 'radial' (I mesh) traverses shown in Figs. 2 and 3, both the angular and scalar fluxes that resulted from the S_N calculations oscillate, here only in about the upper half of the 'angular' (J) mesh, and those from the C-C nodal method are smooth and appear to be converging smoothly and rapidly.

The second test problem studied was composed of the same eccentric two-dimensional cylindrical geometry. In this case, however, the inner cylinder (region 1) was not a 'perfect' absorber; rather, it had total cross section Σ_t

$\mu = 2.40 \text{ cm}^{-1}$ and an absorption cross section $\Sigma_a^1 = 2.0 \text{ cm}^{-1}$. The cross sections in the outer region (region 2) were the same as those in the first test problem, as were all the dimensions. In this second problem, the source also was different. It was a unit (per cm) half-range isotropic (inward-directed) source located on the circumference of the outer cylinder. As in the first test problem non-reentrant vacuum boundary conditions were used on the outer surface of the outer cylinder. This geometry and source arrangement is of interest as a crude representation of an eccentrically shielded detector or some inner chamber of a large facility. It also is relevant to the detection of neutrons and gamma rays returning to bore holes from underground formations in nuclear oil-well logging and uranium exploration. This one-energy-group problem was solved in the S-2 approximation using the same quadratures and weights used for the first test problem. The same grids also were used in region 2, and the grids used in region 1 were special cases of boundary-fitted coordinate grids -- uniform standard cylindrical r - θ grids.

A brief summary of the results for this second test problem is presented in Table 2. Computed values for the total absorption in region 1, the quantity of principal interest, are tabulated for solutions obtained using the C-C DNTM and the S_N method, each on five meshes. In this sequence of grids, the 'angular' (J) mesh was kept constant at twenty, a value that was determined to be adequate for these studies, and the inner 'radial' (I_1) mesh was kept constant at forty, which also was determined to be adequate for the correct computation of the absorption in region 1. Because three mesh numbers were involved in this sequence of grids, and only one was varied, extrapolation to a reliable reference solution was not possible. Hence, a fine mesh S_N result was used as the reference value which, from the systematic convergence of the errors for both the C-C DNTM and the S_N method, appears to be a fairly good

value. A quick glance at the errors in Table 2 shows that the C-C nodal method yields extremely accurate values for the absorption in region 1 in this problem even with only 5 mesh points in the 'radial' direction in region 2; in fact, it yields a smaller error than the S_N method does with forty mesh points in that direction in that region. The ratios of the computing times, S_N to C-C nodal, for comparable error criteria are not as impressive, however. This almost certainly is because refining the 'radial' mesh in the outer region (increasing I_2) does not significantly increase the total number of unknowns or the computation time, when I_1 is so large, until I_2 becomes fairly large. When the S_N grid is sufficiently fine, e.g., $(40+40) \times 20$, the error is fairly small and these results also seem satisfactory. However, when the grid is coarse the S_N error becomes quite large, with the exception of the $(40+10) \times 20$ case which appears to be fortuitous with a relatively small negative error that is quite out of pattern with the other S_N results. On the other hand, one might argue that the very large errors that result from the $(40+5) \times 20$ and $(40+20) \times 20$ S_N calculations are the unusual ones because of the negative fluxes that are obtained in those computations. In fact, negative fluxes plagued many of the boundary-fitted coordinate S_N calculations summarized here with negative flux fix-ups on the angular fluxes being required even at the end of the final iteration. Conversely, the appearance of negative fluxes in the nodal methods was extremely rare, especially in the C-C DNM.

CONCLUSION

In an effort to make possible improved deterministic transport computations for irregularly shaped radiation shields, reactor fuel pin cells and fuel bundles, and other applications such as nuclear well-logging, etc., we have begun the development of boundary-fitted coordinate transport methods. We have developed, encoded and tested constant-constant and linear-linear discrete

nodal transport methods and an S_N transport method, all three for boundary-fitted coordinate geometries. The results for the test problems studied show that these methods are accurate and have good computational efficiency. However, the numerical examples must be taken as preliminary, since a broad spectrum of test problems has not been studied using extensive sets of practical performance criteria. Nevertheless, the present results do establish the feasibility and value of combining discrete nodal transport methods and S_N methods, developed here for general curvilinear coordinates, with boundary-fitted coordinate transformations using elliptic grid generation techniques for irregular geometries which so frequently are of practical interest. Both the boundary-fitted coordinate S_N method and the boundary-fitted coordinate DNTM eventually should have their places in deterministic transport computations for irregular geometries.

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APPENDIX: The Explicit Form of the Two-Dimensional Transport Equation in General Curvilinear Coordinates

A general development of the three-dimensional transport equation in general curvilinear coordinates already has been given⁽¹⁵⁾. The final result obtained there for the transport equation in rectangular coordinates was

$$\text{div}(MN) + \sigma N = S \quad (\text{A-1})$$

where M is a contravariant vector in a five-dimensional space with a Riemannian metric. Since this equation is a five-dimensional tensor equation, it follows from the principle of covariance that it holds in any five-dimensional coordinate system.

The explicit forms of the transport equation in cylindrical coordinates and in spherical coordinates were derived from Eq. (A-1) in Ref. 15, but the analogous explicit form for general curvilinear coordinates was not. The general development there⁽¹⁵⁾ ended with Eq. (A-1). Since the explicit form of the transport equation for the general two-dimensional curvilinear geometry case is needed here to accommodate the general two-dimensional boundary-fitted coordinate transformations, we continue from Eq. (A-1) above, as given in Ref. 15, to develop this explicit form via steps completely analogous to those used to develop the explicit form for cylindrical geometry⁽¹⁵⁾. Recalling the transport equation in rectangular coordinates, with $n_x = n \cdot \hat{x} = (1-\zeta^2)^{1/2} \cos(\omega')$, $n_y = n \cdot \hat{y} = (1-\zeta^2)^{1/2} \sin(\omega')$, $n_z = n \cdot \hat{z} = \zeta$, and $n_x^2 + n_y^2 + n_z^2 = 1$,

$$n_x \frac{\partial N}{\partial x} + n_y \frac{\partial N}{\partial y} + n_z \frac{\partial N}{\partial z} + \sigma N = S \quad (\text{A-2})$$

and the corresponding contravariant vector

$$M_{\text{rect}} = (n_x, n_y, n_z, 0, 0), \quad (\text{A-3})$$

we introduce the general curvilinear coordinates (ξ, η) in the (x, y) plane perpendicular to the straight z coordinate to form the general coordinates $u^1 = \xi$, $u^2 = \eta$, $u^3 = z$, $u^4 = \omega$, and $u^5 = \zeta$. The resulting transformation equations from the curvilinear coordinates to the rectangular coordinates are

$$x_1 = x = x(\xi, \eta) \quad (A-4a)$$

$$x_2 = y = y(\xi, \eta) \quad (A-4b)$$

$$x_3 = z = z \quad (A-4c)$$

$$x_4 = \omega' = \omega + \theta \quad (A-4d)$$

$$x_5 = \zeta = \zeta \quad (A-4e)$$

where ω is the angle formed by the projection of Ω onto the (ξ, η) plane and the ξ -axis, and θ is the local rotation angle of the orthogonal curvilinear coordinates (ξ, η) with respect to the fixed rectangular coordinates (x, y) . Figure A-1 shows the angles ω , ω' and θ and the relationship between the curvilinear coordinates and the rectangular coordinates in the (x, y) or (ξ, η) plane.

The resulting Jacobian of the transformation from the curvilinear coordinates to the rectangular coordinates is

$$\left| \frac{\partial x^i}{\partial u^j} \right| = \begin{vmatrix} x_\xi & y_\xi & 0 & A & 0 \\ x_\eta & y_\eta & 0 & B & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{vmatrix} \quad (A-5)$$

and the Jacobian for the inverse transformation is

$$\left| \frac{\partial u^i}{\partial x^j} \right| = \begin{vmatrix} \xi_x & \eta_x & 0 & C & 0 \\ \xi_y & \eta_y & 0 & D & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{vmatrix} \quad (\Lambda-6)$$

where

$$A = \frac{\partial}{\partial \xi} \left\{ -\tan^{-1}\left(-\frac{x_\eta}{y_\eta}\right) \right\}; \quad B = \frac{\partial}{\partial \eta} \left\{ -\tan^{-1}\left(-\frac{x_\eta}{y_\eta}\right) \right\} \quad (\Lambda-7)$$

$$C = -\frac{\partial}{\partial x} \left\{ \tan^{-1}\left(\frac{\xi_y}{\xi_x}\right) \right\}; \quad D = -\frac{\partial}{\partial y} \left\{ \tan^{-1}\left(\frac{\xi_y}{\xi_x}\right) \right\} \quad (\Lambda-8)$$

The metric tensor a_{ij} in the curvilinear system follows from

$$a_{ij} = g_{k\ell} \frac{\partial x^k}{\partial u^i} \frac{\partial x^\ell}{\partial u^j} \quad (\Lambda-9)$$

which yields

$$J^2 = |a_{ij}| = (x_\xi^2 + y_\xi^2)(x_\eta^2 + y_\eta^2) - (x_\xi x_\eta + y_\xi y_\eta)^2 \quad (\Lambda-10)$$

From the contravariant vector in the rectangular system, we have

$$M_{\text{curv}}^i = M_{\text{rect}}^j \frac{\partial u^i}{\partial x^j} = (\Omega_x, \Omega_y, \zeta, 0, 0) \frac{\partial u^i}{\partial x^j} \quad (\Lambda-11)$$

More explicitly, the components are

$$M_{\text{curv}}^1 = \Omega_x \xi_x + \Omega_y \xi_y \quad (\text{A-12a})$$

$$M_{\text{curv}}^2 = \Omega_x \eta_x + \Omega_y \eta_y \quad (\text{A-12b})$$

$$M_{\text{curv}}^3 = \zeta \quad (\text{A-12c})$$

$$M_{\text{curv}}^4 = \Omega_x C + \Omega_y D \quad (\text{A-12d})$$

$$M_{\text{curv}}^5 = 0. \quad (\text{A-12e})$$

In the curvilinear system, the divergence becomes

$$\text{div } \mathbf{M} = \frac{1}{J} \frac{\partial}{\partial u^i} (J M^i) \quad (\text{A-13})$$

and the divergence form of the transport equation, Eq. (A-1), in the curvilinear coordinates is

$$\begin{aligned} \frac{1}{J} \left[\frac{\partial}{\partial \xi} \{J(\Omega_x \xi_x + \Omega_y \xi_y)N\} + \frac{\partial}{\partial \eta} \{J(\Omega_x \eta_x + \Omega_y \eta_y)N\} + \frac{\partial}{\partial z} (J\zeta N) \right. \\ \left. + \frac{\partial}{\partial \omega} \{J(\Omega_x C + \Omega_y D)N\} \right] + \sigma N = S. \end{aligned} \quad (\text{A-14})$$

Now using the conditions for the orthogonal coordinate transformation

$$\sin \theta = \frac{-y_\xi}{(x_\xi^2 + y_\xi^2)^{1/2}} = \frac{x_\eta}{(x_\eta^2 + y_\eta^2)^{1/2}} \quad (\text{A-15a})$$

$$\cos \theta = \frac{x_\xi}{(x_\xi^2 + y_\xi^2)^{1/2}} = \frac{y_\eta}{(x_\eta^2 + y_\eta^2)^{1/2}} \quad (\text{A-15b})$$

$$x_\xi x_\eta + y_\xi y_\eta = 0 \quad (\text{A-15c})$$

and the general relationships between the coordinates

$$\xi_x = y_\eta/J, \quad \xi_y = -x_\eta/J, \quad \eta_x = -y_\xi/J, \quad \eta_y = x_\xi/J. \quad (\text{A-16})$$

the contravariant terms multiplied by J, written in Eq. (A-14) in terms of the derivatives of the curvilinear coordinates with respect to the rectangular coordinates, are rewritten in terms of the derivatives of the rectangular coordinates with respect to the curvilinear coordinates

$$J(\Omega_x \xi_x + \Omega_y \xi_y) = \mu (x_\eta^2 + y_\eta^2)^{1/2} \quad (\text{A-17a})$$

$$J(\Omega_x \eta_x + \Omega_y \eta_y) = \nu (x_\xi^2 + y_\xi^2)^{1/2} \quad (\text{A-17b})$$

$$J\zeta = \zeta (x_\eta^2 + y_\eta^2)^{1/2} (x_\xi^2 + y_\xi^2)^{1/2} \quad (\text{A-17c})$$

$$J(\Omega_x C + \Omega_y D) = \mu \frac{\partial}{\partial \eta} (x_\xi^2 + y_\xi^2)^{1/2} - \nu \frac{\partial}{\partial \xi} (x_\eta^2 + y_\eta^2)^{1/2} \quad (\text{A-17d})$$

where

$$\mu \equiv (1 - \zeta^2)^{1/2} \cos(\omega); \quad \nu \equiv (1 - \zeta^2)^{1/2} \sin(\omega) \quad (\text{A-17e})$$

Thus, finally the transformed transport equation in the two curvilinear coordinates (ξ, η) and one straight coordinate (z) becomes, in conservative form,

$$\begin{aligned} & \frac{1}{(x_\xi^2 + y_\xi^2)^{1/2} (x_\eta^2 + y_\eta^2)^{1/2}} \left[\mu \frac{\partial}{\partial \xi} ((x_\eta^2 + y_\eta^2)^{1/2} N) + \nu \frac{\partial}{\partial \eta} ((x_\xi^2 + y_\xi^2)^{1/2} N) + \right. \\ & \left. \frac{\partial}{\partial z} \left\{ \zeta (x_\eta^2 + y_\eta^2)^{1/2} (x_\xi^2 + y_\xi^2)^{1/2} N \right\} + \frac{\partial}{\partial \omega} \left\{ \left(\mu \frac{\partial (x_\xi^2 + y_\xi^2)^{1/2}}{\partial \eta} - \nu \frac{\partial (x_\eta^2 + y_\eta^2)^{1/2}}{\partial \xi} \right) N \right\} \right] \\ & + \sigma N = S, \end{aligned} \quad (\text{A-18})$$

For a system with geometry, sources, and boundary conditions uniform in the z -direction the derivative with respect to z vanishes, and this reduces the transport equation for two-dimensional general curvilinear coordinates, Eq. (5) in the main text, which subsequently is used there to accommodate the general boundary-fitted computational coordinates.

In non-conservative form the transformed transport equation, Eq. (A-18), becomes

$$\frac{\mu}{(x_{\xi}^2 + y_{\xi}^2)^{1/2}} \frac{\partial N}{\partial \xi} + \frac{\nu}{(x_{\eta}^2 + y_{\eta}^2)^{1/2}} \frac{\partial N}{\partial \eta} + \zeta \frac{\partial N}{\partial z} +$$

$$\frac{1}{(x_{\xi}^2 + y_{\xi}^2)^{1/2} (x_{\eta}^2 + y_{\eta}^2)^{1/2}} \frac{\partial}{\partial \omega} \left\{ \left(\mu \frac{\partial (x_{\xi}^2 + y_{\xi}^2)^{1/2}}{\partial \eta} - \nu \frac{\partial (x_{\eta}^2 + y_{\eta}^2)^{1/2}}{\partial \xi} \right) N \right\} + \sigma N = S. \quad (A-19)$$

Table 1. Comparison Among DNTM C-C, DNTM L-L, and S_N Method for Test Problem No. 1^{a,b}

MESH	TOTAL LEAKAGE		ERROR ^c (PERCENT)		NUMBER OF ITERATIONS		ITERATION TIME(sec) ^d
IxJ	NCE (NL)	S_N	NC (NL)	S_N	NC (NL)	S_N	NC (NL)
5x5	.67350 E-3	n.c. ^f	-15.38	n.c.	19	n.c.	0.16
	(.62935 E-3)g		(-20.92)		(20)		(5.26)
10x10	.73309 E-3	.32665 E-3	- 7.89	-58.96	22	17	0.62
	(.74808 E-3)		(- 6.00)		(24)		(24.74)
20x20	.77566 E-3	.65376 E-3h	- 2.54	-17.86	23	20	2.45
	(.78377 E-3)		(- 1.52)		(24)		(97.45)
40x40	.79073 E-3	.75858 E-3	- 0.65	- 4.69	24	20	10.16
80x80	-	.78633 E-3	-	- 1.20	-	22	-
							24.42

- a. $\Sigma_t = 1.25 \text{ cm}^{-1}$, $\Sigma_a = 1.00 \text{ cm}^{-1}$, $R_1 = 4 \text{ cm}$, $R_2 = 14 \text{ cm}$, distance between centers = 6 cm.
b. Convergence criterion on scalar flux = 10^{-7} .
c. Reference value .79558 E-3, from h^2 extrapolation of 40x40-80x80 S_N .
d. CPU time (sec) on CDC 180/855.
e. NC - Constant-Constant Nodal; (NL) - Linear-Linear Nodal.
f. (n.c.) - Solution does not converge.
g. Negative scalar flux occurs in final iteration. No fix-ups used in Nodal methods.
h. Negative scalar flux occurs in final iteration even after fix-up.

Table 2. Comparison Between DNTM C-C and S_N Method for Test Problem No. 2a,b

MESH	TOTAL ABSORPTION IN REGION ONE		ERROR ^c (PERCENT)		NUMBER OF ITERATIONS		ITERATION TIME(sec) ^d	
	NC ^f	S _N	NC	S _N	NC	S _N	NC	S _N
(I ₁ +I ₂)xJ ^e								
(40+ 5)x20	.72859 E-3 ^g	.19844 E-3 ^h	-3.23	71.88	23	26	5.85	5.71
(40+10)x20	.71275 E-3	.74815 E-3	-0.99	-6.01	21	20	5.90	5.03
(40+20)x20	.70811 E-3	.60389 E-3 ^h	-0.33	14.44	20	20	6.76	6.15
(40+40)x20	.70688 E-3	.67899 E-3	-0.16	3.79	20	21	9.02	8.60
(40+80)x20	.70657 E-3	.70174 E-3	-0.11	0.57	20	41	13.61	25.75

- $\Sigma_t^1 = 2.40 \text{ cm}^{-1}$, $\Sigma_a^1 = 2.00 \text{ cm}^{-1}$, $\Sigma_c^2 = 1.25 \text{ cm}^{-1}$, $\Sigma_a^2 = 1.00 \text{ cm}^{-1}$, $R_1 = 4 \text{ cm}$, $R_2 = 14 \text{ cm}$, distance between centers = 6 cm.
- Convergence criterion on scalar flux = 10^{-7} .
- Reference value .70577 E-3, from (40+120)x20 S_N calculation.
- CPU time (sec) on CDC 180/855.
- I₁ - radial mesh in region 1; I₂ - radial mesh in region 2; J - spatial angular mesh.
- NC - Constant-Constant Nodal.
- Negative scalar flux occurs in final iteration. No fix-ups used in Nodal method.
- Negative scalar flux occurs in final iteration even after fix-up.

Figure 1. The 80x80 boundary-fitted coordinate grid used in test Problem Number 1, and in Region 2 of test Problem Number 2.

Figure 2. 'Radial' traverses of the node outer surface averaged angular fluxes, for Test Problem Number 1, in the direction to the left of the outward normals, plotted at the mid-points of the surfaces of the computational elements, along the $j = 39$ strip on a $J = 40$ grid. (The abscissa is indexed for the 20×40 grid; hence, the values must be multiplied by 2, 4 and 6, respectively, for the 40×40 , 80×40 and 120×40 grids.)

Figure 3. 'Radial' traverses of the node averaged scalar fluxes, for Test Problem Number 1, plotted at the centers of the computational elements along the $j = 39$ strip on a $J = 40$ grid. (The abscissa is indexed for the 20×40 grid; hence, the values must be multiplied by 2, 4 and 6, respectively, for the 40×40 , 80×40 and 120×40 grids.)

Figure 4. The node outer surface averaged outgoing angular fluxes, for Test Problem Number 1, in the direction to the left of the outward normals, plotted at the mid-points of the surfaces of the outermost computational elements (along the circumference of the outer cylinder).

Figure 5. The node averaged scalar fluxes (equal to the total outgoing fluxes), for on Test Problem Number 1, plotted at the mid-points of the outer surfaces of the outermost computational elements (along the circumference of the outer cylinder).

Figure A.1. The general curvilinear coordinates (ξ, η) and the rectangular coordinates (x, y) in the plane perpendicular to the straight coordinate (z) . The angle θ is the local rotational angle of the orthogonal curvilinear coordinate system (ξ, η) with respect to the fixed rectangular coordinate system (x, y) . The normal vector to the $\xi(x, y) = C_1$ curve is $\nabla F(x, y) = \xi_x \hat{x} + \xi_y \hat{y}$ where $F(x, y) = \xi(x, y) - C_1 = 0$, and $\tan(\theta) = \xi_y / \xi_x$.

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