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THREE-DIMENSIONAL NODAL DIFFUSION AND TRANSPORT METHODS FOR THE ANALYSIS OF FAST-REACTOR CRITICAL EXPERIMENTS*

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R. D. Lawrence
Applied Physics Division
Argonne National Laboratory
Argonne, IL 60439

Summary

This paper describes two new nodal methods for solving the multigroup neutron diffusion and transport equations in three-dimensional Cartesian geometry. These methods have been developed for the global analysis of fast-reactor critical experiments once cell-averaged multigroup cross sections for each matrix position or "drawer" have been computed using appropriate cell-homogenization procedures. Brief descriptions of the nodal diffusion and transport schemes are presented here, along with results of two- and three-dimensional calculations for a current Zero Power Plutonium Reactor (ZPPR) configuration.

The Cartesian-geometry nodal diffusion and transport methods discussed here are based on an interface-current formulation analogous to that developed previously[1] for the solution of the diffusion equation in hexagonal geometry. The discretized equations for both schemes are derived by approximating the one-dimensional equations obtained via the transverse-integration procedure common to most recent nodal methods.[2] In Cartesian-geometry diffusion theory, the one-dimensional fluxes are approximated by a polynomial equivalent to that used in the nodal expansion method[3] (NEM) developed for light-water-reactor calculations, although the final form of the computational equations is quite different in the two formulations. As in the NEM, a weighted-residual procedure is used to compute the higher-order expansion coefficients. Equations for the face-averaged, outgoing partial currents are derived by inserting the one-dimensional polynomials into Fick's Law evaluated on the nodal surfaces. Combining results in the three coordinate directions yields an inhomogeneous response matrix equation for the k-th node:

$$\underline{J}_g^{out,k} = [P_g^k] \left\{ \underline{Q}_g^k - \underline{L}_g^k \right\} + [R_g^k] \, \underline{J}_g^{in,k} \quad . \tag{1}$$

Here, $\underline{J}_g^{out,k}$ and $\underline{J}_g^{in,k}$ contain, respectively, the six outgoing and six incoming face-averaged partial currents for the k-th node, $\underline{Q}_g^k$ contains the zero-moment (node-averaged) group source plus the higher-order source moments introduced via the weighted residual approximation, and $\underline{L}_g^k$ contains the higher-order spatial moments of the transverse leakages. The transverse-leakage moments are computed using the quadratic fit used in most recent nodal schemes.[2] The matrices $[P_g^k]$ and $[R_g^k]$ contain nodal coupling coefficients which are computed and stored for unique nodes characterized by mesh spacings and material zone assignment.

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As in the nodal discrete-ordinates method[4] (NDOM) developed by Wagner, the nodal transport scheme is based on the solution of one-dimensional (1D) transport equations derived, for example, by integrating the two-dimensional transport equation over the y-direction and the azimuthal angle with respect to the x-axis. The 1D equations are discretized in the NDOM using a 1D discrete-ordinates approximation applied on a fine mesh introduced within the node. Our approach is based on approximation of exact integral equations for the 1D scalar fluxes and for the outgoing angular fluxes on the surfaces of the node. The 1D scalar fluxes are approximated by quadratic polynomials with coefficients computed using a weighted-residual procedure applied to the 1D integral equations. The surface angular fluxes are approximated by a double-P_1 expansion. As in the NDOM, the transverse leakage is assumed to be isotropic, and thus is treated in the same manner as in diffusion theory.

Extension of this development to three dimensions is straightforward, and leads eventually to the following transport-theory analog of Eq. (1):

$$\underline{\psi}_g^{out,k} = [\tilde{P}_g^k] \left\{ \underline{Q}_g^k - \underline{L}_g^k \right\} + [\tilde{R}_g^k] \, \underline{\psi}_g^{in,k} \quad . \tag{2}$$

Here, $\underline{\psi}_g^{out,k}$ contains the six outgoing face-averaged partial currents plus the six outgoing half-angle-integrated fluxes due to the double-P_1 surface expansions, and $\underline{Q}_g^k$ and $\underline{L}_g^k$ are defined as in diffusion theory. The entries in the transport-theory matrices $[\tilde{P}_g^k]$ and $[\tilde{R}_g^k]$ are evaluated analytically in terms of exponential integral $[E_n]$ functions introduced by the exact one-dimensional angular integrations. The source contribution due to within-group scattering is included in the calculation of these matrices, and thus, in contrast to nodal transport methods[5-7] based on multidimensional discrete-ordinates approximations, the present method does not require the traditional inner iteration on the within-group scattering source. Instead, Eq. (2) is solved using iterative procedures identical to those used to solve the diffusion-theory equations [Eq. (1)]. The elimination of the scattering-source iteration can lead to very significant reductions in computational cost, particularly for problems (such as fast-reactor criticals) characterized by high scattering ratios.

The nodal diffusion and transport schemes discussed above have been implemented as options in a test version of the DIF3D finite-difference code.[8] These methods have been applied to a 3-group model of a ZPPR-13 mockup of a radially-heterogeneous 700 MWe LMFBR. The quarter-core planar layout consists of a 36 by 36 array of square (homogenized) drawers with dimensions of 5.52 cm. Half-core axial symmetry was used in the three-dimensional calculations. All calculations were performed on the ANL IBM 3033 computer.

Table I summarizes two-dimensional diffusion and transport calculations for ZPPR-13 using the DIF3D code. The nodal diffusion-theory (NDT) results show that the nodal option with a single mesh per drawer (mpd) produces spatially-converged solutions to the diffusion equation in CPU times nearly a factor of 4 less than finite-difference diffusion theory (FDDT) with 2 × 2 mpd. However, transport effects are important in this problem as shown by the large errors (e.g. 0.52% in k-eff) in the NDT calculation relative to the

exact transport-theory (TT) solution. The nodal transport-theory (NTT) option eliminates over 80% of the errors due to the diffusion approximation, with a CPU time that is only slightly greater than nodal diffusion theory. The NTT solution is not quite as accurate as the S_4 solution, and this probably is due to the assumption of isotropic transverse leakage. Very dramatic reductions in CPU time are observed relative to the S_n calculations, although it should be noted that the DIF3D diamond-difference option[9] typically runs slower by a factor of ~5 than the diffusion-accelerated TWODANT code.[10]

Table II summarizes three-dimensional calculations for ZPPR-13. The nodal and finite-difference calculations used axial mesh spacings of ~22.9 cm and ~4.5 cm, respectively, in the active core. The nodal option achieves very acceptable accuracy using this very coarse axial mesh and a single mesh per drawer. The nodal calculation is nearly an order of magnitude more accurate than the 4 mpd FDDT calculation, with a reduction in computational cost by a factor of 15. Standard analysis calculations usually employ 28 groups (versus the three groups used here), and thus three-dimensional calculations with 4 mpd often are considered prohibitively expensive. Instead, "mesh corrections" are applied to coarse-mesh (i.e. 1 mpd) finite-difference calculations in order to obtain more accurate approximations to the true diffusion-theory solution. It is clear that the use of the DIF3D nodal option eliminates the uncertainties (and inconvenience) associated with such corrections.

The calculations summarized in Table II further demonstrate the very high computational efficiency of the DIF3D nodal transport scheme. The NTT calculation cost only 50% more than the NDT calculation, and is a factor of two cheaper than coarse-mesh finite-difference diffusion theory. Although an exact transport-theory solution is not available for the three-dimensional model, the 0.57% difference in k-eff between nodal diffusion theory and transport theory appears consistent with the two-dimensional results and other predictions (using r-z models) of the axial transport effect. Further benchmarking of the method is underway.

In summary, use of the nodal diffusion-theory method eliminates the need for mesh corrections to diffusion calculations, while making possible significant reductions in the computational costs associated with global calculations of critical experiments. Transport effects in these assemblies are significant, and use of the DIF3D nodal transport option eliminates over 80% of the errors due to the use of diffusion theory. The very high computational efficiency of the present nodal transport method, in combination with likely improvements to the angular approximations, promises to make accurate three-dimensional transport calculations for critical assemblies possible on a routine basis.

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Table I. Summary of Two-Dimensional Diffusion and Transport Calculations for ZPPR-13

Method[a]	Mesh Per Drawer	k-eff	ε_k(%)[b]	ε_{CRP}(%)[c]	CPU Time (min)
NDT	1 × 1	0.98411	0.003	-0.01	0.25
FDDT	1 × 1	0.98620	0.212	-1.78	0.18
FDDT	2 × 2	0.98459	0.051	-0.48	0.97
Reference (DT)		0.98408	-	-	
NDT	1 × 1	0.98411	-0.52	+5.9	0.25
NTT	1 × 1	0.98842	-0.09	+1.0	0.30
S_4	2 × 2	0.98957	+0.03	+0.5	21.8
S_8	2 × 2	0.98921	-0.01	+0.2	>54.0
Reference (TT)		0.9893	-	-	

[a] NDT ≡ Nodal Diffusion Theory
FDDT ≡ Finite-Difference Diffusion Theory
NTT ≡ Nodal Transport Theory
S_n ≡ DIF3D diamond-difference transport option

[b] ε_k ≡ Error in k-effective relative to the respective reference solutions, which are exact solutions to the multigroup diffusion (DT) and transport (TT) equations.

[c] ε_{CRP} ≡ Error in group 1 flux in control rod position.

Table II. Summary of Three-Dimensional Diffusion and Transport Calculations for ZPPR-13

Method[a]	No. of Axial Mesh Planes	Mesh Per Drawer	k-eff	ϵ_k(%)[b]	CPU Time (min)	Cost ($)
NDT	5	1 × 1	0.98348	0.018	2.1	18
FDDT	25	1 × 1	0.98622	0.292	6.1	50
FDDT	25	2 × 2	0.98441	0.111	28.5	269
Reference (DT)			0.98330	-		
NTT	5	1 × 1	0.98915		3.0	28

[a] NDT ≡ Nodal Diffusion Theory

FDDT ≡ Finite-Difference Diffusion Theory

NTT ≡ Nodal Transport Theory

[b] ϵ_k ≡ Error in k-effective relative to the reference solution, which is the exact solution to the multigroup diffusion equation.