BNL-NUREG--37002

TI86 000028

CONF-851115--19

A GEOMETRY-INDEPENDENT APPROACH TO COARSE-MESH NEUTRON DIFFUSION CALCULATIONS

P. Kohut
Department of Nuclear Energy
Brookhaven National Laboratory
Upton, New York 11973

June 1985

Paper Submitted to the 1985 Winter Meeting of the American Nuclear Society, San Francisco, California, November 10-14, 1985

A GEOMETRY-INDEPENDENT APPROACH TO COARSE-MESH NEUTRON DIFFUSION CALCULATIONS*

P. Kohut

Department of Nuclear Energy
Brookhaven National Laboratory
Upton, New York 11973

Powerful coarse-mesh[1] and nodal[2,3] methods have been recently developed to calculate accurate node-average fluxes and eigenvalues. The nodal methods solve for the node-average flux by reducing the multidimensional diffusion problem to a coupled system of 1-D equations. These schemes are mainly limited to rectangular (xyz) nodes and cannot easily be extended to other geometries. The polynomial-based coarse-mesh methods have been applied to θRZ and HEXZ geometries.[4] However, the complex integral terms arising in this formulation are difficult to evaluate. It is of practical interest, especially in fast reactor and advanced gas-cooled reactor design studies, to develop an ultra-coarse-mesh multigroup method for the solution of the neutron diffusion equation in general geometries. The neutron distribution inside a homogeneous body is uniquely defined by the boundary surface fluxes and by the interior sources. This fact may be used to formulate the neutron diffusion problem in integral form containing surface quantities only. The advantages of evaluating only node boundary fluxes are a) the possibility of arbitrary node geometry, and b) the use of ultra-coarse-mesh without loss of accuracy. This summary describes the development of a boundary coarse-mesh nodal method applicable to arbitrary geometries using the boundary integral technique coupled with nodal source expansion.

---

*Work performed under the auspices of the U.S. Nuclear Regulatory Commission.

The starting point of this boundary-integral-expansion method is the integral formulation of the diffusion equation with the Green's function as the spatial diffusion kernel. The boundary conditions are selected in such a way that the nodal multidimensional Green's function, $G(r_o|r')$, satisfies zero identically on the node boundary. Other Green's functions can also be considered, in particular, the free-space solution. However, the selection of the zero-boundary-flux condition has the advantage that the surface currents are eliminated from the nodal equations.

The multigroup flux at any point inside an arbitrary node may be written in the usual form as:

$$\phi^g(r) = \int_V G^g(r'|r)\, s^g(r')\, dr' + \int_\Gamma \phi^g(r_s')\, I^g(r_s'|r_s)\, dr_s' , \qquad (1)$$

where $I^g(r_s'|r_s)$ is the normal component of $-D^g \nabla G^g(r_s'|r_s)$. The source term $s^g(r')$ includes all in-scattering and fission neutron productions, and the nodal properties are assumed to be spatially constant inside the node. The surface currents, $-D\nabla\phi(r_s)$, are eliminated in this formulation since $G(r_s|r) \equiv 0$ by definition. Let the point r approach the surface point r_s from the node interior to obtain a similar integral equation for the nodal surface flux at point r_s, in terms of the boundary fluxes $\phi(r_s')$, and the internal sources $s(r')$. Even though the Green's function is singular (in 2- and 3-D), the limiting process is well defined and the volume and surface integrals remain convergent.

For a homogeneous region with arbitrary geometry, the following procedure may be used to evaluate the multidimensional zero-boundary-flux Green's function, $G(r_o|r')$:

1. An integral equation is constructed for $G(r_o|r')$, using the free-space Green's function, $E(r_o|r')$.
2. Let r_o and r' approach the region boundary from the node interior ($r_o \to r_s$ and $r' \to r'_s$) to obtain

$$cE(r_s|r'_s) = \int_\Gamma E(r_s|r)\, I(r'_s|r)\, d\Gamma_r,$$

where $c = 1/2$ for a smooth surface. This is an inhomogeneous Fredholm-integral equation for $I(r'_s|r)$ and once a solution is found, $G(r'_s|r)$ can easily be recovered. The fact that the functions $G(r'_s|r)$ and $I(r'_s|r)$ are equivalent will be used to simplify the source term.

3. The boundary integral equation is solved using the boundary-element technique, by dividing the surface Γ to elements Γ_i's and discretizing $I(r'_s|r)$ to $I_{\ell n}$, i.e.,

$$cE_{m\ell} = \sum_i \hat{H}_{mi} I_{\ell n}$$

where the coefficients $\hat{H}_{mi}$, are weighted integrals of the free-space Green's function. The weight functions are determined by the order of approximation (constant, linear, etc.)

Once the surface-to-surface Green's function (or equivalently, the surface normal gradient of $G(r'_s|r)$) is known, the surface integral part of

Equation (1) for $\phi(r_s)$ can be reduced to simple algebraic form using the same boundary-element technique, i.e.,

$$c\phi_m^g = \sum_\ell H_{m\ell}^g \phi_\ell^g + \text{SOURCE TERM} .$$

Here ϕ_ℓ is the nodal surface flux at point r_s', $(\phi_\ell(r_s) \equiv \phi_m)$, and $H_{m\ell}$ is a weighted integral of $I(r_s'|r)$ on the node surface.

In order to evaluate the volume source (fission and in-scattering production), the node interior flux is expanded in polynomial basis functions, similar to finite-element schemes. The coefficients of these polynomials are determined by a localized least-square method to satisfy prescribed boundary values. The complexity of the node geometry enters through the basis functions, which are independent of the nodal flux and can be evaluated before the flux iteration. This approximation leads to a simplification in the source term, reducing it to integrals of $G(r'|r_s)$ with basis function weighting. Finally, the source term can also be manipulated to an algebraic expression using the integral definition of $G(r'|r_s)$, in terms of $E(r'|r_s)$ and $I(r'|r_s)$. In the resulting equation, the node surface flux, $\phi_m(r_s)$ is expressed as a combination of or response to the boundary fluxes, $\phi_\ell(r_s')$ on the same nodal surface, i.e.,

$$c\phi_m^g = \sum_{g'} \sum_\ell \hat{T}_\ell^{g'} \phi_\ell^{g'} + \sum_\ell H_{m\ell}^g \phi_\ell^g , \qquad (2)$$

where $\hat{T}_\ell^{g'}$ contains terms related to volume-to-surface and surface-to-surface diffusion.

Global coupling is insured by flux continuity on adjoining node surfaces. Based on Equation (2), matrix equations can be constructed and solved for each node corresponding to the inner iteration of other schemes. Since surface currents are not required in this method, the number of equations are greatly reduced. A 1-D proof-of-principle problem has been constructed with satisfactory results.

The boundary-element-expansion method presented above shows considerable promise as an efficient coarse-mesh nodal scheme for problems with complex periodic geometries. For arbitrary non-periodic geometries, the free-space Green's function could be more advantageous to use. In this case Equation (2) will have an additional term on the RHS, proportional to the surface flux gradient ($\nabla\phi_{\ell}^{g}$). The method also has the advantage that the interior homogeneous flux distribution can easily be recovered, since it directly solves for the node boundary flux.

REFERENCES

1. S. Langebuch, W. Maurer, W. Werner, "Coarse-Mesh Nodal Diffusion Method for the Analysis of Space-Time Effects in Large Light Water Reactors," Nucl. Sci. Eng., 63, 437 (1977).

2. R. D. Lawrence, J. J. Dorning, "A Nodal Green's Function Method for Multidimensional Neutron Diffusion Calculations," Nucl. Sci. Eng., 76, 218 (1980).

3. R. A. Shober, R. N. Sims, A. F. Henry, "Two Nodal Methods for Solving the Time-Dependent Group Diffusion Equations," Nucl. Sci. Eng., 64, 582 (1977).

4. R. A. Rydin, M. A. Robinson, P. J. Wantuck, "Recent Advances in the Quad and Cube Coarse-Mesh Diffusion Theory Methods," Proc. ANS Topical Meeting Computational Methods in Nuclear Engineering, Williamsburg, Virginia, April 23-25, 1979, NTIS-1979.

5. Y. A. Chao, J. A. Penkrot, "A Nodal Method for Direct Intra-Node Distribution Calculations," Proc. ANS Topical Meeting Advances in Reactor Physics and Core Thermal Hydraulics, Kiamesha Lake, New York, 1982.