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Parallel Shooting Solution of the Neutron Transport Equation in Spherical Geometry

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A direct and efficient parallel-shooting method is given for the solution of the spherical harmonics approximation to the neutron transport equation in spherical geometry with arbitrary anisotropic scattering and source. The special numerical difficulties due to the singularity at the center of the sphere are solved in a simple and efficient way. The algorithm "measures" the roundoff instability of the problem and eliminates it by performing a minimum of matrix transformations that ensure the linear independence of the matrix columns.

I. INTRODUCTION

We present a new direct method for the numerical solution of the spherical harmonics approximation to the neutron transport equation in spherical geometry with arbitrary anisotropic scattering and source. The spherical harmonics equations in spherical geometry are an essentially different problem than for slab geometry; this is because the center of the sphere is a singular point of the equations. Although the singularity does not create any difficulty for the analytic solution of the continuous equations for homogeneous spheres with isotropic scattering, the treatment of the center in the finite-difference approximation to the equations presents very severe numerical difficulties not encountered in slab geometry [1]. The finite-difference approximation has considerable practical importance because it can be used to obtain solutions for problems in inhomogeneous media with arbitrary anisotropic scattering.

The main new result of this work is to extend to spherical geometry the direct parallel or multiple-shooting method developed recently for slab geometry [2, 3], after modifying it properly to account for the singularity at the center. Although there are certain formal similarities between the treatment given here and our previous work in slab geometry, the numerical solution of the transport equation in spherical geometry poses a problem which is quite different than in slab geometry. One essential property of the method used is that it allows us to define stabilizing

transformations when marching only in one direction, i.e., from the sphere's boundary to its center. As the singularity at the center does not allow marching from the center toward the surface, other multiple shooting methods that require marching in both directions across the domain are not applicable to problems with singular points; this is for example the case of the stabilized march technique of Lucey and Hansen [4].

The known numerical instability of a simple direct solution of the spherical harmonics equations is due to the existence of independent solutions which grow and decay exponentially with distance, this instability is common to slab and spherical geometries; for spheres, we have the added instability due to the singularity at the center. The spherical harmonics equations are first reduced by finite differences to an algebraic problem in block form. The numerical instability is then eliminated by performing linear transformations of the matrices of the problem, which ensure the linear independence of the matrix columns. The main novelty and advantage of the method lies in that only a minimum number of matrix transformations is performed, the precise number being determined dynamically and efficiently by the program itself in the course of the computation. Thus, in stable problems where the algorithm does not encounter instability, the optimal direct solution is obtained without performing any matrix transformations whatever. The presentation of this paper follows closely that given in [2] for slab geometry.

Results of criticality and critical length computations are given both for stable and unstable problems with isotropic and anisotropic scattering. These results compare very favorably in accuracy and efficiency with those obtained by the S_n method of Carlson and co-workers [5, 6].

II. The Transport Equation in Spherical Geometry

The Boltzmann equation in spherical geometry with arbitrary anisotropic scattering and source reads [7, 8]

$$\mu \frac{\partial \phi(x, \mu)}{\partial x} + \frac{1 - \mu^2}{x} \frac{\partial \phi(x, \mu)}{\partial \mu} + \Sigma_t(x)\, \phi(x, \mu) = \int_{-1}^{1} \Sigma_s(x, \mu, \mu')\, \phi(x, \mu')\, d\mu' + S(x, \mu), \tag{1}$$

where x is the distance from the center of the sphere; μ is the cosine of the angle between the neutron velocity and the radius vector; $\phi(x, \mu)$ is the angular flux; $\Sigma_t(x)$ is the total cross section; $\Sigma_s(x, \mu, \mu')$ is the scattering cross section from μ' to μ; and $S(x, \mu)$ is the anisotropic neutron source. The derivation of the spherical

harmonics approximation to Eq. (1) is standard and can be found in detail in [8, 9]. Briefly, in the P_L approximation the spherical harmonics equations are obtained by expanding

$$\phi(x, \mu) \cong \sum_{l=0}^{L} \tfrac{1}{2}(2l + 1) f_l(x) P_l(\mu), \tag{2}$$

$$\Sigma_s(x, \mu, \mu') = (1/2\pi) \Sigma_s(x, \mu_0)$$

$$\cong (1/2\pi) \sum_{l=0}^{L} \tfrac{1}{2}(2l + 1) \Sigma_{sl}(x) P_l(\mu_0), \tag{3}$$

$$S(x, \mu) \cong \sum_{l=0}^{L} \tfrac{1}{2}(2l + 1) S_l(x) P_l(\mu), \tag{4}$$

where μ_0 is the cosine of the angle between the neutron velocities in the directions μ' and μ, and $P_l(\mu)$ are the Legendre polynomials. If we substitute (2), (3), and (4) into (1), and perform the necessary angular integrations using the addition theorem for the Legendre polynomials and their orthogonality properties, we obtain the spherical harmonics equations in the P_L approximation:

$$A \frac{d\mathbf{f}(x)}{dx} + \frac{1}{x} B\mathbf{f} + C(x)\mathbf{f} = \mathbf{s}(x). \tag{5}$$

The vectors $\mathbf{f}(x)$, $\mathbf{s}(x)$ and the matrices A, B, and $C(x)$ are given explicitly in Appendix A. Equations (5) are a system of $L + 1$ inhomogeneous ordinary differential equations. Their general solution has $L + 1$ arbitrary constants of integration, which are determined by imposing $L + 1$ appropriate boundary conditions.

A. *Boundary Conditions*

The interface and boundary conditions are discussed in [8, 9]. For odd-L approximations, the spatial moments f_l are continuous across interfaces of different media. The simple requirement that the solution of (5) must be everywhere finite yields exactly $(1/2)(L + 1)$ conditions which eliminate $(1/2)(L + 1)$ constants of integration. As a consequence, at the center of the sphere one has

$$f_l(0) = 0 \qquad l = 1, 2, \ldots, L, \tag{6}$$

i.e., the angular flux is isotropic (see Eq. (2)), which is clear on physical grounds. The vacuum boundary condition at the sphere's surface requiring that no neutrons return from the vacuum,

$$\phi(R, \mu) = 0 \qquad \mu < 0, \tag{7}$$

cannot be exactly satisfied by any finite expansion (2). Two commonly used approximate boundary conditions due to Marshak [8] and Federighi [10] can both be written in the form

$$\mathbf{f}_o(R) = G\mathbf{f}_e(R), \tag{8}$$

where the subindexes o and e designate the odd and even components of the vectors, i.e.,

$$\mathbf{f}_o(R) \equiv \begin{bmatrix} f_1(R) \\ f_3(R) \\ \vdots \\ f_L(R) \end{bmatrix}, \qquad \mathbf{f}_e(R) \equiv \begin{bmatrix} f_0(R) \\ f_2(R) \\ \vdots \\ f_{L-1}(R) \end{bmatrix}, \tag{9}$$

and the two approximations differ in the elements of the square $(1/2)(L+1)$-order matrix G, for which values are available [10, 3]. The relative merits of both approximations have been discussed by a number of authors [10–14].

To summarize, the spherical harmonics equations (5) are a two-point boundary value problem for a system of ordinary differential equations with left boundary conditions (6) and right boundary conditions (8). The direct numerical solution of this problem is the subject of the remaining sections of this paper.

B. *Effects of the Singularity*

Before obtaining a finite-difference approximation to Eqs. (5), it is essential to consider the effects of the singularity at the sphere center on the spherical harmonics equations. Just as for slab geometry, it is convenient to premultiply Eq. (5) by A^{-1} and obtain

$$(d\mathbf{f}(x)/dx) + (1/x)\, M\mathbf{f} + N(x)\mathbf{f} = \mathbf{v}(x), \tag{10}$$

where we have used the following definitions

$$M \equiv A^{-1}B, \qquad N(x) \equiv A^{-1}C(x), \qquad v(x) \equiv A^{-1}\mathbf{s}(x). \tag{10a}$$

Briefly, given the angular flux at the center $f_0(0)$ [see Eqs. (2) and (6)], it is not possible to obtain from this the moments $f_l(x)$ in some neighborhood of the center. The proof of this fact was given by Gelbard *et al.* for the discrete ordinates approximation to the neutron transport equation [7], but it applies also to the spherical harmonics equations as both formulations are equivalent. If we expand the moments and source term in Eqs. (10) in a Taylor series about the center of the sphere, $x = 0$, we get

$$\mathbf{f}(x) = \sum_{n=0}^{\infty} \mathbf{d}_n x^n, \qquad \mathbf{v}(x) = \sum_{n=0}^{\infty} \mathbf{e}_n x^n. \tag{11}$$

Substituting (11) into (10), we find

$$(nI + M)\,\mathbf{d}_n + N\mathbf{d}_{n-1} = \mathbf{e}_{n-1}\,, \qquad n = 1, 2,..., \infty, \tag{12}$$

where it has been assumed that the cross sections are constant in some neighborhood of the center. We have found [15] that the eigenvalues of the matrix M are 0, 2, -2, 4, -4,..., $-(L-1)$, $(L+1)$; thus, for any approximation higher than P_1, -2 is an eigenvalue of M and the matrix $nI + M$, $n = 2$, is singular. Equation (12) shows then clearly that it is impossible to determine d_2. Physically, as the angular flux is isotropic at the center, it is given only by one single number (i.e., the scalar flux), and this is not enough to determine the angular flux in the neighborhood of the center. This means that it is not possible to develop a numerical algorithm that will construct the solution of the spherical harmonics equations by marching from the sphere center to its boundary. To circumvent this difficulty associated with the singularity, it is known that numerical algorithms can be developed which starting with the solution at the boundary, obtain the rest of the solution by marching toward the center. However, when the cross sections σ_i [see (A8)] are space independent, a simple direct numerical integration of (10) is unstable because the roundoff errors grow exponentially with distance. This is because some of the eigenvalues of N are real and occur in positive and negative pairs [8]. This basic numerical instability of the spherical harmonics equations is known to exist also for nonhomogeneous problems when the matrix $N(x)$ is space dependent. The main contribution of this work is to have developed a direct and numerically stable method which obtains the solution by marching from the sphere boundary to its center.

III. Algebraic Problem for the Spherical Harmonics Equations

As the solution of the finite-difference approximation is to be obtained by marching from the sphere's surface to its center, it is convenient to use a spatial mesh where distances are measured from the surface. The simplest way to obtain a finite-difference approximation to Eqs. (10) is to difference them centrally, so as to get

$$\begin{aligned}\mathbf{f}_j - \mathbf{f}_{j-1} + [h_{j-1}/(x_{j-1} + x_j)]\, M(\mathbf{f}_{j-1} + \mathbf{f}_j) + (1/2)\, h_{j-1} N_{j-1}(\mathbf{f}_{j-1} + \mathbf{f}_j) \\ = (1/2)\, h_{j-1}(\mathbf{v}_{j-1} + \mathbf{v}_j); \qquad j = 2, 3,..., n,\end{aligned} \tag{13}$$

where the index $j = 1$ corresponds to the sphere's surface etc., and $j = n$ to its center. In discrete form, the boundary conditions at the sphere's surface and center, Eqs. (8) and (6), can be expressed respectively as

$$(\mathbf{f}_1)_o = G(\mathbf{f}_1)_e\,, \qquad (\mathbf{f}_n)_o = \mathbf{0}. \tag{14}$$

It should be remarked that although we know that all moments at the sphere center except the first are zero [Eq. (6)], in discrete form we only require that the odd components be zero [see second equation in (14)]; this is necessary so as to have a well posed algebraic problem with the same number of equations as unknowns. The fact that we compute the other components not assumed zero, i.e., $f_2(0), f_4(0), \ldots, f_{L-1}(0)$, provides a built-in check of the numerical accuracy of the algorithm, because we should get at the center $f_2(0) = f_4(0) = \cdots = f_{L-1}(0) = 0$. In our calculations, the computed values for all these moments are of the order of 10^{-6} or less in double precision; this is to be contrasted with other methods where the numerical inaccuracies result in a scalar flux with its maximum slightly displaced to the right of the sphere's center [1].

The algebraic problem defined by Eqs. (13) and (14) is now in a similar form to that obtained before for slab geometry (see Eqs. (14) and (15) of [2]). Its solution, from this point, is almost identical to that given in [2] for plane geometry, and the reader might consult this reference for more details.

As the boundary conditions (14) separate sharply the even from the odd components of $\mathbf{f}$ at the boundary points, it is convenient to rearrange the solution vectors $\mathbf{f}_j$ throughout the grid, putting the even and odd components at the top and bottom halves, respectively. This simplifies the analysis of the algebraic system (13) and (14). We thus use the definitions

$$\mathbf{g}_j \equiv \begin{bmatrix} \mathbf{f}_e \\ \mathbf{f}_o \end{bmatrix}_j \tag{15}$$

$$D_{j-1,j-1} \equiv [-I + h_{j-1}M/(x_{j-1} + x_j) + (1/2)\, h_{j-1}N_{j-1}]', \tag{16}$$

$$D_{j-1,j} \equiv [I + h_{j-1}M/(x_{j-1} + x_j) + (1/2)\, h_{j-1}N_{j-1}]', \tag{17}$$

$$\mathbf{w}_{j-1} \equiv (1/2)\, h_{j-1}(\mathbf{v}_{j-1} + \mathbf{v}_j), \tag{18}$$

where the primes denote the reordering of the columns of the matrices inside the parentheses by parity, i.e., the first half of the columns of the D's are the 1st, 3rd, 5-th,..., L-th columns of the matrix inside the parentheses, and the second half are the 2nd, 4-th, 6-th,..., $(L + 1)$-th columns. Using (15), (16), (17), and (18), we write the algebraic problem (13) and (14) in full:

$$\begin{aligned}
D_{11}\mathbf{g}_1 + D_{12}\mathbf{g}_2 &= \mathbf{w}_1 \\
D_{22}\mathbf{g}_2 + D_{23}\mathbf{g}_3 &= \mathbf{w}_2 \\
&\cdots \\
D_{n-1,n-1}\mathbf{g}_{n-1} + D_{n-1,n}\mathbf{g}_n &= \mathbf{w}_{n-1} \\
\mathbf{g}_1{}^{b} = G\mathbf{g}_1{}^{t}, \qquad \mathbf{g}_n{}^{b} &= \mathbf{0},
\end{aligned} \tag{19}$$

where the superscripts b and t designate the bottom and top halves of the respective vectors, the D's are space-dependent $(L + 1)$-th order square matrices, and the $\mathbf{g}$'s and $\mathbf{w}$'s are $(L + 1)$-component column vectors.

One attractive property of the spherical harmonics method is that the algebraic problem (19) can be generated numerically from the analytic formulas given in the text, independently of the number of terms $L + 1$ (P_L approximation) kept in the expansions (2), (3), and (4); it should also be noted that the form of (19) and therefore its solution remain the same independently of the anisotropy of the scattering cross section and of the source. Finally, it can be shown that the finite-difference approximation used is $O(h^2)$, where h is the mesh size.

IV. Direct Solution of Algebraic Problem

The essential difference between the algebraic problem (19) and the corresponding one for plane geometry (Eq. (19) of [2]) is that the D matrices in (19) are a function of distance, whether the sphere is homogeneous or nonhomogeneous. Therefore, the direct solution of (19) always requires the inversion of one D matrix for each row of the block system (19). Otherwise, the solution of (19) is almost identical to that of Eq. (19) of [2], and is now described briefly for the sake of clarity. The very simple structure of (19) suggests an obvious direct solution by substitution. We first define the following sequence of rectangular matrices of order $(L + 1) \times (1/2)(L + 1)$:

$$F_1 = \begin{bmatrix} I \\ G \end{bmatrix}, \qquad F_2 = \pi_1 F_1 , \qquad F_3 = \pi_2 \pi_1 F_1 ,\ldots, \qquad F_n = \pi_{n-1}\pi_{n-2} \cdots \pi_1 F_1 , \tag{20}$$

$$\pi_i \equiv -D_{i,i+1}^{-1} D_{ii} .$$

In (20) F_1 is chosen so as to satisfy the left boundary conditions [its upper half is the unit matrix and its lower half is the boundary condition matrix G in (19)]; the other terms in the sequence are found by substitution in (19) without the inhomogeneous terms. By substitution in the full inhomogeneous system (19), we define the following sequence of $(L + 1)$-component vectors

$$\mathbf{a}_1 = \mathbf{0}, \qquad \mathbf{a}_2 = D_{12}^{-1}\mathbf{w}_1 + \pi_1 \mathbf{a}_1 , \qquad \mathbf{a}_3 = D_{23}^{-1}\mathbf{w}_2 + \pi_2 \mathbf{a}_2 ,\ldots, \tag{21}$$

$$\mathbf{a}_n = D_{n-1,n}^{-1}\mathbf{w}_{n-1} + \pi_{n-1}\mathbf{a}_{n-1} .$$

If the vector $\boldsymbol{l}_1$ designates the upper half of $\mathbf{g}_1$ (the lower half is $G\boldsymbol{l}_1$ from the left boundary condition), then the exact mathematical solution of (19) is

$$\mathbf{g}_i = F_i \boldsymbol{l}_1 + \mathbf{a}_i , \qquad i = 1, 2,\ldots, n. \tag{22}$$

where the $(1/2)(L + 1)$-component vector $\boldsymbol{l}_1$ is the solution of the inhomogeneous system of equations

$$F_n{}^b \boldsymbol{l}_1 = -\mathbf{a}_n{}^b, \tag{23}$$

obtained using the right boundary condition; the superscript b designates the lower half of the corresponding matrices and vectors. This method is the discrete finite-differences analog of the well-known simple shooting technique based on initial value problems [16].

As discussed in the previous sections, in many problems the computation of this exact solution is unstable against the propagation of roundoff errors. These errors result in many cases in the extreme ill-conditioning of the matrix $F_n{}^b$ in the left of Eq. (23), making its numerical solution impossible. The degree of numerical instability depends on many variables, such as the sphere radius (in units of mean free paths), the anisotropy of the scattering cross section, the order of the P_L approximation, etc. As it is not possible to know a priori how unstable a given problem is, it is then imperative to "measure" the instability during the computation and eliminate it in the most efficient way.

A. *Stabilizing Transformations*

The idea behind the stabilizing transformations is quite simple: the exact mathematical solution of our problem (19), given by (22) and (23), is to be transformed so that the new solution is given only in terms of matrices and vectors that are arbitrarily well conditioned for computation. Obviously, the transformed solution has to be mathematically identical to the untransformed solution.

Although the stabilizing transformations are achieved by rather complicated linear algebra manipulations, the underlying idea behind them is very simple. It is to be noticed that the starting matrix and vector F_1 and $\mathbf{a}_1$ of the sequences (20) and (21) are perfectly well conditioned because their tops are the unit matrix and null vector, respectively, and thus the columns of F_1 and $\mathbf{a}_1$ form a set of linearly independent vectors. As the computation of the sequences F_i and $\mathbf{a}_i$ proceeds, the columns of F_i and $\mathbf{a}_i$ progressively become more linearly dependent. However, before the sequences become too ill-conditioned, certain linear transformations of F_{c_i} and $\mathbf{a}_{c_i}$ are performed at a conditioning point c_i (see Fig. 1) with the result

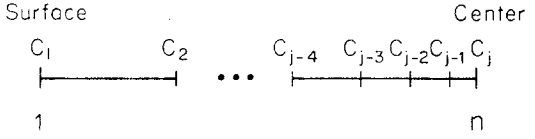

FIG. 1. Illustration showing the j conditioning points with a higher density near the sphere's center.

that the tops of the transformed or reconditioned matrix and vector U_{c_i} and $\mathbf{u}_{c_i}$ are reset again equal to the unit matrix and the null vector [see Eqs. (B3) and (B4)]. The process of computation of the matrix and vector sequences is restarted anew from the well conditioned pair U_{c_i} and $\mathbf{u}_{c_i}$. So, by a proper frequency of conditioning, we can assure that our matrix and vector sequences are arbitrarily well conditioned, and the numerical instability is thus eliminated.

In [2], it is shown that the solution of (19) can be given in the well conditioned form

$$\begin{aligned} \mathbf{g}_i &= U_i \boldsymbol{l}_k + \mathbf{u}_i \qquad c_k \leqslant i \leqslant c_{k+1} \\ \mathbf{g}_n &= U_n \boldsymbol{l}_j + \mathbf{u}_n , \end{aligned} \tag{25}$$

where the $(1/2)(L + 1)$-component vectors $\boldsymbol{l}_k$ are given by

$$\begin{aligned} \boldsymbol{l}_{k-1} &= T_{c_k}(\boldsymbol{l}_k - \mathbf{t}_{c_k}), \qquad k = 2, 3, \ldots, j - 1, \\ \boldsymbol{l}_{j-1} &= T_n(\boldsymbol{l}_j - \mathbf{t}_n), \end{aligned} \tag{26}$$

and $\boldsymbol{l}_j$ is the solution of the following system of equations:

$$U_n{}^{\mathrm{b}} \boldsymbol{l}_j = -\mathbf{u}_n{}^{\mathrm{b}}. \tag{27}$$

For completeness and reference, the transformation matrices and vectors T_c and $\mathbf{t}_{c_i}$ and the reconditioned matrices and vectors U_{c_i} and $\mathbf{u}_{c_i}$ are given explicitly in Appendix B.

Once $\boldsymbol{l}_j$ is obtained by solving the arbitrarily well-conditioned system of equations (27), all the other $\boldsymbol{l}$ vectors are obtained recursively from the formulas (26); therefore, the solution vectors $\mathbf{g}_{c_i}$ at all the conditioning points are obtained from (25) by solving only one system of equations, i.e., (27). This method is the finite-difference analog of the multiple shooting technique for the solution of two-point boundary value problems [16], and is based on the extension and generalization of previous methods due to Godunov [17] and Conte [18].

B. *The Numerical Algorithm*

The numerical algorithm for the direct solution of (19) is essentially the same as that discussed in considerable detail in [1], to which we refer the reader. Briefly, the first step is the computation of the untransformed (simple shooting) solution of (19) given by (22) and (23). The solution of (23) is obtained by a linear system solver (LINSY1) based on gaussian elimination with pivoting and iterative improvement of the solution, as described by Forsythe and Moler [19]. If system (23) is well conditioned, as determined by LINSY1, its solution gives the angular flux at the sphere's surface $\mathbf{g}_1$, and the solution at the other mesh points are

obtained by substitution in (19). Instead, if (23) is ill-conditioned in the sense discussed in [19], LINSY1 sets a signal for the main program; then the spatial grid (see Fig. 1) is divided into two marching intervals by a reconditioning point inside the grid c_2. The reconditioning transformations at c_2 and at the sphere center, $c_3 = n$, require the numerical inversion of the matrices $F^t_{c_2}$ and $F_n{}^t T_1 T_{c_2}$ [see (B1) and (B3)]; only when $F^t_{c_2}$ is inverted by LINSY1 without any error messages is the U_{c_2} matrix computed and stored, and the computation is continued to the sphere center. Whenever the *first* ill-conditioned matrix is detected, the sweep is immediately stopped and the number of marching intervals doubled. The procedure is pursued in this way until all the matrices involved in a given sweep are well-conditioned. Finally, the well-conditioned system (27) is solved, and the solution obtained at all the conditioning points by means of (26) and (27). In between conditioning points the solution is obtained by marching (substitution) through the inhomogeneous system (19).

V. Numerical Results and Discussion

A. *Isotropic Scattering Problems*

We first give the results of critical length computations for homogeneous spheres with isotropic scattering; exact values for the critical radii have been published by Carlson and Bell [5], and approximations obtained with the S_n method are reported in the recent book by Bell and Glasstone [6]. The transport equation solved is

$$\mu \frac{\partial \phi(x, \mu)}{\partial x} + \frac{1 - \mu^2}{x} \frac{\partial \phi(x, \mu)}{\partial \mu} + \phi(x, \mu) = \tfrac{1}{2} c \int_{-1}^{1} \phi(x, \mu')\, d\mu', \qquad (28)$$

with the boundary conditions, $\phi(x, \mu)$ finite and

$$\phi(R, \mu) = 0 \qquad -1 < \mu < 0. \qquad (29)$$

In (28) c is the average number of neutrons emitted per collision. For a given c, the critical length problem is to determine the sphere radius in units of mean free paths such that the steady-state equations (28) and (29) are satisfied [2].

The results of the computations for all the values of c given in [5] are shown in Table I. The most numerically unstable problems are those for the thicker spheres, and the table illustrates the power and efficiency of our method for automatically selecting the required number of reconditioning points. Except for the case $c = 1.02$, it is seen that Federighi's boundary conditions give closer agreement with the exact values than Marshak's; this effect was already observed

TABLE I

Sphere Critical Radii in Units of Mean Free Paths. Isotropic Scattering

Secondary neutrons per collision, c	Order of Approximation[a]					
	P_3 Boundary conditions		P_5 Boundary conditions		S_{16}[b]	Exact[c]
	Marshak	Federighi	Marshak	Federighi		
1.02	12.026(2)	12.023(2)	12.025(8)	12.023(8)	12.032	12.027
1.05	7.280(0)	7.276(0)	7.278(4)	7.276(4)	7.276	7.277
1.1	4.875(0)	4.872(0)	4.874(4)	4.873(4)	4.871	4.873
1.2	3.174(0)	3.172(0)	3.173(0)	3.172(0)	3.170	3.172
1.4	1.9868(0)	1.9857(0)	1.9859(0)	1.9855(0)	1.983	1.9855
1.6	1.4770(0)	1.4764(0)	1.4765(0)	1.4762(0)	1.474	1.4761
1.8	1.1839(0)	1.1835(0)	1.1836(0)	1.1834(0)		1.1833
2.0	0.9911(0)	0.9908(0)	0.9908(0)	0.9907(0)		0.9906

[a] The number of reconditioning points required is given in parentheses; double precision arithmetic; 64 equal space intervals.

[b] Ref. [6], with 64 equal space intervals.

[c] Ref. [5].

both in the neutron transport and radiative transfer computations done in plane geometry [2, 3]. It is known [6] that the S_{16} approximation is mathematically equivalent to a P_{15} approximation (both are a two-point boundary value problem for a system of 16 differential equations). The reason why our P_3 computations give better results than the S_{16} computations performed by Lee [6] is because he uses Mark boundary conditions and these are known to give much poorer answers than Marshak's or Federighi's. It is seen that our P_5 computations with Federighi's conditions agree with the exact values to almost five significant figures.

To give an idea of the efficiency of the method, we have timed some of the computations given in Table I in an IBM 360/195 computing system. The P_5 computation for $c = 1.02$ required 10 sec of computer time; in this case the system of equations (19), where the D matrices are 6×6, had to be solved 143 times because of the slow convergence of the power method (Rayleigh quotients) for the determination of the criticality eigenvalue of each successive size [2]. The P_5 computation for $c = 2.0$ required 3 sec of computer time; in this case, the system (19) had to be solved only 15 times.

In Table II, we give the results of some criticality computations for some spheres with isotropic scattering. Once the radius R is fixed, the problem is to determine the average number of neutrons emitted per collision which are necessary to maintain criticality. The aim of these computations was to compare the accuracy

TABLE II

Number of Secondary Neutrons (c) per Collision Necessary to Maintain Criticality as a Function of the Sphere Radius R (in Mean Free Paths). Isotropic Scattering

R	Number of Secondaries, c				Computer time (sec) IBM 360/195
	Method				
	IT_3[a]	S_8[a]	S_{16}[a]	P_3[b]	
0.1	13.4286	13.32	13.39	13.4296	0.6
0.5	3.23718	3.219	3.230	3.23746	0.8
1.0	1.98839	1.981	1.986	1.98860	0.9
5.0	1.09576	1.0955	1.0957	1.09575	2.8
10.0	1.02815	1.02281	1.02282	1.02814	6.3

[a] See Ref. [20].

[b] With Federighi's boundary conditions and 64 equal space intervals.

and efficiency of our method with the recent IT_N method of Hembd and Kschwendt, and with the S_N method [20]. As ours is a completely general method, for a fixed P_N approximation the computer time required is exactly the same whether the scattering is isotropic or anisotropic. For the radii 0.1, 0.5, and 1.0, our P_3 computations with Federighi's boundary conditions agree to five significant figures with the IT_3 computations; for the radii 5.0 and 10.0, the agreement is of six significant figures. The computer time given in Table II is to be compared with that required by the IT_3 method, which is of about 1 sec in an IBM 360/65 [20]. The reason for the considerably higher accuracy of our P_3 results compared with the S_8 and S_{16} results is the same as discussed before in connection with Table I.

B. *Anisotropic Scattering Problems*

We have obtained the critical radii of some homogeneous spheres with anisotropic scattering. Explicitly the transport equation solved was the following:

$$\mu \frac{\partial \phi(x, \mu)}{\partial x} + \frac{1 - \mu^2}{x} \frac{\partial \phi(x, \mu)}{\partial \mu} + \phi$$

$$= \tfrac{1}{2}(\Sigma_s^{\text{iso}} + \nu\Sigma_f) \int_{-1}^{1} \phi(x, \mu')\, d\mu'$$

$$+ \Sigma_s^{\text{aniso}} \sum_{n=0}^{4} \tfrac{1}{2}(2n + 1)\, b_n P_n(\mu) \int_{-1}^{1} P_n(\mu')\, \phi(x, \mu')\, d\mu', \qquad (30)$$

with the same center and vacuum boundary conditions used for the isotropic problems [see (28) and (29)]. For given values of the secondary neutron ratio $c + c'$, where

$$c = \Sigma_s^{\text{aniso}} \tag{31}$$

is the anisotropic-scattering ratio, and

$$c' = \Sigma_s^{\text{iso}} + \nu\Sigma_f\,, \tag{32}$$

is the isotropic secondary-neutron ratio, the critical length problem is again to determine the sphere radii such that the steady-state equation (30) with the proper boundary conditions are satisfied. The values of b_n are those for elastic hydrogen scattering

$$b_0 = 1, \qquad b_1 = 2/3, \qquad b_2 = 1/4, \qquad b_3 = 0, \qquad b_4 = -1/24. \tag{33}$$

For a given value of $c + c'$, c is increased to observe the effects of the anisotropy of the scattering. The results of our P_L computations are shown in Table III, where they are compared with S_{32} computations done by Lathrop [21]. For the secondary neutron ratio $c + c' = 1.05$, the agreement between our P_3 computations with Federighi's conditions and the S_{32} computations is of almost five significant figures. It should be recalled that mathematically, S_{32} computations are equivalent in principle to P_{31} computations; for this case $c + c' = 1.05$, the spherical harmonics method with Federighi's conditions provides the solution much more efficiently than the S_n method. (We should point out, however, that we do not know whether lower order S_n computations for this problem would already have converged to essentially the same results as those given with S_{32}.) When $c + c' = 1.4$, the agreement between our P_9 computations and the S_{32} computations is of four significant figures. Although not as notable as for the case $c + c' = 1.05$, the efficiency of the spherical harmonics method with Federighi's conditions is considerably higher than that of the S_n method. Some typical values of the computer time required are also given in the table.

A very significant difference between the anisotropic P_L computations for spherical geometry and the corresponding ones for plane geometry [1] has been observed. In plane geometry [2, 3] the ill-conditioning of the matrices was mostly due to the slab thickness, and always occurred as soon as the marching width exceeded a length of the order of one mean free path. For very thick spheres, this instability is also observed. This is as expected, because for large radii the $1/r$ term in the sphere transport equation is negligible several mean free paths away from the center, and the behavior here is close to that for plane geometry. However, Table III shows that the numerical instability for the cases $c + c' = 1.4$ is much

TABLE III

Sphere Critical Radii in Units of Mean Free Paths. Anisotropic Scattering[a]

c	P_3	S_{32}[b]	Computer time (sec) IBM 360/195
	$c + c' = 1.05$		
0.1	7.5012(0)	7.5012	1.1
0.3	8.0244(2)	8.0246	
0.5	8.6812(2)	8.6815	
0.7	9.5413(2)	9.5419	
0.9	10.7403(4)	10.7415	1.2
	$c + c' = 1.4$		
c	P_9	S_{32}[b]	Computer time (sec) IBM 360/195
0.1	2.0274(8)	2.0267	
0.3	2.1212(8)	2.1205	
0.5	2.2313(8)	2.2304	
0.7	2.3630(8)	2.3620	
0.9	2.5249(8)	2.5238	4.5

[a] The P_L computations were done with Federighi's boundary conditions, double precision arithmetic and 64 equal space intervals. The number of reconditioning points required is indicated inside the parentheses.

[b] K. D. Lathrop, private communication (1970); with 75 equal space intervals.

worse than for $c + c' = 1.05$, despite the fact that the radii are larger in the latter cases. In contrast (Table 4 of [1]), there is no instability in plane geometry with the same absorption and scattering cross sections for the cases $c + c' = 1.4$. We observed that for the same transport equation in spherical geometry the origin of this instability is due to the singularity at the center. When performing the computations for $c + c' = 1.4$, it was observed that the matrices became always ill-conditioned at the sphere center. To improve the efficiency of our algorithm, the density of the conditioning points near the center was increased, in accordance with an empirical logarithmic law. In this way, the number of reconditioning points required for stability was reduced approximately by a factor of two.

APPENDIX A

The vectors $\mathbf{f}(x)$, $\mathbf{s}(x)$ and the matrices A, B, and $C(x)$ of the text in Eq. (5) are given by

$$\mathbf{f}(x) \equiv \begin{bmatrix} f_0(x) \\ f_1(x) \\ \vdots \\ f_L(x) \end{bmatrix} \tag{A1}$$

$$f_l(x) \equiv \int_{-1}^{1} \phi(x, \mu)\, P_l(\mu)\, d\mu; \tag{A2}$$

$$\mathbf{s}(x) \equiv \begin{bmatrix} S_0(x) \\ S_1(x) \\ \vdots \\ S_L(x) \end{bmatrix}; \tag{A3}$$

$$S_l(x) \equiv \int_{-1}^{1} S(x, \mu)\, P_l(\mu)\, d\mu; \tag{A4}$$

$$A \equiv \begin{bmatrix} 0 & 1 & & & & \\ 1/3 & 0 & 2/3 & & & \bigcirc \\ & 2/5 & 0 & 3/5 & & \\ & \ddots & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \ddots & \\ & & \dfrac{L-1}{2L-1} & 0 & \dfrac{L}{2L-1} & \\ & \bigcirc & & & & \\ & & & \dfrac{L}{2L+1} & 0 & \end{bmatrix}; \tag{A5}$$

$$B \equiv \begin{bmatrix} 0 & \dfrac{2}{1} & & & & \\ 0 & 0 & \dfrac{2.3}{3} & & & \bigcirc \\ & -\dfrac{1.2}{5} & 0 & \dfrac{3.4}{5} & & \\ & & \dfrac{2.3}{7} & 0 & \dfrac{4.5}{7} & \\ & & & \ddots & \ddots & \ddots \\ & \bigcirc & & -\dfrac{(L-2)(L-1)}{2L-1} & 0 & \dfrac{L(L+1)}{2L-1} \\ & & & & \dfrac{(L-1)L}{2L+1} & 0 \end{bmatrix}; \tag{A6}$$

$$C(x) \equiv \begin{bmatrix} \sigma_0(x) & & & \bigcirc \\ & \sigma_1(x) & & \\ & & \ddots & \\ \bigcirc & & & \sigma_L(x) \end{bmatrix}; \tag{A7}$$

$$\sigma_l(x) \equiv \Sigma_t(x) - \Sigma_{sl}(x) \equiv \Sigma_t(x) - \int_{-1}^{1} \Sigma_s(x, \mu_0)\, P_l(\mu_0)\, d\mu_0 . \tag{A8}$$

Appendix B

In our well conditioned solution, see Eqs. (25)–(27) of the text, the following transformation matrices and vectors were used:

$$\begin{aligned} T_1 &= I, \\ T_{c_2} &= (F_{c_2}^{\mathrm{t}} T_1)^{-1} = (F_{c_2}^{\mathrm{t}})^{-1}, \\ T_{c_3} &= (F_{c_3}^{\mathrm{t}} T_1 T_{c_2})^{-1}, \\ &\cdots \\ T_n &= (F_n{}^{\mathrm{t}} T_1 T_{c_2} \cdots T_{c_{j-1}})^{-1}, \end{aligned} \tag{B1}$$

and

$$\begin{aligned} \mathbf{t}_1 &= \mathbf{0}, \\ \mathbf{t}_{c_2} &= (\mathbf{a}_{c_2} - F_{c_2} T_1 \mathbf{t}_1)^t = \mathbf{a}_{c_2}^t, \\ \mathbf{t}_{c_3} &= (\mathbf{a}_{c_3} - F_{c_3} T_1 T_{c_2} \mathbf{t}_{c_2})^{\mathrm{t}}, \\ &\cdots \\ \mathbf{t}_n &= (\mathbf{a}_n - F_n T_1 T_{c_2} \mathbf{t}_{c_2} - \cdots - F_n T_1 T_{c_2} \cdots T_{c_{j-1}} \mathbf{t}_{c_{j-1}})^{\mathrm{t}}, \end{aligned} \tag{B2}$$

where the matrix and vector sequences F_i and $\mathbf{a}_i$ are given in Eqs. (20) and (21) of the main text. The sequences of reconditioned matrices and vectors are given respectively by

$$U_i = \begin{cases} \begin{bmatrix} I \\ G \end{bmatrix} & i = 1 \\ F_i T_1 \equiv F_i I \equiv F_i & i = 2, 3, \ldots, c_2 - 1 \\ \left[(F_{c_2}^{\mathrm{b}} T_1) \quad \overset{I}{} \quad (F_{c_2}^{\mathrm{t}} T_1)^{-1} \right] & i = c_2 \\ F_i T_1 T_{c_2} & i = c_2 + 1, c_2 + 2, \ldots, c_3 - 1 \\ \cdots & \\ \left[(F_n^{\mathrm{b}} T_1 T_{c_2} \cdots T_{c_{j-1}}) \quad \overset{I}{} \quad (F_n^{\mathrm{t}} T_1 T_{c_2} \cdots T_{c_{j-1}})^{-1} \right] & i = c_j = n \end{cases} \tag{B3}$$

and

$$\begin{aligned} \mathbf{u}_1 &= \mathbf{0}, \\ \mathbf{u}_{c_2} &= \mathbf{a}_{c_2} - F_{c_2} T_1 T_{c_2} \mathbf{t}_{c_2} = \mathbf{a}_{c_2} - U_{c_2} \mathbf{t}_{c_2}, \\ \mathbf{u}_{c_3} &= \mathbf{a}_{c_3} - F_{c_3} T_1 T_{c_2} \mathbf{t}_{c_2} - F_{c_3} T_1 T_{c_2} T_{c_3} \mathbf{t}_{c_3} = \mathbf{a}_{c_3} - F_{c_3} T_1 T_{c_2} \mathbf{t}_{c_2} - U_{c_3} \mathbf{t}_{c_3}, \\ &\vdots \\ \mathbf{u}_n &= \mathbf{a}_n - F_n T_1 T_{c_2} \mathbf{t}_{c_2} - F_n T_1 T_{c_2} T_{c_3} \mathbf{t}_{c_3} - \cdots - F_n T_1 T_{c_2} \cdots T_{c_{j-1}} T_n \mathbf{t}_n \\ &= \mathbf{a}_n - F_n T_1 T_{c_2} \mathbf{t}_{c_2} - F_n T_1 T_{c_2} T_{c_3} \mathbf{t}_{c_3} - \cdots - F_n T_1 \cdots T_{c_{j-1}} \mathbf{t}_{c_{j-1}} - U_n \mathbf{t}_n, \end{aligned} \tag{B4}$$

where the superscripts t and b designate the top and bottom halves of the respective matrix and vector. In between conditioning points, the vector sequence u_i is determined by substitution in (19) using as starting values the u_{c_k} given in (B4) [see Eq. (21)]. It is to be noticed that the transformation vectors $\mathbf{t}_{c_k}$ (B2) are chosen so that the top halves of the reconditioned vectors (B4) are the null vector.

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