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The Boundary Element Formulation of the One Group 1D Nodal Equations

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The nodal method is a powerful numerical tool with which to treat neutron diffusion in heterogeneous media.[1,2] The popularity of nodal methods stems from the common features they share with finite element and finite difference methods. In particular, like finite element methods, in nodal methods, the flux is approximated over a coarse grid, possibly by piecewise continuous functions to provide an accurate representation of the flux and/or current map. Like finite difference approximations, the coupling matrix that results from the application of the nodal approach is relatively sparse and can usually be treated by routine numerical inversion. In addition, nodal methods are compatible with modern homogenization techniques that characterize fuel pin geometry in an efficient and accurate manner. Finally, nodal methods (especially those of the analytical variety) ensure neutron balance and therefore have a degree of robustness not found in finite difference techniques.

There are many derivations of nodal methods that can be found in the literature[1] that relate the flux and/or current within a cell to values on the cell boundaries. Here, we will again consider the 1D steady state neutron diffusion equation through the application of the boundary element method applied to a single cell. The advantage of this approach is its succinctness and completeness, simultaneously yielding all possible analytical nodal equations in a 1D heterogeneous medium setting. Also the approach is extendable to multigroup formulations and multidimensions which is to be the subject of future investigations. While the solutions obtained are well known, what is new is the procedure from which they are derived providing a variety of solutions. This effort represents a first step in the development of a highly accurate multidimensional benchmarking tool that will be used to assess multidimensional Pebble Bed Reactor (PBR) production codes.[3] To this end, analytical nodal formulation will be compared to a proposed 1D finite difference (FD) scheme.

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Reformulation of the Diffusion Equation

We consider the one group, 1D diffusion equation in the *j*th region (thickness Δ_j) of a heterogeneous reactor, where the *j*th region means the interval (x_{j-1}, x_j):

$$\left[\frac{d^2}{dx^2} + B_j^2\right]\Phi_j(x) = -\frac{S_j(x)}{D_j} = -q_j(x) \qquad (1)$$

$$B_j^2 \equiv \left[\frac{\nu\Sigma_{fj} - \Sigma_{aj}}{D_j}\right]$$

with interfacial continuity of flux and current

$$\Phi_j \equiv \Phi_j(x_j)$$

$$\Phi_{j-1} \equiv \Phi_{j-1}(x_{j-1}) = \Phi_j(x_{j-1})$$

$$J_j \equiv J_j(x_j)$$

$$J_{j-1} \equiv J_{j-1}(x_{j-1}) = J_j(x_{j-1}).$$

A zero net current is assumed at the reactor centerline as is a zero flux at the outer surface.

The derivation begins with the extension of the flux in region *j* to all space through

$$\Psi_j(x) \equiv \rho_j(x)\Phi_j(x)$$

$$\rho_j(x) \equiv \Theta(x - x_{j-1}) - \Theta(x - x_j)$$

where ρ_j is the characteristic function that ensures the flux outside the specific slab of interest is zero, since it does not concern us as long as the boundary fluxes are properly set. Θ is recognized as the Heavyside step function. When a second spatial derivative is taken of Ψ_j, and Eq.(1) is taken into account, there results

$$\left[\frac{d^2}{dx^2}+B_j^2\right]\Psi_j(x)=$$
$$\left[\delta'\left(x-x_{j-1}\right)-\delta'\left(x-x_j\right)\right]\Phi_j(x)+ \quad (2)$$
$$+2\left[\delta\left(x-x_{j-1}\right)-\delta\left(x-x_j\right)\right]\frac{d}{dx}\Phi_j(x)-$$
$$-\rho_j(x)q_j(x).$$

Thus, artificial boundary sources have been introduced consisting of yet-to-be- determined boundary fluxes with their presence ensured by Dirac-delta functions and their derivatives. In this way, particle balance is rigorously maintained. It is this equation that is new.

The Green's Function and Solution

The Green's function, satisfying

$$\left[\frac{d^2}{dx^2}+B_j^2\right]G_j(x,x')=-\delta(x-x'),$$

can be shown to be simply (using Fourier transforms)

$$G_j(x,x')=-\frac{1}{2B_j}\sin\left(B_j|x-x'|\right). \quad (3)$$

When the Green's function is integrated against Eq.(2) over all space, we find the solution

$$\Psi_j(x)=$$
$$=\frac{1}{2}\frac{1}{D_jB_j}\left[\begin{array}{l}J_j\left(x_j\right)\sin\left(B_j|x_j-x|\right)-\\-J_j\left(x_{j-1}\right)\sin\left(B_j|x_{j-1}-x|\right)\end{array}\right]+ \quad (4)$$
$$+\frac{1}{2}\left[\begin{array}{l}\Phi_j\left(x_j\right)\cos\left(B_j|x_j-x|\right)\mathrm{sgn}\left(x_j-x\right)-\\-\Phi_j\left(x_{j-1}\right)\cos\left(B_j|x_{j-1}-x|\right)\mathrm{sgn}\left(x_{j-1}-x\right)\end{array}\right]$$
$$+Q_j(x)$$

where

$$Q_j(x)\equiv\int_{x_{j-1}}^{x_j}dx'q_j(x')G_j(x,x').$$

Useful relationships between the boundary flux and current are obtained by introducing $x=x_{j-1}+\varepsilon$ and $x=x_j+\varepsilon$ into Eq.(4) to obtain

$$\Phi_{j-1}=\frac{1}{D_jB_j}J_j\sin\left(B_j\Delta_j\right)+$$
$$+\Phi_j\cos\left(B_j\Delta_j\right)+2Q_j\left(x_{j-1}\right) \quad (5a)$$

$$\Phi_j=-\frac{1}{D_jB_j}J_{j-1}\sin\left(B_j\Delta_j\right)+$$
$$+\Phi_{j-1}\cos\left(B_j\Delta_j\right)+2Q_j\left(x_j\right). \quad (5b)$$

By restricting x to the interval $\left[x_{j-1},x_j\right]$, Eqs. (4) and (5) lead to the following relationships for

--the interior flux to boundary fluxes

$$\Phi_j(x)=\left[\Phi_j-Q_j\left(x_j\right)\right]\mathrm{X}_j^-(x)+$$
$$+\left[\Phi_{j-1}-Q_j\left(x_{j-1}\right)\right]\mathrm{X}_j^+(x)+Q_j(x) \quad (6a)$$

--the interior current to the boundary currents

$$J_j(x)=\left[J_j+D_jB_jQ_{cj}\left(x_j\right)\right]\mathrm{X}_j^-(x)+$$
$$+\left[J_{j-1}-Q_{cj}\left(x_{j-1}\right)\right]\mathrm{X}_j^+(x)+Q_{cj}(x) \quad (6b)$$

with

$$Q_{cj}(x)\equiv-\int_{x_{j-1}}^{x_j}dx'q_j(x')\frac{dG_j(x,x')}{dx}\mathrm{sgn}\left(x-x'\right).$$

and

$$\mathrm{X}_j^-(x)\equiv\left[\frac{\sin\left(B_j\left(x-x_{j-1}\right)\right)}{S_j}\right]$$
$$\mathrm{X}_j^+(x)\equiv\left[\frac{\sin\left(B_j\left(x_j-x\right)\right)}{S_j}\right]$$
$$S_j\equiv\sin\left(B_j\Delta_j\right).$$

These are just two of the possible eight relationships that can be obtained from Eq.(4). The solution is finalized, say for Eq.(6a), when the boundary fluxes are found recursively by requiring current continuity

$$\Phi_j+b_j\Phi_{j-1}+\gamma_j\Phi_{j-2}=f_j \quad (7)$$

where the coefficients are known in terms of the nuclear parameters of regions j and j-1. The numerical solution to Eq.(7) is most effectively obtained using a tridiagonal solver. Although a solution to Eq.(2) has previously been obtained through approaches based on the repeated use of finite domain Green's functions for each homogeneous sub-domain, it is noteworthy that the present work obtains the relations directly from a single Green's function for the entire heterogeneous domain. Once the collected ensemble of all types of Eq.(6) for all cases are solved, the remainder of the method presented here allows the determination of fluxes (and

currents if desired) throughout the domain [per Eqs.(5a) and (5b)].

To emphasize the novelty of the development, it should be noted that the boundary element methods prescribes the most efficient form of the homogeneous solution when given two boundary conditions on either the flux or current. In addition, a direct extension to multigroup is possible.

A Benchmarking Application

In this section, an application of the above analytical result to assess the performance of a proposed FD approximation is presented.

Consider a grid of *Ln* intervals (slabs) representing a particular subdivision of a heterogeneous medium where the different material boundaries are maintained; however, the contiguous material regions can be further subdivided into subregions. Also let each material thickness be removed from the diffusion equation by the transformation $x \to x/\Delta_j$. If Eq.(1) is integrated over the *j*th interval assuming a uniform source, then

$$J_j\left(x_{j-1}\right) - J_j\left(x_j\right) + \\ + D_j B_j^2 \int_{h_j} dx \Phi\left(x\right) = -hS_j \qquad (8)$$

with

$$h \equiv x_j - x_{j-1} = 1/N .$$

N is the number of discrete nodes per region (either fuel or water). If a trapezoidal rule integration is assumed and if

$$J_j\left(x_j\right) = -D_j\left[\frac{\Phi_j - \Phi_{j-1}}{h}\right] \quad ;$$

consequently, since

$$J_j\left(x_{j-1}\right) = J_{j-1}\left(x_{j-1}\right) = -D_{j-1}\left[\frac{\Phi_{j-1} - \Phi_{j-2}}{h}\right] \quad ,$$

we find a three-point (finite-difference) recurrence for Eq.(8) in terms of cell edge fluxes

$$\Phi_j\left(x\right) + b_j'\Phi_{j-1} + \gamma_j'\Phi_{j-2} = f_j'$$

$$b_j' \equiv -\frac{1 + D_{j-1}/D_j - B_j^2 h^2/2}{1 + B_j^2 h^2/2}$$

$$\gamma_j' \equiv \frac{D_{j-1}/D_j}{1 + B_j^2 h^2/2}$$

$$f_j' \equiv -\frac{h^2 q_j}{1 + B_j^2 h^2/2}.$$

For zero current at the centerline, the recurrence for $j = 2$ can be shown to be as above except with

$$b_2' \to b_2' + \gamma_2' b_1 \quad \gamma_2' \to 0$$
$$f_2' \to \gamma_2' f_1' + f_2'.$$

As an example, consider a heterogeneous half symmetry subcritical MTR reactor of slabs of alternating water and BWR fuel of thicknesses 1.1158 and 3.231cm respectively. A uniform source exists in each water channel to simulate the thermalized fast flux. The flux variation from Eq.(6a) is shown in Fig. 1 for *Ln* = 30, 60, 120 slabs. The stability and fidelity of the analytical solver is evident as seen from the repetitive nature of the flux approaching an infinite heterogeneous MTR reactor.

Figure 2 shows the relative error of the FD scheme in comparison to the analytical flux

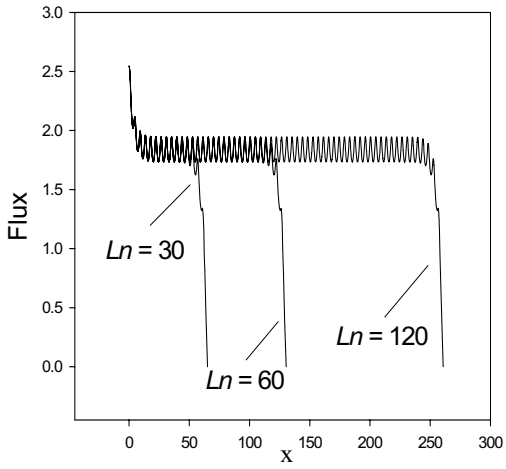

Fig. 1. MTR reactor with increasing number of fuel cells.

for increasing discretization. For the largest number of discrete nodes, the FD scheme can deliver accuracy better than 10^{-3} which is an indication of a robust FD scheme. The motivation for this comparison is the 2D application. It is anticipated to eventually be able to use a 2D finite difference formulation with convergence acceleration as a legitimate benchmark—but you will have to wait for this one since convergence acceleration will first be applied to the above 1D scheme to assess its accuracy.

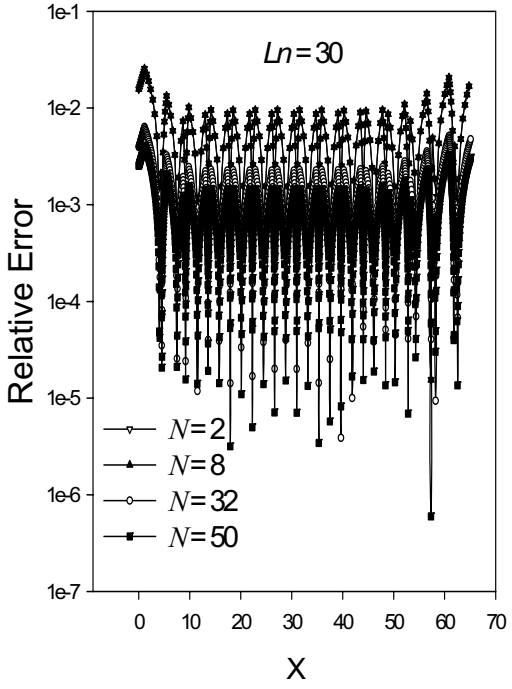

Fig. 2. Relative error comparison.

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