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Improved Iteration in Neutron Transport
Calculations by Alternating between
Diffusion and S_n Cycles.

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In a recent article on numerical transport theory¹ the author obtained, by combining the equations for the S_2 approximation, the following difference equations for simple diffusion:

$$(1) \quad A_{i+1}I_{i+1} - A_iI_i + B_{j+1}J_{j+1} - B_jJ_j + \sigma_0(N_{i+1} + N_i) = S_0$$

$$(2a) \quad a(N_{i+1} - N_i) + \sigma_1(I_{i+1} + I_i) = S_a + R_a$$

$$(2b) \quad b(N_{j+1} - N_j) + \sigma_1(J_{j+1} + J_j) = S_b + R_b$$

These equations apply to the case of two space variables with no time dependence and are to be solved for each neutron velocity group separately. All quantities which appear in (1) and (2) have double subscripts for position but, by convention, centered subscripts are omitted. For example,

$I_{i+1,j+1/2}$ is written I_{i+1} and $\sigma_{0,i+1/2,j+1/2}$ becomes σ_0 .

A_i , B_j , and V denote the area and volume elements and a and b are abbreviations for $(A_{i+1} + A_i)/2$ and $(B_{j+1} + B_j)/2$. In (x,y) geometry for example, $A_i = \Delta y$, $B_j = \Delta x$, and $V = \Delta x \cdot \Delta y$. The quantities σ_0 and σ_1 are equal to the total cross section less the isotropic and linearly anisotropic components, respectively, of the self-scattering cross section. By self-scattering is meant scattering without change of group. σ_0 includes a factor $V/2$ and σ_1 a factor $3V/2$. The units for A_i , B_j , a , b , σ_0 , and σ_1 are length squared.

The function N represents the average neutron flux; I and J denote the neutron currents or net flux, one for each space variable; and S_0 , S_a , and

¹The Numerical Theory of Neutron Transport. "Methods in Computational Physics." Vol. I, (1963), pp. 31-32. Academic Press, New York and London.

S_0 the components of the neutron source, of the isotropic and two anisotropic components, respectively. Here S_0 , S_a , and S_b are linear combinations, over velocity groups, of the N's, I's, and the J's, respectively. The coefficients involved are transfer cross sections times V. The units for I, J, and N are inverse length squared per second.

The quantities R_a and R_b are identically equal to zero in the case of simple diffusion. This is also true for S_2 in (x,y) space but not quite true for S_2 in curved geometries. But, more important, R_a and R_b can be stated explicitly in terms of quantities which appear in the S_n equations. R_a and R_b can therefore be calculated after any inner S_n cycle, that is, after any set of computations which includes one sweep over the space mesh for each discrete ray within the group. To determine the expressions for R_a and R_b for arbitrary even n, one adds, over ray index, the S_n equations using certain weights, w_μ and w_η^1 , and then identifies the resulting expressions with (2a) and (2b).

The main result of this paper is, therefore, a much improved inner iteration procedure in transport calculations which entails alternate cycles of simple diffusion and S_n calculations. One starts by solving (1) and (2) for the functions N, I, and J using $R_a = R_b = 0$ unless R_a and R_b are available in updated form. In the second step, one uses the new data for N, I, and J in an S_n cycle to generate the detailed angular flux which is the basis for updating R_a and R_b . One repeats these two steps until some convergence criterion has been met.

The case of simple diffusion theory becomes in this way numerically imbedded (as it is analytically) in transport theory. Therefore, one also has the capability of limiting the calculation to the first diffusion cycle, if this seems reasonable, for selected, in some cases all, velocity groups.

The iterative procedure sketched above is particularly attractive for one dimensional problems, stationary or time dependent, for in these cases, as is well known, one can solve the diffusion equations explicitly (without iteration). The direct method is based on a familiar reflection or imbedding principle and is outlined below for the case with non-zero S_a .

One assumes the following relations between net and average flux:

$$(3a) \quad I_i = p_i N_i - q_i \quad (3b) \quad I_{i+1} = p_{i+1} N_{i+1} - q_{i+1}$$

with the objective of finding recursion relations for p_i and q_i . The first step is to find I_{i+1} and N_{i+1} in terms of I_i and N_i using equations (1) and (2a) with $J \equiv 0$. The second step is to substitute the expression for I_{i+1} and N_{i+1} in (3b) and equate to (3a), which then yields:

$$(4a) \quad p_i = [2a\sigma_0 + (aA_{i+1} + \sigma_0\sigma_1) p_{i+1}] / [aA_i + \sigma_0\sigma_1 + 2a\sigma_1 p_{i+1}]$$

$$(4b) \quad q_i = [(a + \sigma_1 p_{i+1}) S_0 - (\sigma_0 + A_{i+1} p_{i+1}) S_a + (aA_{i+1} - \sigma_0\sigma_1) q_{i+1}] / [\text{as in (4a)}]$$

The problem is now solved a) by applying the boundary conditions at $i = i_{\max}$ to generate p and q , b) by applying the conditions at $i = 0$ using p and q to generate N , $i = 0, 1, \dots, i_{\max}$, and, finally, c) by calculating I using equation (3a). A zero boundary condition implies: $p_{i_{\max}} = \sqrt{3}/3$ (for S_2), $q_{i_{\max}} = 0$; a reflective condition: $p_{i_{\max}} = 0$, $q_{i_{\max}} = 0$; and a periodic condition: $p_{i_{\max}} = p_1$, $q_{i_{\max}} = q_1$. All are simple to apply except the last which requires a component (two-boundary) treatment.

It would be very desirable to have the above direct method available in the case of two space variables. If, however, explicit solution of the diffusion equations is not possible here, a fast iterative method consistent with equations (1) and (2) would be quite satisfactory, a modification, possibly, of one of the methods now in use.