The F_N Method for Multigroup Transport Theory with Upscattering

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Abstract – An integral transform technique and the F_N method are used to develop solutions to a class of multigroup radiation-transport problems. The multigroup model considered allows an anisotropic scattering law and transfer from any group to any group. Computational aspects of the developed solution are discussed, and especially accurate numerical results are reported for two test cases.

I. INTRODUCTION

While multigroup transport theory has a long history in the nuclear engineering community (see, for example, Refs. 1 and 2), attention has mostly been focused on cases where there is only downscattering or weak upscattering.^{3–5} Even though elaborate schemes for improving the convergence rate of iterative solutions of upscatter problems have been proposed,^{6–10} we believe that various multigroup codes currently in use are still largely inefficient for problems that involve strong upscattering.

To provide an alternative procedure to iterating over the groups, a spherical-harmonics method that solves directly the vector equation of transfer has recently been developed and reported in the radiative-transfer literature.¹¹ We note also that Kelley¹² has constructed a version of the discrete ordinates method that has been used to obtain numerical results for the six-group test problem introduced in Ref. 11. Kelley's results for the group fluxes and currents for the considered problem agreed with Siewert's results¹¹ to within ± 1 in the fifth significant figure for all considered points interior to the surfaces of the one-dimensional layer. On the other hand, the fluxes at the boundaries of the layer were reported in Refs. 11 and 12 with no more than three significant figures; in particular, the flux and current on the right boundary for one of the groups were reported in these works with only one figure.

We note that early attempts to solve the test problem of Ref. 11 with the ANISN code⁵ were not successful^{13,14} nor were similar attempts with another standard S_N code.¹⁴ The kinds of difficulties observed in these studies are clearly displayed in Fig. 2 of Ref. 14. In this figure, one can see that the scalar flux computed with ANISN for group 3 of the six-group problem introduced in Ref. 11 underestimates the true scalar flux by \sim 200% near the boundary of incidence. The same behavior was observed in other test problems (including a strongly coupled two-group problem) and when the twodimensional discrete ordinates codes DOT and TWO-TRAN were used.¹³ More recently, it was observed¹⁵ that the use of a relaxation factor (input parameter RYF) for dealing with the upscatter convergence in ANISN can greatly improve the results for the six-group problem near the boundary of incidence, but at the expense of reduced efficiency; in addition, the results at or near the other boundary still show big discrepancies. Thus, regardless of the geometry, the treatment of the energy dependence of transport problems by iterative techniques in discrete ordinates codes seems to be problematic for calculations that require good energy resolution in the thermal range.

Here, to provide a compact computational method that yields high-quality results on the boundaries (as well as for the interior) of a plane-parallel layer, we generalize our previous work (see, for example, Refs. 16 through 19) on the F_N method to the case of fully coupled multigroup transport theory.

We consider the multigroup transport equation written as

$$\mu \frac{\partial}{\partial z} \Psi(z,\mu) + \mathbf{S}\Psi(z,\mu)$$
$$= \frac{1}{2} \sum_{l=0}^{L} P_l(\mu) \mathbf{T}_l \int_{-1}^{1} P_l(\mu') \Psi(z,\mu') d\mu' \qquad (1)$$

for $z \in (0, z_0)$ and $\mu \in [-1,1]$. Here the Legendre polynomials are denoted by $P_l(\mu)$, and the transfer matrices \mathbf{T}_l are such that particle transfer (by, for example, scattering and/or fission) between and within all energy groups is allowed. In addition, the elements $\psi_1(z,\mu), \psi_2(z,\mu), \dots, \psi_M(z,\mu)$ of the *M*-vector $\Psi(z,\mu)$ are the group angular fluxes; the elements s_1, s_2, \dots, s_M of the diagonal **S** matrix are the group total cross sections expressed in cm⁻¹; *z* is the position variable measured in cm; and μ is the direction cosine, with respect to the positive *z* axis, that defines the direction of particle motion.

Along with Eq. (1), we consider boundary conditions of the form

$$\Psi(0,\mu) = \mathbf{F}_1(\mu) \tag{2a}$$

and

$$\Psi(z_0, -\mu) = \mathbf{F}_2(\mu) \tag{2b}$$

for $\mu \in (0,1]$. Here $\mathbf{F}_1(\mu)$ and $\mathbf{F}_2(\mu)$ are considered given.

To use dimensionless units, we introduce an optical variable $\tau = zs_{min}$ and an optical thickness $\tau_0 = z_0 s_{min}$, where s_{min} is the minimum of the set $\{s_i\}$, and rewrite Eqs. (1) and (2) as

$$\mu \frac{\partial}{\partial \tau} \Psi(\tau, \mu) + \Sigma \Psi(\tau, \mu)$$
$$= \frac{1}{2} \sum_{l=0}^{L} P_l(\mu) \mathbf{C}_l \int_{-1}^{1} P_l(\mu') \Psi(\tau, \mu') d\mu' , \quad (3)$$

for $\tau \in (0, \tau_0)$ and $\mu \in [-1, 1]$, and

$$\Psi(0,\mu) = \mathbf{F}_1(\mu) \tag{4a}$$

and

$$\Psi(\tau_0, -\mu) = \mathbf{F}_2(\mu) \quad , \tag{4b}$$

for $\mu \in (0,1]$. Here the diagonal matrix Σ has entries $\sigma_i = s_i/s_{min}$, and the dimensionless transfer matrices are defined by $\mathbf{C}_l = \mathbf{T}_l/s_{min}$.

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II. SINGULAR INTEGRAL EQUATIONS AND CONSTRAINTS

In this section we use an integral transform procedure to reduce the problem formulated by Eqs. (3) and (4) to a linear system of singular integral equations and constraints for two vector quantities (\mathbf{Y} and \mathbf{Z}) that are related in a simple way to the angular-flux vectors at two arbitrary locations in the layer. We next specialize this system so that the resulting solution can be used to determine the exiting angular-flux vectors $\Psi(0, -\mu)$ and $\Psi(\tau_0, \mu)$ for $\mu \in (0, 1]$. Assuming that the exiting angular-flux vectors have been found, we then go back to the original system and show how to use it for computing the interior angular-flux vector $\Psi(\tau, \mu)$ for any $\tau \in (0, \tau_0)$ and $\mu \in [-1, 1]$.

In the manner of Ref. 18, we begin our derivation by changing μ to $-\mu$ in Eq. (3), multiplying the resulting equation by $\exp(-\tau/s)$, and integrating over τ from $\tau = a$ to $\tau = b$, with $0 \le a < b \le \tau_0$. We find, after an integration by parts,

$$(\boldsymbol{\mu}\mathbf{I} - s\boldsymbol{\Sigma})\boldsymbol{\Psi}^*(s, -\boldsymbol{\mu}) + \frac{s}{2}\sum_{l=0}^{L}(-1)^l P_l(\boldsymbol{\mu})\mathbf{C}_l\boldsymbol{\Psi}_l^*(s)$$
$$= \boldsymbol{\mu}s\mathbf{B}(\boldsymbol{\mu}, s) \quad , \tag{5}$$

where

$$\mathbf{B}(\mu,s) = \mathbf{\Psi}(a,-\mu)e^{-a/s} - \mathbf{\Psi}(b,-\mu)e^{-b/s} , \qquad (6)$$

$$\Psi^*(s,-\mu) = \int_a^b \Psi(\tau,-\mu) e^{-\tau/s} d\tau \quad , \tag{7}$$

and

$$\Psi_l^*(s) = \int_a^b \Psi_l(\tau) e^{-\tau/s} d\tau$$
(8)

for l = 0, 1, ..., L. Here we have also introduced the notation

$$\Psi_l(\tau) = \int_{-1}^{1} P_l(\mu) \Psi(\tau, \mu) d\mu \quad . \tag{9}$$

We consider now that $s \notin [-1,1]$ so that we can rewrite Eq. (5) as

$$\Psi^*(s,-\mu) + \frac{s}{2} \mathbf{D}(\mu,s) \sum_{\alpha=0}^{L} (-1)^{\alpha} P_{\alpha}(\mu) \mathbf{C}_{\alpha} \Psi^*_{\alpha}(s)$$
$$= \mu s \mathbf{D}(\mu,s) \mathbf{B}(\mu,s) \quad , \tag{10}$$

where

$$\mathbf{D}(\boldsymbol{\mu}, \boldsymbol{s}) = (\boldsymbol{\mu}\mathbf{I} - \boldsymbol{s}\boldsymbol{\Sigma})^{-1} \quad . \tag{11}$$

At this point we multiply Eq. (10) by $P_l(\mu)$, for l = 0, 1, ..., L, and integrate over all μ to obtain

$$(-1)^{l} \boldsymbol{\Psi}_{l}^{*}(s) + \frac{s}{2} \sum_{\alpha=0}^{L} (-1)^{\alpha} \\ \times \int_{-1}^{1} P_{l}(\mu) \mathbf{D}(\mu, s) P_{\alpha}(\mu) d\mu \mathbf{C}_{\alpha} \boldsymbol{\Psi}_{\alpha}^{*}(s) = \mathbf{\Gamma}_{l}(s) ,$$
(12)

where

$$\mathbf{\Gamma}_{l}(s) = s \int_{-1}^{1} \mu P_{l}(\mu) \mathbf{D}(\mu, s) \mathbf{B}(\mu, s) \, d\mu \quad . \tag{13}$$

Multigroup versions $G_l(\xi)$ of the Chandrasekhar polynomials were defined in Ref. 20 by the starting value

$$\mathbf{G}_0(\boldsymbol{\xi}) = \mathbf{I} \tag{14}$$

and the three-term recursion formula

$$\xi \mathbf{h}_{l} \mathbf{G}_{l}(\xi) = (l+1) \mathbf{G}_{l+1}(\xi) + l \mathbf{G}_{l-1}(\xi)$$
(15)

for $l \ge 0$. Here

$$\mathbf{h}_{l} = (2l+1)\mathbf{\Sigma} - \mathbf{C}_{l}, \text{ for } l = 0, 1, \dots, L, (16a)$$

and

$$\mathbf{h}_l = (2l+1)\mathbf{\Sigma} \quad , \text{ for } l > L \quad . \tag{16b}$$

Now we introduce a set of matrices $\mathbf{G}_{l}^{\dagger}(\xi)$ relevant to the adjoint problem: We define these matrices by the starting value

$$\mathbf{G}_{0}^{\dagger}(\boldsymbol{\xi}) = \mathbf{I} \tag{17}$$

and the three-term recursion formula

$$\boldsymbol{\xi} \tilde{\mathbf{h}}_{l} \mathbf{G}_{l}^{\dagger}(\boldsymbol{\xi}) = (l+1) \mathbf{G}_{l+1}^{\dagger}(\boldsymbol{\xi}) + l \mathbf{G}_{l-1}^{\dagger}(\boldsymbol{\xi})$$
(18)

for $l \ge 0$, where the tilde is used (throughout this work) to denote the transpose operation.

We now multiply Eq. (12) by $\tilde{\mathbf{G}}_{l}^{\dagger}(s)\mathbf{C}_{l}$ and sum the resulting equation over *l* to obtain

$$\sum_{l=0}^{L} (-1)^{l} \mathbf{M}_{l}(s) \mathbf{C}_{l} \boldsymbol{\Psi}_{l}^{*}(s) = \sum_{l=0}^{L} \tilde{\mathbf{G}}_{l}^{\dagger}(s) \mathbf{C}_{l} \mathbf{\Gamma}_{l}(s) , \quad (19)$$

where

$$\mathbf{M}_{l}(s) = \widetilde{\mathbf{G}}_{l}^{\dagger}(s) + \frac{s}{2} \sum_{\alpha=0}^{L} \widetilde{\mathbf{G}}_{\alpha}^{\dagger}(s) \mathbf{C}_{\alpha}$$
$$\times \int_{-1}^{1} P_{\alpha}(\mu) \mathbf{D}(\mu, s) P_{l}(\mu) d\mu \quad . \tag{20}$$

Multiplying Eq. (20) by (2l + 1)s and using the threeterm recursion formula

$$(2l+1)\mu P_l(\mu) = (l+1)P_{l+1}(\mu) + lP_{l-1}(\mu) \quad (21)$$

for the Legendre polynomials, we can now show that

$$\mathbf{M}_{l}(s) = \mathbf{\Omega}(s)\mathbf{P}_{l}(s\mathbf{\Sigma}) \quad , \tag{22}$$

where

$$\mathbf{\Omega}(s) = \mathbf{I} + \frac{s}{2} \sum_{l=0}^{L} \widetilde{\mathbf{G}}_{l}^{\dagger}(s) \mathbf{C}_{l} \int_{-1}^{1} \mathbf{D}(\boldsymbol{\mu}, s) P_{l}(\boldsymbol{\mu}) d\boldsymbol{\mu}$$
(23)

and

$$\mathbf{P}_{l}(s\mathbf{\Sigma}) = \operatorname{diag}\{\dots, P_{l}(\sigma_{i}s), \dots\} \quad (24)$$

We note that in this work we use the notation $\mathbf{A}(x\boldsymbol{\Sigma})$ to indicate that $\sigma_i x$ is the argument of the *i*'th component of **A**, when **A** represents a vector, or the argument of the *i*'th diagonal element of **A**, when **A** represents a diagonal matrix. Clearly, the definition given by Eq. (24) refers to the latter case. It follows that we can use Eq. (22) to rewrite Eq. (19) as

$$\mathbf{\Omega}(s)\mathbf{X}(s) = s \sum_{l=0}^{L} \widetilde{\mathbf{G}}_{l}^{\dagger}(s)\mathbf{C}_{l}$$
$$\times \int_{-1}^{1} \mu P_{l}(\mu)\mathbf{D}(\mu,s)\mathbf{B}(\mu,s) \,d\mu \quad , \quad (25)$$

where

$$\mathbf{X}(s) = \sum_{l=0}^{L} (-1)^{l} \mathbf{P}_{l}(s \mathbf{\Sigma}) \mathbf{C}_{l} \boldsymbol{\Psi}_{l}^{*}(s) \quad .$$
 (26)

At this point we find it convenient to change the integration variable in Eq. (23) so that we can write

$$\mathbf{\Omega}(s) = \mathbf{I} + \frac{s}{2} \int_{-1}^{1} \mathbf{G}^{\dagger}(s, x \mathbf{\Sigma}) \mathbf{\Theta}(x) \frac{dx}{x - s} , \qquad (27)$$

where

$$\mathbf{G}^{\dagger}(s, x\mathbf{\Sigma}) = \sum_{l=0}^{L} \widetilde{\mathbf{G}}_{l}^{\dagger}(s) \mathbf{C}_{l} \mathbf{P}_{l}(x\mathbf{\Sigma})$$
(28)

and where

$$\Theta(x) = \operatorname{diag}\{\dots, \theta_i(x), \dots\}$$
(29)

with $\theta_i(x) = 1$ for $x \in [-1/\sigma_i, 1/\sigma_i]$ and $\theta_i(x) = 0$, otherwise. By making a similar change of variable in the right-hand side of Eq. (25), we can rewrite that equation as

$$\mathbf{\Omega}(s)\mathbf{X}(s) = s \int_{-1}^{1} x \mathbf{G}^{\dagger}(s, x \mathbf{\Sigma}) \mathbf{\Sigma} \mathbf{\Theta}(x) \mathbf{B}(x \mathbf{\Sigma}, s) \frac{dx}{x - s} .$$
(30)

Rather than consider that s can take values in both the left and right half planes, we prefer to write Eq. (30) twice and consider only values of s in the right half plane. We thus let

$$\mathbf{\Upsilon}(a,b:s) = \frac{1}{s} \mathbf{X}(s) e^{a/s}$$
(31a)

and

$$\mathbf{\Xi}(a,b:s) = \frac{1}{s} \mathbf{X}(-s) e^{-b/s}$$
(31b)

and consider

$$\mathbf{\Omega}(s)\mathbf{\Upsilon}(a,b:s) = \mathbf{R}_1(s) + \mathbf{R}_2(s)$$
(32a)

and

$$\mathbf{\Omega}(s)\mathbf{\Xi}(a,b:s) = \mathbf{R}_3(s) + \mathbf{R}_4(s)$$
(32b)

for $\Re s > 0$. Here

$$\mathbf{R}_{1}(s) = \int_{0}^{1} x \mathbf{G}^{\dagger}(s, x \mathbf{\Sigma}) \mathbf{\Sigma} \Theta(x) [\Psi(a, -x \mathbf{\Sigma}) - \Psi(b, -x \mathbf{\Sigma}) e^{-(b-a)/s}] \frac{dx}{x-s} , \qquad (33a)$$

$$\mathbf{R}_{2}(s) = \int_{0}^{1} x \mathbf{G}^{\dagger}(s, -x\boldsymbol{\Sigma}) \boldsymbol{\Sigma} \boldsymbol{\Theta}(x) [\boldsymbol{\Psi}(a, x\boldsymbol{\Sigma}) - \boldsymbol{\Psi}(b, x\boldsymbol{\Sigma}) e^{-(b-a)/s}] \frac{dx}{x+s} , \qquad (33b)$$

$$\mathbf{R}_{3}(s) = \int_{0}^{1} x \mathbf{G}^{\dagger}(s, x \mathbf{\Sigma}) \mathbf{\Sigma} \mathbf{\Theta}(x) [\mathbf{\Psi}(b, x \mathbf{\Sigma}) - \mathbf{\Psi}(a, x \mathbf{\Sigma}) e^{-(b-a)/s}] \frac{dx}{x-s} , \qquad (33c)$$

$$\mathbf{R}_{4}(s) = \int_{0}^{1} x \mathbf{G}^{\dagger}(s, -x\boldsymbol{\Sigma}) \boldsymbol{\Sigma} \boldsymbol{\Theta}(x) [\boldsymbol{\Psi}(b, -x\boldsymbol{\Sigma}) - \boldsymbol{\Psi}(a, -x\boldsymbol{\Sigma})e^{-(b-a)/s}] \frac{dx}{x+s} \quad .$$
(33d)

Following Ref. 18, we now let *s* approach $\nu \in (0,1)$, but $\nu \notin \{1/\sigma_i\}$, from the upper half plane and from the lower half plane and use the Plemelj formulas²¹ to find from Eqs. (32)

$$\boldsymbol{\omega}(\nu)\mathbf{Y}(a,b:\nu) = \mathbf{r}_1(\nu) + \mathbf{R}_2(\nu) \quad , \tag{34a}$$

$$\boldsymbol{\omega}(\nu)\boldsymbol{\Xi}(a,b:\nu) = \mathbf{r}_3(\nu) + \mathbf{R}_4(\nu) \quad , \tag{34b}$$

$$\frac{1}{2}\mathbf{G}^{\dagger}(\nu,\nu\mathbf{\Sigma})\boldsymbol{\Theta}(\nu)\mathbf{Y}(a,b:\nu) = \mathbf{G}^{\dagger}(\nu,\nu\mathbf{\Sigma})\mathbf{\Sigma}\boldsymbol{\Theta}(\nu)[\boldsymbol{\Psi}(a,-\nu\mathbf{\Sigma})-\boldsymbol{\Psi}(b,-\nu\mathbf{\Sigma})e^{-(b-a)/\nu}], \quad (35a)$$

and

$$\frac{1}{2}\mathbf{G}^{\dagger}(\nu,\nu\boldsymbol{\Sigma})\boldsymbol{\Theta}(\nu)\boldsymbol{\Xi}(a,b:\nu) = \mathbf{G}^{\dagger}(\nu,\nu\boldsymbol{\Sigma})\boldsymbol{\Sigma}\boldsymbol{\Theta}(\nu)[\boldsymbol{\Psi}(b,\nu\boldsymbol{\Sigma}) - \boldsymbol{\Psi}(a,\nu\boldsymbol{\Sigma})e^{-(b-a)/\nu}] .$$
(35b)

Here

$$\boldsymbol{\omega}(\nu) = \mathbf{I} + \frac{\nu}{2} \int_{-1}^{1} \mathbf{G}^{\dagger}(\nu, x \boldsymbol{\Sigma}) \boldsymbol{\Theta}(x) \frac{dx}{x - \nu} , \qquad (36)$$

$$\mathbf{r}_{1}(\nu) = \int_{0}^{1} x \mathbf{G}^{\dagger}(\nu, x \mathbf{\Sigma}) \mathbf{\Sigma} \Theta(x) [\Psi(a, -x \mathbf{\Sigma}) - \Psi(b, -x \mathbf{\Sigma}) e^{-(b-a)/\nu}] \frac{dx}{x - \nu} , \qquad (37a)$$

and

$$\mathbf{r}_{3}(\nu) = \int_{0}^{1} x \mathbf{G}^{\dagger}(\nu, x \mathbf{\Sigma}) \mathbf{\Sigma} \Theta(x) [\Psi(b, x \mathbf{\Sigma}) - \Psi(a, x \mathbf{\Sigma}) e^{-(b-a)/\nu}] \frac{dx}{x - \nu} , \qquad (37b)$$

where the symbol f is used to indicate that the integral is to be evaluated in the Cauchy principal-value sense. We note that in using the Plemelj formulas to deduce Eqs. (34), we have excluded the "endpoints" 0 and $\{1/\sigma_i\}$; however, in subsequent equations these endpoint restrictions can effectively be removed.

To satisfy Eqs. (35), we let, for $x \in (0,1]$,

$$\boldsymbol{\Sigma}\boldsymbol{\Theta}(x)\boldsymbol{\Psi}(a,-x\boldsymbol{\Sigma}) = \boldsymbol{\Sigma}\boldsymbol{\Theta}(x)\boldsymbol{\Psi}(b,-x\boldsymbol{\Sigma})e^{-(b-a)/x} + \frac{1}{2}\boldsymbol{\Theta}(x)\boldsymbol{\Upsilon}(a,b:x)$$
(38a)

and

$$\boldsymbol{\Sigma}\boldsymbol{\Theta}(x)\boldsymbol{\Psi}(b,x\boldsymbol{\Sigma}) = \boldsymbol{\Sigma}\boldsymbol{\Theta}(x)\boldsymbol{\Psi}(a,x\boldsymbol{\Sigma})e^{-(b-a)/x} + \frac{1}{2}\boldsymbol{\Theta}(x)\boldsymbol{\Xi}(a,b:x)$$
(38b)

which can be substituted into Eqs. (34) to yield

$$\boldsymbol{\omega}(\nu)\boldsymbol{\Upsilon}(a,b:\nu) + \frac{1}{2} \int_{0}^{1} x \mathbf{G}^{\dagger}(\nu, x\boldsymbol{\Sigma})\boldsymbol{\Theta}(x)\boldsymbol{\Upsilon}(a,b:x) \frac{dx}{\nu - x} + \frac{1}{2} e^{-(b-a)/\nu} \int_{0}^{1} x \mathbf{G}^{\dagger}(\nu, -x\boldsymbol{\Sigma})\boldsymbol{\Theta}(x)\boldsymbol{\Xi}(a,b:x) \frac{dx}{\nu + x} = \mathbf{T}_{1}(a,b:\nu)$$
(39a)

$$\boldsymbol{\omega}(\nu)\boldsymbol{\Xi}(a,b:\nu) + \frac{1}{2} \int_{0}^{1} x \mathbf{G}^{\dagger}(\nu, x\boldsymbol{\Sigma}) \boldsymbol{\Theta}(x) \boldsymbol{\Xi}(a,b:x) \frac{dx}{\nu - x} + \frac{1}{2} e^{-(b-a)/\nu} \int_{0}^{1} x \mathbf{G}^{\dagger}(\nu, -x\boldsymbol{\Sigma}) \boldsymbol{\Theta}(x) \mathbf{Y}(a,b:x) \frac{dx}{\nu + x} = \mathbf{T}_{2}(a,b:\nu)$$
(39b)

for $\nu \in [0,1]$. We can use the definitions

$$C(\tau : x, y) = \frac{e^{-\tau/x} - e^{-\tau/y}}{x - y}$$
(40a)

and

$$S(\tau : x, y) = \frac{1 - e^{-\tau/x} e^{-\tau/y}}{x + y}$$
(40b)

to write

$$\mathbf{T}_{1}(a,b:\xi)$$

$$= \int_{0}^{1} x [\mathbf{G}^{\dagger}(\xi,-x\boldsymbol{\Sigma})\boldsymbol{\Sigma}\boldsymbol{\Theta}(x)\boldsymbol{\Psi}(a,x\boldsymbol{\Sigma})S(b-a:x,\xi)$$

$$+ \mathbf{G}^{\dagger}(\xi,x\boldsymbol{\Sigma})\boldsymbol{\Sigma}\boldsymbol{\Theta}(x)\boldsymbol{\Psi}(b,-x\boldsymbol{\Sigma})$$

$$\times C(b-a:x,\xi)] dx \qquad (41a)$$

and

$$\mathbf{T}_{2}(a,b:\xi)$$

$$= \int_{0}^{1} x [\mathbf{G}^{\dagger}(\xi,-x\boldsymbol{\Sigma})\boldsymbol{\Sigma}\boldsymbol{\Theta}(x)\boldsymbol{\Psi}(b,-x\boldsymbol{\Sigma})S(b-a:x,\xi)$$

$$+ \mathbf{G}^{\dagger}(\xi,x\boldsymbol{\Sigma})\boldsymbol{\Sigma}\boldsymbol{\Theta}(x)\boldsymbol{\Psi}(a,x\boldsymbol{\Sigma})$$

$$\times C(b-a:x,\xi)] dx \quad . \tag{41b}$$

We note that Eqs. (41) can also be written as

$$\mathbf{T}_{1}(a,b:\xi) = \sum_{l=0}^{L} \widetilde{\mathbf{G}}_{l}^{\dagger}(\xi) \mathbf{C}_{l} \mathbf{\Sigma}^{-1} \int_{0}^{1} \mu P_{l}(\mu)$$

$$\times \left[(-1)^{l} \mathbf{S}(b-a:\mu \mathbf{\Sigma}^{-1},\xi) \mathbf{\Psi}(a,\mu) + \mathbf{C}(b-a:\mu \mathbf{\Sigma}^{-1},\xi) \mathbf{\Psi}(b,-\mu) \right] d\mu$$
(42a)

and

$$\begin{aligned} \mathbf{T}_{2}(a,b:\xi) &= \sum_{l=0}^{L} \widetilde{\mathbf{G}}_{l}^{\dagger}(\xi) \mathbf{C}_{l} \mathbf{\Sigma}^{-1} \int_{0}^{1} \mu P_{l}(\mu) \\ &\times \left[(-1)^{l} \mathbf{S}(b-a:\mu \mathbf{\Sigma}^{-1},\xi) \mathbf{\Psi}(b,-\mu) \right. \\ &+ \mathbf{C}(b-a:\mu \mathbf{\Sigma}^{-1},\xi) \mathbf{\Psi}(a,\mu) \right] d\mu , \end{aligned}$$

$$\end{aligned}$$

$$(42b)$$

where

$$\mathbf{C}(\tau: x \mathbf{\Sigma}^{-1}, y) = \operatorname{diag}\{\dots, C(\tau: x/\sigma_i, y), \dots\}$$
(43a)

and

$$\mathbf{S}(\tau : x \mathbf{\Sigma}^{-1}, y) = \text{diag}\{\dots, S(\tau : x/\sigma_i, y), \dots\} \quad (43b)$$

In addition to the values of the transform variable $s = \nu \in [0,1]$, we also consider a discrete spectrum in the right half plane $s = \nu_j, \nu_j \notin [0,1], j = 1,2,...,\aleph$, defined by

$$\det \mathbf{\Omega}(\nu_j) = 0 \quad . \tag{44}$$

Thus, if we let $\mathbf{M}(\nu_j)$ be a vector in the null space of $\mathbf{\Omega}(\nu_j)$, i.e.,

$$\mathbf{M}(\nu_i)\mathbf{\Omega}(\nu_i) = \mathbf{0} \quad , \tag{45}$$

we can deduce from Eqs. (32) the additional equations

$$\frac{1}{2} \mathbf{M}(\nu_j) \int_0^1 x \mathbf{G}^{\dagger}(\nu_j, x \mathbf{\Sigma}) \mathbf{\Theta}(x) \mathbf{Y}(a, b:x) \frac{dx}{\nu_j - x} + \frac{1}{2} e^{-(b-a)/\nu_j} \mathbf{M}(\nu_j) \times \int_0^1 x \mathbf{G}^{\dagger}(\nu_j, -x \mathbf{\Sigma}) \mathbf{\Theta}(x) \mathbf{\Xi}(a, b:x) \frac{dx}{\nu_j + x} = \mathbf{M}(\nu_j) \mathbf{T}_1(a, b:\nu_j)$$
(46a)

and

$$\frac{1}{2} \mathbf{M}(\nu_j) \int_0^1 x \mathbf{G}^{\dagger}(\nu_j, x \mathbf{\Sigma}) \mathbf{\Theta}(x) \mathbf{\Xi}(a, b:x) \frac{dx}{\nu_j - x} + \frac{1}{2} e^{-(b-a)/\nu_j} \mathbf{M}(\nu_j) \times \int_0^1 x \mathbf{G}^{\dagger}(\nu_j, -x \mathbf{\Sigma}) \mathbf{\Theta}(x) \mathbf{Y}(a, b:x) \frac{dx}{\nu_j + x} = \mathbf{M}(\nu_j) \mathbf{T}_2(a, b:\nu_j)$$
(46b)

for $j = 1, 2, ..., \aleph$.

At this point, we note that the unknown vectors $\mathbf{Y}(a, b: \mu)$ and $\mathbf{\Xi}(a, b: \mu)$ in Eqs. (39) and (46) are related to the angular-flux vectors at the positions a and b, as can be seen from Eqs. (38). Moreover, on the right-hand sides of Eqs. (39) and (46), we require the incoming angular-flux vectors $\Psi(a, \mu)$ and $\Psi(b, -\mu)$, $\mu \in (0, 1]$, which are only known for a = 0 and $b = \tau_0$, as specified by Eqs. (4). It is thus clear that we must start our solution by specializing Eqs. (39) and (46) to the case a = 0 and $b = \tau_0$. We find, for $\nu \in [0, 1]$,

$$\boldsymbol{\omega}(\nu)\boldsymbol{\Upsilon}(0,\tau_0:\nu) + \frac{1}{2} \int_0^1 x \mathbf{G}^{\dagger}(\nu, x\boldsymbol{\Sigma})\boldsymbol{\Theta}(x)\boldsymbol{\Upsilon}(0,\tau_0:x) \frac{dx}{\nu-x} + \frac{1}{2} e^{-\tau_0/\nu} \int_0^1 x \mathbf{G}^{\dagger}(\nu, -x\boldsymbol{\Sigma})\boldsymbol{\Theta}(x)\boldsymbol{\Xi}(0,\tau_0:x) \frac{dx}{\nu+x} = \mathbf{K}_1(0:\nu)$$
(47a)

$$\boldsymbol{\omega}(\nu)\boldsymbol{\Xi}(0,\tau_0:\nu) + \frac{1}{2} \int_0^1 x \mathbf{G}^{\dagger}(\nu, x\boldsymbol{\Sigma}) \boldsymbol{\Theta}(x) \boldsymbol{\Xi}(0,\tau_0:x) \frac{dx}{\nu-x} + \frac{1}{2} e^{-\tau_0/\nu} \int_0^1 x \mathbf{G}^{\dagger}(\nu, -x\boldsymbol{\Sigma}) \boldsymbol{\Theta}(x) \mathbf{Y}(0,\tau_0:x) \frac{dx}{\nu+x} = \mathbf{K}_2(\tau_0:\nu) \quad ,$$
(47b)

and, for $j = 1, 2, ..., \aleph$,

$$\frac{1}{2} \mathbf{M}(\nu_j) \int_0^1 x \mathbf{G}^{\dagger}(\nu_j, x \mathbf{\Sigma}) \mathbf{\Theta}(x) \mathbf{\Upsilon}(0, \tau_0 : x) \frac{dx}{\nu_j - x} + \frac{1}{2} e^{-\tau_0/\nu_j} \mathbf{M}(\nu_j) \int_0^1 x \mathbf{G}^{\dagger}(\nu_j, -x \mathbf{\Sigma}) \mathbf{\Theta}(x) \mathbf{\Xi}(0, \tau_0 : x) \frac{dx}{\nu_j + x} = \mathbf{M}(\nu_j) \mathbf{K}_1(0 : \nu_j)$$
(48a)

and

$$\frac{1}{2} \mathbf{M}(\nu_j) \int_0^1 x \mathbf{G}^{\dagger}(\nu_j, x \mathbf{\Sigma}) \mathbf{\Theta}(x) \mathbf{\Xi}(0, \tau_0; x) \frac{dx}{\nu_j - x} + \frac{1}{2} e^{-\tau_0/\nu_j} \mathbf{M}(\nu_j) \int_0^1 x \mathbf{G}^{\dagger}(\nu_j, -x \mathbf{\Sigma}) \mathbf{\Theta}(x) \mathbf{Y}(0, \tau_0; x) \frac{dx}{\nu_j + x}$$
$$= \mathbf{M}(\nu_j) \mathbf{K}_2(\tau_0; \nu_j) \quad , \tag{48b}$$

where, in general,

$$\mathbf{K}_{1}(\tau;\xi) = \int_{0}^{1} x \mathbf{G}^{\dagger}(\xi, -x\boldsymbol{\Sigma}) \boldsymbol{\Sigma} \boldsymbol{\Theta}(x) \mathbf{F}_{1}(x\boldsymbol{\Sigma}) e^{-\tau/x} S(\tau_{0} - \tau; x, \xi) dx + \int_{0}^{1} x \mathbf{G}^{\dagger}(\xi, x\boldsymbol{\Sigma}) \boldsymbol{\Sigma} \boldsymbol{\Theta}(x) \mathbf{F}_{2}(x\boldsymbol{\Sigma}) C(\tau_{0} - \tau; x, \xi) dx$$
(49a)

and

$$\mathbf{K}_{2}(\tau;\xi) = \int_{0}^{1} x \mathbf{G}^{\dagger}(\xi, -x\boldsymbol{\Sigma}) \boldsymbol{\Sigma} \boldsymbol{\Theta}(x) \mathbf{F}_{2}(x\boldsymbol{\Sigma}) e^{-(\tau_{0} - \tau)/x} S(\tau; x, \xi) dx + \int_{0}^{1} x \mathbf{G}^{\dagger}(\xi, x\boldsymbol{\Sigma}) \boldsymbol{\Sigma} \boldsymbol{\Theta}(x) \mathbf{F}_{1}(x\boldsymbol{\Sigma}) C(\tau; x, \xi) dx .$$
(49b)

Equations (47) and (48) define a set of linear singular-integral equations and integral constraints for the vectors $\mathbf{Y}(0,\tau_0;\mu)$ and $\mathbf{\Xi}(0,\tau_0;\mu)$ for $\mu \in (0,1]$. Our intention, therefore, is to solve in some approximate manner Eqs. (47) and (48) and then to compute the desired exiting angular fluxes from

$$\Psi(0,-\mu) = e^{-\tau_0 \Sigma/\mu} \mathbf{F}_2(\mu) + \frac{1}{2} \Sigma^{-1} \Upsilon(0,\tau_0;\mu \Sigma^{-1})$$
(50a)

and

$$\boldsymbol{\Psi}(\tau_0,\mu) = e^{-\tau_0 \boldsymbol{\Sigma}/\mu} \mathbf{F}_1(\mu) + \frac{1}{2} \boldsymbol{\Sigma}^{-1} \boldsymbol{\Xi}(0,\tau_0;\mu\boldsymbol{\Sigma}^{-1})$$
(50b)

for $\mu \in (0,1]$. We note that these expressions were derived by changing the angular variable and setting a = 0 and $b = \tau_0$ in Eqs. (38) and by making use of the boundary conditions given by Eqs. (4). In addition, the matrix exponential used in Eqs. (50) is defined as

$$e^{-\tau \mathbf{\Sigma}/\mu} = \operatorname{diag}\{\dots, e^{-\sigma_i \tau/\mu}, \dots\}$$
 (51)

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Now, to find the interior angular-flux vector $\Psi(\tau, \mu)$, $\tau \in (0, \tau_0)$ and $\mu \in [-1, 1]$, we first consider Eqs. (39a) and (46a) with $a = \tau$ and $b = \tau_0$ and Eqs. (39b) and (46b) with a = 0 and $b = \tau$. We find, for $\nu \in [0,1]$,

$$\boldsymbol{\omega}(\nu)\boldsymbol{\Upsilon}(\tau,\tau_0:\nu) + \frac{1}{2} \int_0^1 x \mathbf{G}^{\dagger}(\nu, x\boldsymbol{\Sigma}) \boldsymbol{\Theta}(x) \boldsymbol{\Upsilon}(\tau,\tau_0:x) \frac{dx}{\nu-x} - \frac{1}{2} \int_0^1 x \mathbf{G}^{\dagger}(\nu, -x\boldsymbol{\Sigma}) \boldsymbol{\Theta}(x) \boldsymbol{\Xi}(0,\tau:x) \frac{dx}{\nu+x}$$
$$= \mathbf{K}_1(\tau:\nu) - \frac{1}{2} e^{-(\tau_0-\tau)/\nu} \int_0^1 x \mathbf{G}^{\dagger}(\nu, -x\boldsymbol{\Sigma}) \boldsymbol{\Theta}(x) \boldsymbol{\Xi}(0,\tau_0:x) \frac{dx}{\nu+x}$$
(52a)

and

$$\boldsymbol{\omega}(\nu) \boldsymbol{\Xi}(0,\tau:\nu) + \frac{1}{2} \int_{0}^{1} x \mathbf{G}^{\dagger}(\nu, x\boldsymbol{\Sigma}) \boldsymbol{\Theta}(x) \boldsymbol{\Xi}(0,\tau:x) \frac{dx}{\nu-x} - \frac{1}{2} \int_{0}^{1} x \mathbf{G}^{\dagger}(\nu, -x\boldsymbol{\Sigma}) \boldsymbol{\Theta}(x) \boldsymbol{\Upsilon}(\tau, \tau_{0}:x) \frac{dx}{\nu+x}$$
$$= \mathbf{K}_{2}(\tau:\nu) - \frac{1}{2} e^{-\tau/\nu} \int_{0}^{1} x \mathbf{G}^{\dagger}(\nu, -x\boldsymbol{\Sigma}) \boldsymbol{\Theta}(x) \boldsymbol{\Upsilon}(0, \tau_{0}:x) \frac{dx}{\nu+x} , \qquad (52b)$$

and, for $j = 1, 2, ..., \aleph$,

$$\frac{1}{2} \mathbf{M}(\nu_j) \int_0^1 x \mathbf{G}^{\dagger}(\nu_j, x \mathbf{\Sigma}) \mathbf{\Theta}(x) \mathbf{Y}(\tau, \tau_0; x) \frac{dx}{\nu_j - x} - \frac{1}{2} \mathbf{M}(\nu_j) \int_0^1 x \mathbf{G}^{\dagger}(\nu_j, -x \mathbf{\Sigma}) \mathbf{\Theta}(x) \mathbf{\Xi}(0, \tau; x) \frac{dx}{\nu_j + x}$$
$$= \mathbf{M}(\nu_j) \mathbf{K}_1(\tau; \nu_j) - \frac{1}{2} e^{-(\tau_0 - \tau)/\nu_j} \mathbf{M}(\nu_j) \int_0^1 x \mathbf{G}^{\dagger}(\nu_j, -x \mathbf{\Sigma}) \mathbf{\Theta}(x) \mathbf{\Xi}(0, \tau_0; x) \frac{dx}{\nu_j + x}$$
(53a)

and

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$$\frac{1}{2} \mathbf{M}(\nu_j) \int_0^1 x \mathbf{G}^{\dagger}(\nu_j, x \mathbf{\Sigma}) \mathbf{\Theta}(x) \mathbf{\Xi}(0, \tau : x) \frac{dx}{\nu_j - x} - \frac{1}{2} \mathbf{M}(\nu_j) \int_0^1 x \mathbf{G}^{\dagger}(\nu_j, -x \mathbf{\Sigma}) \mathbf{\Theta}(x) \mathbf{Y}(\tau, \tau_0 : x) \frac{dx}{\nu_j + x}$$
$$= \mathbf{M}(\nu_j) \mathbf{K}_2(\tau : \nu_j) - \frac{1}{2} e^{-\tau/\nu_j} \mathbf{M}(\nu_j) \int_0^1 x \mathbf{G}^{\dagger}(\nu_j, -x \mathbf{\Sigma}) \mathbf{\Theta}(x) \mathbf{Y}(0, \tau_0 : x) \frac{dx}{\nu_j + x}$$
(53b)

We note that once Eqs. (47) and (48) are solved, the vectors $\mathbf{\Upsilon}(0, \tau_0; \mu)$ and $\mathbf{\Xi}(0, \tau_0; \mu)$ become available, and so the right-hand sides of Eqs. (52) and (53) are completely determined. Therefore, we can also solve in an approximate manner the set of linear singular-integral equations and integral constraints defined by Eqs. (52) and (53) for the unknown vectors $\mathbf{Y}(\tau, \tau_0; \mu)$ and $\Xi(0,\tau:\mu)$. We can then compute the interior angular fluxes from the expressions, for $\mu \in [0,1]$,

$$\Psi(\tau,-\mu) = e^{-(\tau_0-\tau)\Sigma/\mu} \mathbf{F}_2(\mu) + \frac{1}{2} \Sigma^{-1} \Upsilon(\tau,\tau_0:\mu\Sigma^{-1})$$
(54a)

and

$$\Psi(\tau,\mu) = e^{-\tau \Sigma/\mu} \mathbf{F}_1(\mu) + \frac{1}{2} \Sigma^{-1} \Xi(0,\tau : \mu \Sigma^{-1}) ,$$
(54b)

which can be derived by setting $a = \tau$ and $b = \tau_0$ in Eq. (38a), a = 0 and $b = \tau$ in Eq. (38b), and by changing the angular variable in the resulting equations.

III. THE F_N METHOD

The F_N method²² is a collocation technique for solving linear systems of singular-integral equations and constraints in an approximate, but accurate, manner. As the method has been comprehensively reviewed in the literature,^{23,24} no additional review is given here. However, we do note that Kelley²⁵ has discussed convergence aspects of the method in the context of multigroup theory applied to an isotropically scattering half-space.

To start our solution of the boundary system defined by Eqs. (47) and (48), we approximate $\Upsilon(0, \tau_0; \mu)$ and $\Xi(0,\tau_0;\mu)$, for $\mu \in (0,1]$, by the finite-dimensional representations

$$\mathbf{f}(0,\tau_0:\boldsymbol{\mu}) = 2\sum_{\alpha=0}^{N} \Phi_{\alpha}(\boldsymbol{\mu}) \mathbf{a}_{\alpha}$$
(55a)

and

$$\boldsymbol{\Xi}(0,\tau_0:\boldsymbol{\mu}) = 2\sum_{\alpha=0}^N \Phi_\alpha(\boldsymbol{\mu}) \mathbf{b}_\alpha \quad , \tag{55b}$$

where $\{\Phi_{\alpha}(\mu)\}\$ is a set of basis functions to be specified. Once the vectors $\{\mathbf{a}_{\alpha}\}\$ and $\{\mathbf{b}_{\alpha}\}\$ have been determined, we can use Eqs. (55) in Eqs. (50) to find the desired results:

$$\Psi(0,-\mu) = e^{-\tau_0 \mathbf{\Sigma}/\mu} \mathbf{F}_2(\mu) + \mathbf{\Sigma}^{-1} \sum_{\alpha=0}^N \mathbf{\Phi}_\alpha(\mu \mathbf{\Sigma}^{-1}) \mathbf{a}_\alpha$$
(56a)

and

$$\Psi(\tau_0,\mu) = e^{-\tau_0 \mathbf{\Sigma}/\mu} \mathbf{F}_1(\mu) + \mathbf{\Sigma}^{-1} \sum_{\alpha=0}^N \mathbf{\Phi}_\alpha(\mu \mathbf{\Sigma}^{-1}) \mathbf{b}_\alpha$$
(56b)

for $\mu \in (0,1]$. Here, in accordance with our previously defined notation,

$$\boldsymbol{\Phi}_{\alpha}(\boldsymbol{\mu}\boldsymbol{\Sigma}^{-1}) = \text{diag}\{\dots, \boldsymbol{\Phi}_{\alpha}(\boldsymbol{\mu}/\sigma_{i}), \dots\} \quad (57)$$

If we now substitute Eqs. (55) into Eqs. (47) and (48), we find

$$\sum_{\alpha=0}^{N} \left[\mathbf{B}_{\alpha}(\xi) \mathbf{a}_{\alpha} + e^{-\tau_0/\xi} \mathbf{A}_{\alpha}(\xi) \mathbf{b}_{\alpha} \right] = \mathbf{V}_1(0 : \xi) \quad (58a)$$

and

$$\sum_{\alpha=0}^{N} \left[\mathbf{B}_{\alpha}(\xi) \mathbf{b}_{\alpha} + e^{-\tau_{0}/\xi} \mathbf{A}_{\alpha}(\xi) \mathbf{a}_{\alpha} \right] = \mathbf{V}_{2}(\tau_{0} : \xi) , \quad (58b)$$

for $\xi = \nu_j, j = 1, 2, ..., \aleph$, or $\xi = \nu \in [0, 1]$. Here, we have defined the *M*-dimensional row vectors

$$\mathbf{A}_{\alpha}(\nu_{j}) = \mathbf{M}(\nu_{j}) \sum_{l=0}^{L} (-1)^{l} \widetilde{\mathbf{G}}_{l}^{\dagger}(\nu_{j}) \mathbf{C}_{l} \mathbf{\Sigma}^{-1}$$
$$\times \int_{0}^{1} \mu P_{l}(\mu) \mathbf{D}(\mu, -\nu_{j}) \mathbf{\Phi}_{\alpha}(\mu \mathbf{\Sigma}^{-1}) d\mu$$

and

$$\mathbf{B}_{\alpha}(\nu_{j}) = -\mathbf{M}(\nu_{j}) \sum_{l=0}^{L} \tilde{\mathbf{G}}_{l}^{\dagger}(\nu_{j}) \mathbf{C}_{l} \boldsymbol{\Sigma}^{-1}$$
$$\times \int_{0}^{1} \mu P_{l}(\mu) \mathbf{D}(\mu, \nu_{j}) \boldsymbol{\Phi}_{\alpha}(\mu \boldsymbol{\Sigma}^{-1}) d\mu , \qquad (59b)$$

for $j = 1, 2, ..., \aleph$, and the $M \times M$ matrices

$$\mathbf{A}_{\alpha}(\nu) = \sum_{l=0}^{L} (-1)^{l} \widetilde{\mathbf{G}}_{l}^{\dagger}(\nu) \mathbf{C}_{l} \mathbf{\Sigma}^{-1}$$
$$\times \int_{0}^{1} \mu P_{l}(\mu) \mathbf{D}(\mu, -\nu) \mathbf{\Phi}_{\alpha}(\mu \mathbf{\Sigma}^{-1}) d\mu$$
(60a)

and

$$\mathbf{B}_{\alpha}(\nu) = 2\Phi_{\alpha}(\nu)\boldsymbol{\omega}(\nu) - \sum_{l=0}^{L} \tilde{\mathbf{G}}_{l}^{\dagger}(\nu)\mathbf{C}_{l}\boldsymbol{\Sigma}^{-1}$$

$$\times \int_{0}^{1} \mu P_{l}(\mu)\mathbf{D}(\mu,\nu)\boldsymbol{\Phi}_{\alpha}(\mu\boldsymbol{\Sigma}^{-1}) d\mu ,$$
(60b)

for $\nu \in [0,1]$. In addition, we have also used in Eqs. (58) the general definitions, for $\beta = 1$ or 2,

$$\mathbf{V}_{\beta}(\tau : \xi) = \mathbf{E}(\xi) \mathbf{K}_{\beta}(\tau : \xi) \quad , \tag{61}$$

where, for $\xi = \nu_j$, $j = 1, 2, ..., \aleph$, $\mathbf{E}(\nu_j) = \mathbf{M}(\nu_j)$ and, for $\xi = \nu \in [0,1]$, $\mathbf{E}(\nu) = \mathbf{I}$.

To generate a finite system of linear algebraic equations from which to obtain the required 2M(N + 1) unknowns, i.e., the M(N + 1) elements of \mathbf{a}_{α} , $\alpha = 0, 1, ..., N$, and the M(N + 1) elements of \mathbf{b}_{α} , $\alpha = 0, 1, ..., N$, we use collocation. If we write $\aleph = k_1M + k_2$, where k_1 and k_2 are nonnegative integers (with $k_2 < M$), and let ξ take on the values $\xi_{\beta} = \nu_{\beta}$, $\beta = 1, 2, ..., \aleph$, and $\xi_{\beta} \in [0,1]$, $\beta = \aleph + 1, \aleph + 2, ..., \aleph + N + 1 - k_1$, in Eqs. (58), we obtain a system of $2M(N+1) + 2k_2$ linear algebraic equations. Clearly, the number of equations exceeds the number of unknowns by $2k_2$, and so, in general, the system will be overdetermined, unless $k_2 = 0$. As we prefer to have a collocation strategy that yields always a square system, we follow the lines of a previous work on the F_N method for radiative transfer with polarization²⁶ and define the projection matrices

$$\mathbf{P}_{\boldsymbol{\beta}} = 1$$
 , $\boldsymbol{\beta} = 1, 2, \dots, \aleph$, (62a)

for the discrete spectrum and

(59a)

$$\mathbf{P}_{\beta} = \mathbf{I}$$
, $\beta = \aleph + 1, \aleph + 2, \dots, \aleph + N - k_1$, (62b)

for all points in the continuum except the last one. We assume, for simplicity, that the collocation points in the continuum are ordered by increasing magnitudes, so that the last of these points is closest to 1. Thus, to obtain a square system, we associate with this point a $(M - k_2) \times M$ projection matrix \mathbf{P}_{β} , $\beta = \aleph + N + 1 - k_1$, defined in a way that the elements of row *i* are unity for columns $i, i + 1, \ldots, i + k_2$ and zero otherwise. For example, when $k_2 = 0$, this projection matrix is simply the identity matrix, and when $k_2 = M - 1$, it reduces to a row vector of dimension M with all elements equal to unity. With these definitions, we can now solve the square system formed by

$$\mathbf{P}_{\beta} \sum_{\alpha=0}^{N} \left[\mathbf{B}_{\alpha}(\xi_{\beta}) \mathbf{a}_{\alpha} + e^{-\tau_{0}/\xi_{\beta}} \mathbf{A}_{\alpha}(\xi_{\beta}) \mathbf{b}_{\alpha} \right] = \mathbf{P}_{\beta} \mathbf{V}_{1}(0 : \xi_{\beta})$$
(63a)

$$\mathbf{P}_{\beta} \sum_{\alpha=0}^{N} \left[\mathbf{B}_{\alpha}(\xi_{\beta}) \mathbf{b}_{\alpha} + e^{-\tau_{0}/\xi_{\beta}} \mathbf{A}_{\alpha}(\xi_{\beta}) \mathbf{a}_{\alpha} \right] = \mathbf{P}_{\beta} \mathbf{V}_{2}(\tau_{0} : \xi_{\beta}) ,$$
(63b)

for $\beta = 1, 2, ..., \aleph + N + 1 - k_1$, to find the vectors $\{\mathbf{a}_{\alpha}\}$ and $\{\mathbf{b}_{\alpha}\}$ required in Eqs. (56).

Once we solve Eqs. (63), we can turn our attention to the calculation of the interior angular-flux vector $\Psi(\tau,\mu)$ for any $\tau \in (0,\tau_0)$ and $\mu \in [-1,1]$. First, we introduce the approximations

$$\mathbf{\Upsilon}(\tau,\tau_0:\boldsymbol{\mu}) = 2\sum_{\alpha=0}^N \Phi_\alpha(\boldsymbol{\mu})\mathbf{c}_\alpha(\tau)$$
(64a)

and

$$\mathbf{\Xi}(0,\tau:\mu) = 2\sum_{\alpha=0}^{N} \Phi_{\alpha}(\mu) \mathbf{d}_{\alpha}(\tau) \quad , \qquad (64b)$$

for $\mu \in [0,1]$, into Eqs. (52) and (53) and use the same collocation strategy used for the boundary system to obtain the square system

$$\mathbf{P}_{\beta} \sum_{\alpha=0}^{N} \left[\mathbf{B}_{\alpha}(\xi_{\beta}) \mathbf{c}_{\alpha}(\tau) - \mathbf{A}_{\alpha}(\xi_{\beta}) \mathbf{d}_{\alpha}(\tau) \right]$$
$$= \mathbf{P}_{\beta} \mathbf{V}_{1}(\tau : \xi_{\beta}) - e^{-(\tau_{0} - \tau)/\xi_{\beta}} \mathbf{P}_{\beta} \sum_{\alpha=0}^{N} \mathbf{A}_{\alpha}(\xi_{\beta}) \mathbf{b}_{\alpha}$$
(65a)

and

$$\mathbf{P}_{\beta} \sum_{\alpha=0}^{N} \left[\mathbf{B}_{\alpha}(\xi_{\beta}) \mathbf{d}_{\alpha}(\tau) - \mathbf{A}_{\alpha}(\xi_{\beta}) \mathbf{c}_{\alpha}(\tau) \right]$$
$$= \mathbf{P}_{\beta} \mathbf{V}_{2}(\tau; \xi_{\beta}) - e^{-\tau/\xi_{\beta}} \mathbf{P}_{\beta} \sum_{\alpha=0}^{N} \mathbf{A}_{\alpha}(\xi_{\beta}) \mathbf{a}_{\alpha} \qquad (65b)$$

for the unknown vectors $\{\mathbf{c}_{\alpha}(\tau)\}\$ and $\{\mathbf{d}_{\alpha}(\tau)\}\$. Clearly, as the matrix of coefficients related to the linear system defined by Eqs. (65) does not depend on τ , a single lowerupper (LU) decomposition of this matrix is sufficient for finding $\{\mathbf{c}_{\alpha}(\tau)\}\$ and $\{\mathbf{d}_{\alpha}(\tau)\}\$ for any number of positions inside the layer. Finally, once these vectors become available, we can substitute Eqs. (64) into Eqs. (54) and use the resulting expressions, i.e.,

$$\Psi(\tau, -\mu) = e^{-(\tau_0 - \tau)\Sigma/\mu} \mathbf{F}_2(\mu)$$

+ $\Sigma^{-1} \sum_{\alpha=0}^{N} \Phi_{\alpha}(\mu\Sigma^{-1}) \mathbf{c}_{\alpha}(\tau)$ (66a)

and

$$\Psi(\tau,\mu) = e^{-\tau \Sigma/\mu} \mathbf{F}_{1}(\mu) + \Sigma^{-1} \sum_{\alpha=0}^{N} \mathbf{\Phi}_{\alpha}(\mu \Sigma^{-1}) \mathbf{d}_{\alpha}(\tau)$$
(66b)

for $\mu \in [0,1]$, to compute our F_N approximations to the interior angular fluxes.

IV. COMPUTATIONAL METHODS

To implement our F_N solution to the considered multigroup problem, we must first compute ν_j , $j = 1, 2, ..., \aleph$, the zeros of det $\Omega(\xi)$ in the right half plane cut from [0,1]. Here we use a procedure similar to that of Siewert and Thomas,²⁰ and so we begin by writing the transpose of Eq. (23), for $\Re \xi \ge 0$ but $\xi \notin [0,1]$, as

$$\tilde{\mathbf{\Omega}}(\xi) = \mathbf{I} + \xi \sum_{l=0}^{L} \mathbf{Q}_{l}(\xi \mathbf{\Sigma}) \tilde{\mathbf{C}}_{l} \mathbf{G}_{l}^{\dagger}(\xi) , \qquad (67)$$

where

$$\mathbf{Q}_{l}(\boldsymbol{\xi}\boldsymbol{\Sigma}) = \frac{1}{2} \int_{-1}^{1} \mathbf{D}(\boldsymbol{\mu}, \boldsymbol{\xi}) P_{l}(\boldsymbol{\mu}) d\boldsymbol{\mu}$$
(68)

satisfies

$$= (l+1)\boldsymbol{\xi}\boldsymbol{\Sigma}\mathbf{Q}_{l}(\boldsymbol{\xi}\boldsymbol{\Sigma})$$
$$= (l+1)\mathbf{Q}_{l+1}(\boldsymbol{\xi}\boldsymbol{\Sigma}) + l\mathbf{Q}_{l-1}(\boldsymbol{\xi}\boldsymbol{\Sigma}) - \delta_{l,0}\mathbf{I} \qquad (69)$$

for $l \ge 0$. If we now subtract Eq. (18) multiplied on the left by $\mathbf{Q}_l(\boldsymbol{\xi}\boldsymbol{\Sigma})$ from Eq. (69) multiplied on the right by $\mathbf{G}_l^{\dagger}(\boldsymbol{\xi})$ and sum the resulting equation from l = 0 up to l = L, we obtain an alternative representation for $\mathbf{\tilde{\Omega}}(\boldsymbol{\xi})$, namely,

$$\widetilde{\mathbf{\Omega}}(\xi) = (L+1) [\mathbf{Q}_{L+1}(\xi \mathbf{\Sigma}) \mathbf{G}_{L}^{\dagger}(\xi) - \mathbf{Q}_{L}(\xi \mathbf{\Sigma}) \mathbf{G}_{L+1}^{\dagger}(\xi)] .$$
(70)

Similarly, we can subtract Eq. (18) multiplied on the left by $\mathbf{P}_l(\xi \mathbf{\Sigma})$ from

$$(2l+1)\boldsymbol{\xi}\boldsymbol{\Sigma}\mathbf{P}_{l}(\boldsymbol{\xi}\boldsymbol{\Sigma}) = (l+1)\mathbf{P}_{l+1}(\boldsymbol{\xi}\boldsymbol{\Sigma}) + l\mathbf{P}_{l-1}(\boldsymbol{\xi}\boldsymbol{\Sigma})$$
(71)

multiplied on the right by $\mathbf{G}_l^{\dagger}(\xi)$ and sum the result from l = 0 up to l = L to find

$$\xi \sum_{l=0}^{L} \mathbf{P}_{l}(\xi \mathbf{\Sigma}) \widetilde{\mathbf{C}}_{l} \mathbf{G}_{l}^{\dagger}(\xi)$$

$$= (L+1) [\mathbf{P}_{L+1}(\xi \mathbf{\Sigma}) \mathbf{G}_{L}^{\dagger}(\xi) - \mathbf{P}_{L}(\xi \mathbf{\Sigma}) \mathbf{G}_{L+1}^{\dagger}(\xi)] .$$
(72)

In addition, we can subtract Eq. (71) multiplied on the left by $\mathbf{Q}_l(\xi \mathbf{\Sigma})$ from Eq. (69) multiplied on the right by $\mathbf{P}_l(\xi \mathbf{\Sigma})$ and sum the result from l = 0 up to l = L to find

$$\mathbf{I} = (L+1) [\mathbf{Q}_{L+1}(\boldsymbol{\xi}\boldsymbol{\Sigma})\mathbf{P}_{L}(\boldsymbol{\xi}\boldsymbol{\Sigma}) - \mathbf{Q}_{L}(\boldsymbol{\xi}\boldsymbol{\Sigma})\mathbf{P}_{L+1}(\boldsymbol{\xi}\boldsymbol{\Sigma})] .$$
(73)

Proceeding with the development of our procedure for computing the discrete spectrum in the right half plane, we multiply Eq. (70) on the left by $\mathbf{P}_L(\boldsymbol{\xi}\boldsymbol{\Sigma})$ and use Eqs. (72) and (73) to obtain

$$\mathbf{P}_{L}(\boldsymbol{\xi}\boldsymbol{\Sigma})\tilde{\boldsymbol{\Omega}}(\boldsymbol{\xi}) = \mathbf{G}_{L}^{\dagger}(\boldsymbol{\xi}) + \boldsymbol{\xi}\mathbf{Q}_{L}(\boldsymbol{\xi}\boldsymbol{\Sigma})\sum_{l=0}^{L}\mathbf{P}_{l}(\boldsymbol{\xi}\boldsymbol{\Sigma})\tilde{\mathbf{C}}_{l}\mathbf{G}_{l}^{\dagger}(\boldsymbol{\xi}) \quad .$$
(74)

Noting that $C_l = 0$ for l > L, we can easily show that Eq. (74) is also valid when *L* is replaced by *K*, for any $K \ge L$. Moreover, since $\xi \notin (0,1)$, we can write Eq. (74) as

$$\widetilde{\mathbf{\Omega}}(\xi) = \mathbf{P}_{K}^{-1}(\xi \mathbf{\Sigma}) \\ \times \left[\mathbf{G}_{K}^{\dagger}(\xi) + \xi \mathbf{Q}_{K}(\xi \mathbf{\Sigma}) \sum_{l=0}^{L} \mathbf{P}_{l}(\xi \mathbf{\Sigma}) \widetilde{\mathbf{C}}_{l} \mathbf{G}_{l}^{\dagger}(\xi) \right]$$
(75)

for any $K \ge L$. Since the Legendre function of the second kind

$$Q_{l}(\xi) = \frac{1}{2} \int_{-1}^{1} P_{l}(\mu) \frac{d\mu}{\xi - \mu} , \quad \xi \notin [-1, 1] , \quad (76)$$

approaches zero as $l \to \infty$ (see, for example, the book by Robin²⁷) and $\mathbf{Q}_l(\xi \boldsymbol{\Sigma})$ can be expressed as

$$\mathbf{Q}_{l}(\boldsymbol{\xi}\boldsymbol{\Sigma}) = \operatorname{diag}\{\ldots, \mathcal{Q}_{l}(\boldsymbol{\sigma}_{i}\boldsymbol{\xi}), \ldots\} \quad (77)$$

we obtain, if we let $K \to \infty$ in Eq. (75),

$$\widetilde{\mathbf{\Omega}}(\xi) = \lim_{K \to \infty} \mathbf{P}_{K}^{-1}(\xi \mathbf{\Sigma}) \mathbf{G}_{K}^{\dagger}(\xi) \quad .$$
(78)

We thus conclude from Eq. (78) that the required zeros of det $\mathbf{\Omega}(\xi)$ can be approximated with increasing accuracy by the zeros of det $\mathbf{G}_{K}^{\dagger}(\xi)$ in the right half plane cut from [0,1] as $K \rightarrow \infty$. In regard to the computational implementation of our procedure, we begin by taking K = $\mathcal{N} + 1$, with \mathcal{N} odd and $\mathcal{N} \ge L$, in Eq. (78) and computing, according to the procedure summarized in the next paragraph, the zeros of det $\mathbf{G}_{\mathcal{N}+1}^{\dagger}(\xi)$. We note that this is a necessary step in the computational implementation of the spherical-harmonics method of order \mathcal{N} for the class of problems we are addressing in this paper.¹¹ However, in this work we are not interested in all the zeros of det $\mathbf{G}_{\mathcal{N}+1}^{\mathsf{T}}(\boldsymbol{\xi})$; only those zeros in the right half plane cut from [0,1] are relevant here. Having found our first approximations for the required zeros of det $\Omega(\xi)$, we then increase the value of \mathcal{N} and repeat the procedure as many times as necessary until convergence within a prescribed tolerance in the approximations is attained. As discussed by Siewert and Thomas,²⁰ there may be situations for which a faster procedure (e.g., Newton's method) is required; here, for the sample problems to be discussed in the next section, we found that this was not necessary.

We now describe our procedure for computing the zeros of det $\mathbf{G}_{\mathcal{N}+1}^{\dagger}(\xi)$. First, in the manner of Ref. 20, we eliminate the odd-order terms in Eq. (18) to obtain, for l = 0, 2, ...,

$$\mathbf{X}_{l}\mathbf{G}_{l-2}^{\dagger}(\xi) + \mathbf{Y}_{l}\mathbf{G}_{l}^{\dagger}(\xi) + \mathbf{Z}_{l}\mathbf{G}_{l+2}^{\dagger}(\xi) = \xi^{2}\mathbf{G}_{l}^{\dagger}(\xi) ,$$
(79)

where

$$\mathbf{X}_l = l(l-1)\tilde{\mathbf{h}}_l^{-1}\tilde{\mathbf{h}}_{l-1}^{-1} , \qquad (80a)$$

$$\mathbf{Y}_{l} = l^{2} \tilde{\mathbf{h}}_{l}^{-1} \tilde{\mathbf{h}}_{l-1}^{-1} + (l+1)^{2} \tilde{\mathbf{h}}_{l}^{-1} \tilde{\mathbf{h}}_{l+1}^{-1} , \qquad (80b)$$

and

$$\mathbf{Z}_{l} = (l+1)(l+2)\tilde{\mathbf{h}}_{l}^{-1}\tilde{\mathbf{h}}_{l+1}^{-1} .$$
(80c)

Next, assuming that ξ is a zero of det $\mathbf{G}_{\mathcal{N}+1}^{\dagger}(\xi)$, we multiply Eq. (79) by $\mathbf{N}(\xi)$, a vector in the null space of $\mathbf{G}_{\mathcal{N}+1}^{\dagger}(\xi)$, and use the resulting equation for $l = 0, 2, ..., \mathcal{N} - 1$ along with

$$\mathbf{G}_{\mathcal{N}+1}^{\dagger}(\boldsymbol{\xi})\mathbf{N}(\boldsymbol{\xi}) = \mathbf{0}$$
(81)

to obtain the eigenvalue problem

$$\mathbf{A}\mathbf{U} = \boldsymbol{\xi}^2 \mathbf{U} \quad , \tag{82}$$

where

$$\mathbf{A} = \begin{pmatrix} \mathbf{Y}_{0} & \mathbf{Z}_{0} & \mathbf{0} & \dots & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{X}_{2} & \mathbf{Y}_{2} & \mathbf{Z}_{2} & \dots & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{X}_{4} & \mathbf{Y}_{4} & \dots & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \dots & \mathbf{Y}_{\mathcal{N}-5} & \mathbf{Z}_{\mathcal{N}-5} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \dots & \mathbf{X}_{\mathcal{N}-3} & \mathbf{Y}_{\mathcal{N}-3} & \mathbf{Z}_{\mathcal{N}-3} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \dots & \mathbf{0} & \mathbf{X}_{\mathcal{N}-1} & \mathbf{Y}_{\mathcal{N}-1} \end{pmatrix}$$

$$(83)$$

is a M(N+1)/2 square matrix and

$$\mathbf{U} = \text{diag}\{\mathbf{G}_0^{\dagger}(\boldsymbol{\xi}), \mathbf{G}_2^{\dagger}(\boldsymbol{\xi}), \dots, \mathbf{G}_{\mathcal{N}-1}^{\dagger}(\boldsymbol{\xi})\}\mathbf{N}(\boldsymbol{\xi})$$
(84)

is a vector of dimension $M(\mathcal{N} + 1)/2$. Clearly, the desired zeros of det $\mathbf{G}_{\mathcal{N}+1}^{\dagger}(\xi)$ are simply the (positive) square roots of the eigenvalues of **A**. In this work we used the subroutines BALANC, ELMHES, and HQR from the EISPACK package²⁸ to compute the eigenvalues of **A**.

We now turn our attention to the computation of the matrix-valued functions $\mathbf{A}_{\alpha}(\xi)$ and $\mathbf{B}_{\alpha}(\xi)$ defined by Eqs. (59) and (60) and required for $\xi \in \{\nu_j\} \cup [0,1]$. Although, in principle, we could have pursued the route of recurrence formulas,^{23,29} we prefer to use Gaussian integration here to evaluate the integrals in Eqs. (59) and (60). Clearly, the application of a standard Gauss-Legendre quadrature for performing the integrals in

Eqs. (59) and (60a) is straightforward, but in the case of Eq. (60b), the singularity must be removed first. By combining the first and second terms on the right-hand side of Eq. (60b), we find we can write this equation as

$$\mathbf{B}_{\alpha}(\nu) = 2\Phi_{\alpha}(\nu)\mathbf{I} - \nu\Phi_{\alpha}(\nu)\sum_{l=0}^{L} (-1)^{l} \tilde{\mathbf{G}}_{l}^{\dagger}(\nu)\mathbf{C}_{l}$$

$$\times \int_{0}^{1} P_{l}(\mu)\mathbf{D}(\mu, -\nu) d\mu$$

$$- \sum_{l=0}^{L} \tilde{\mathbf{G}}_{l}^{\dagger}(\nu)\mathbf{C}_{l} \int_{0}^{1} P_{l}(\mu)\mathbf{D}(\mu, \nu)$$

$$\times \left[\mu \mathbf{\Sigma}^{-1} \mathbf{\Phi}_{\alpha}(\mu \mathbf{\Sigma}^{-1}) - \nu \Phi_{\alpha}(\nu)\mathbf{I}\right] d\mu , \quad (85)$$

a form to which we can readily apply a standard Gauss-Legendre quadrature. The order of the applied quadrature was determined as follows. We first used a 100-point Gauss-Legendre quadrature shifted to the interval [0,1] to compute $\mathbf{A}_{\alpha}(\xi)$ and $\mathbf{B}_{\alpha}(\xi)$ for all values of $\xi \in \{\nu_j\} \cup \{0.0(0.1)1.0\}$ and $\alpha = 0,1,\ldots,N_m$, where N_m is the maximum order of the F_N approximation to be used in the calculation. We note that $N_m = 549$ for the first sample problem described in Sec. V, while $N_m = 129$ for the second. Next, denoting as $A^{ij}_{\alpha}(\xi)$ and $\mathbf{B}^{ij}_{\alpha}(\xi)$, respectively, we computed the quantities

$$n_A(\xi) = \sum_{\alpha=0}^{N_m} \sum_{i=1}^{I} \sum_{j=1}^{M} |A_{\alpha}^{ij}(\xi)|$$
(86a)

and

$$n_B(\xi) = \sum_{\alpha=0}^{N_m} \sum_{i=1}^{I} \sum_{j=1}^{M} |B_{\alpha}^{ij}(\xi)| , \qquad (86b)$$

where I = 1 when $\xi \in \{\nu_j\}$ and I = M when $\xi \in [0,1]$, for all the grid points defined for ξ . We then repeated the procedure increasing the order of the quadrature by 100 each time, until the maximum relative difference ob-

where $\mathbf{H}(\nu_i)$ is a M(L+1) square matrix given by

served for $n_A(\xi)$ and $n_B(\xi)$ in two successive calculations was $< 10^{-10}$. This procedure defined the order of the quadrature as 1400 for the first of our test problems in Sec. V and 300 for the second. It should be noted that the Gaussian integration technique does not yield accurate results for elements of $\mathbf{A}_{\alpha}(\xi)$ and $\mathbf{B}_{\alpha}(\xi)$, which have magnitudes of the order of or smaller than the machine precision (typically $\approx 10^{-16}$ for double-precision calculations in short-word machines). This may occur in high order for $\mathbf{A}_{\alpha}(\xi), \xi \in \{\nu_i\} \cup [0,1]$, and for $\mathbf{B}_{\alpha}(\xi), \xi \in \{\nu_i\}$ $\{\nu_i\}$. Fortunately, this loss of accuracy turns out to be of no concern for us here, as we have found that the sensitivity of the solutions of the linear systems defined by Eqs. (63) and (65) to such small elements of $A_{\alpha}(\xi)$ and $\mathbf{B}_{\alpha}(\xi)$ is extremely small, and consequently these solutions are stable in high order. Even if these elements were computed very accurately, they would end up being corrupted during the Gaussian elimination process used to solve the linear systems.

Finally, we report our methods for computing the matrices $\tilde{\mathbf{G}}_{l}^{\dagger}(\nu)$ for $\nu \in [0,1]$ and the row vectors

$$\widetilde{\mathbf{T}}_{l}^{\dagger}(\nu_{j}) = \mathbf{M}(\nu_{j})\widetilde{\mathbf{G}}_{l}^{\dagger}(\nu_{j})$$
(87)

for $j = 1, 2, ..., \aleph$ —both of which are required in Eqs. (59) and (60) and on the right-hand sides of Eqs. (63) and (65). We note that the required matrices $\tilde{\mathbf{G}}_l^{\dagger}(\nu)$ for $\nu \in [0,1]$ can be easily computed by recurrence, using the initial value given by Eq. (17) along with Eq. (18) in the forward direction for l = 0, 1, ..., L - 1, and then taking the transposes of the matrices so obtained. To develop a method for computing the required vectors $\tilde{\mathbf{T}}_l^{\dagger}(\nu_j)$, we first consider $\xi = \nu_j$ in the transpose of Eq. (70) and multiply the resulting equation on the right by $\tilde{\mathbf{M}}(\nu_j)$ to obtain, for $j = 1, 2, ..., \aleph$,

$$\mathbf{T}_{L+1}^{\dagger}(\nu_j) = \mathbf{Q}_L^{-1}(\nu_j \mathbf{\Sigma}) \mathbf{Q}_{L+1}(\nu_j \mathbf{\Sigma}) \mathbf{T}_L^{\dagger}(\nu_j) \quad .$$
(88)

Multiplying Eq. (18) on the right by $\mathbf{\hat{M}}(\nu_j)$, using the resulting equation for l = 0, 1, ..., L and considering the truncation condition expressed by Eq. (88), we now obtain, for $j = 1, 2, ..., \aleph$,

$$\mathbf{H}(\boldsymbol{\nu}_i)\mathbf{T}(\boldsymbol{\nu}_i) = \mathbf{0} \quad , \tag{89}$$

$$\mathbf{H}(\nu_{j}) = \begin{pmatrix} \nu_{j}\tilde{\mathbf{h}}_{0} & -\mathbf{I} & \mathbf{0} & \dots & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ -\mathbf{I} & \nu_{j}\tilde{\mathbf{h}}_{1} & -2\mathbf{I} & \dots & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & -2\mathbf{I} & \nu_{j}\tilde{\mathbf{h}}_{2} & \dots & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \dots & \nu_{j}\tilde{\mathbf{h}}_{L-2} & -(L-1)\mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \dots & -(L-1)\mathbf{I} & \nu_{j}\tilde{\mathbf{h}}_{L-1} & -L\mathbf{I} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \dots & \mathbf{0} & -L\mathbf{I} & \nu_{j}\tilde{\mathbf{h}}_{L} - \mathbf{R}(\nu_{j}) \end{pmatrix}$$
(90)

Group	$\tau/\tau_0 = 0.0$	$\tau/\tau_0=0.25$	$\tau/ au_0 = 0.5$	$\tau/\tau_0=0.75$	$\tau/\tau_0 = 1.0$
1	1.09412	1.62048E-4 ^a	4.85237E-8	1.45667E-11	4.03114E-15
2	2.29719E-1	3.74472E-2	1.96392E-3	1.02768E-4	1.78976E-6
3	2.91728E-1	1.85473E-1	9.79886E-3	5.12779E-4	4.36490E-6
4	3.05978E-2	2.62814E-2	1.38837E-3	7.26540E-5	4.39421E-7
5	5.99893E-4	6.10777E-4	3.22597E-5	1.68816E-6	7.91259E-9
6	7.30516E-6	7.25931E-6	3.83255E-7	2.00558E-8	7.94257E-11

TABLE I The Group Scalar Fluxes $\Psi_0(au)$

^aRead as 1.62048×10^{-4} .

with
$$\mathbf{R}(\nu_i) = (L+1)\mathbf{Q}_L^{-1}(\nu_i \boldsymbol{\Sigma})\mathbf{Q}_{L+1}(\nu_i \boldsymbol{\Sigma})$$
, and

$$\mathbf{T}(\nu_j) = \begin{pmatrix} \mathbf{T}_0^{\dagger}(\nu_j) \\ \mathbf{T}_1^{\dagger}(\nu_j) \\ \mathbf{T}_2^{\dagger}(\nu_j) \\ \vdots \\ \mathbf{T}_{L-2}^{\dagger}(\nu_j) \\ \mathbf{T}_{L-1}^{\dagger}(\nu_j) \\ \mathbf{T}_{L}^{\dagger}(\nu_j) \end{pmatrix}$$
(91)

In conclusion, the required vectors $\widetilde{\mathbf{T}}_{l}^{T}(\nu_{j})$ can be found from the transposes of the vectors $\mathbf{T}(\nu_{j})$, once these are computed for $j = 1, 2, ..., \aleph$. In this work we used the subroutine MINFIT from the EISPACK package³⁰ to compute singular-value decompositions of the matrices $\mathbf{H}(\nu_{j})$ for $j = 1, 2, ..., \aleph$ that were subsequently used to compute the corresponding \mathbf{T} vectors.

V. SAMPLE PROBLEMS

To demonstrate the quality of the results that can be obtained with the F_N method, we first report in this sec-

tion highly accurate results for a six-group problem with cubic (L = 3) anisotropic scattering that was previously used to test a developed version of the spherical-harmonics method.¹¹ The problem consists of a water layer (with $z_0 = 30$ cm) bombarded on the surface at z = 0 by a uniform and isotropic flux of neutrons with energies in group 1. As the cross sections that define the problem have been tabulated in Ref. 11, we do not repeat these tabulations here. However, we do note that the thickness of the layer is equivalent to 45.156 in units of the optical variable introduced in Sec. I and that the boundary conditions are expressed as

$$\mathbf{F}_{1}(\mu) = (1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0)^{T}$$
(92a)

and

$$\mathbf{F}_2(\mu) = \mathbf{0} \tag{92b}$$

for $\mu \in (0,1]$.

In Tables I and II we report our F_N results, thought to be accurate to all figures given, for the group scalar fluxes

$$\Psi_0(\tau) = \int_{-1}^1 \Psi(\tau, \mu) \, d\mu \tag{93}$$

		1	1()		
Group	$\tau/ au_0 = 0.0$	$\tau/ au_0 = 0.25$	$\tau/ au_0 = 0.5$	$ au/ au_0 = 0.75$	$\tau/\tau_0 = 1.0$
1 2 3 4 5 6	4.71921E-1 ^a -9.92907E-2 -1.62966E-1 -1.70261E-2 -3.27829E-4 -3.86253E-6	1.04414E-4 5.98176E-3 8.77724E-3 5.92290E-4 6.71835E-6 2.88262E-8	3.12929E-8 3.11437E-4 4.69326E-4 3.16933E-5 3.59244E-7 1.53371E-9	9.39417E-12 1.63588E-5 2.46565E-5 1.66505E-6 1.88732E-8 8.05724E-11	2.92352E-15 1.09847E-6 2.51982E-6 2.46538E-7 4.31668E-9 4.10414E-11

TABLE II The Group Currents $\Psi_1(\tau)$

^aRead as 4.71921×10^{-1} .

and the group currents

$$\Psi_{1}(\tau) = \int_{-1}^{1} \mu \Psi(\tau, \mu) \, d\mu \quad . \tag{94}$$

We note that to find these results, we used the basis functions

$$\Phi_{\alpha}(\mu) = P_{\alpha}(2\mu - 1) \quad , \tag{95}$$

where $P_{\alpha}(2\mu - 1)$ are the shifted Legendre polynomials, in the F_N approximations given by Eqs. (55) and (64). In addition, we used the multigroup version of a collocation scheme³¹ based on the (positive) discrete spectrum and the zeros of a Chebyshev polynomial of the second kind shifted to (0,1), namely,

$$\xi_{\beta} = \nu_{\beta}, \quad \beta = 1, 2, \dots, \aleph \quad , \tag{96a}$$

and

 μ

$$\xi_{\beta} = \frac{1}{2} \left[1 + \cos\left(\frac{\beta - \aleph}{N + 2 - k_1} \pi\right) \right],$$

$$\beta = \aleph + 1, \aleph + 2, \dots, \aleph + N + 1 - k_1, \qquad (96b)$$

to define the linear systems of Eqs. (63) and (65). We note that these systems were solved with subroutines DGECO and DGESL from the LINPACK package.³²

 $\tau/\tau_0 = 0.0$

To provide a more extensive set of results that can be useful for benchmarking purposes, we also list in Tables III through VIII our F_N results for the group angular fluxes, thought to be accurate to within ± 1 in the last reported figure. While the results in Tables I and II were obtained with N = 149, the results in Tables III to VIII are based on a much higher value of N (N = 549) due to the slow convergence rate of the boundary angular fluxes for $|\mu| \rightarrow 0$ that is typical of the F_N method (and also of the spherical-harmonics method).

As a second (and more challenging) test problem, we consider a calculation that is of particular interest for reactor-shield design, as discussed in detail by Selph.³³ A 100-cm-thick concrete slab is irradiated on the surface z = 0 by a normally incident, uniform beam of thermal neutrons in a specified energy group. The group structure used for this problem consists of 42 thermal groups in the energy range from 0 to 4 eV, and so the boundary conditions expressed by Eqs. (4) are given in this case by

$$\Psi(0,\mu) = \mathbf{F}\delta(\mu - \mu_0) \tag{97a}$$

and

$$\Psi(\tau_0, -\mu) = \mathbf{0} \tag{97b}$$

 $\tau / \tau_0 = 1.0$

for $\mu \in (0,1]$. Here $\mu_0 = 1.0$ is the cosine of the angle of incidence and the vector **F** has components $F_i = \delta_{i,i}$ for

 $\tau / \tau_0 = 0.75$

TABLE III The Exit and Interior Angular Fluxes for Group 1

 $\tau / \tau_0 = 0.5$

 $\tau / \tau_0 = 0.25$

-1.0 $2.6054E - 2^{a}$ 4.0455E - 61.2072E-9 3.6236E-13 2.7698E - 2-0.95.1802E-6 1.5505E-9 4.6545E-13 -0.83.2092E-2 6.2324E-6 1.8679E-9 5.6075E-13 7.2863E-6 -0.73.9697E-2 2.1846E-9 6.5582E-13 -0.65.1100E - 28.4424E - 62.5307E-9 7.5973E-13 -0.56.7080E-2 9.8228E-6 2.9429E-9 8.8346E-13 -0.48.8703E-2 1.1577E-5 3.4659E-9 1.0405E-12 -0.31.1754E-1 1.3889E-5 4.1551E-9 1.2473E-12 -0.21.5612E-1 1.6991E-5 5.0798E-9 1.5249E-12 2.0958E-1 -0.12.1175E-5 6.3278E-9 1.8995E-12 -0.03.0161E-1 2.6818E-5 8.0122E-9 2.4051E-12 0.0 2.6818E-5 8.0122E-9 2.4051E-12 6.0808E-16 0.1 3.4416E-5 1.0281E-8 3.0862E-12 8.5506E-16 0.2 4.4628E-5 4.0022E-12 1.1500E-15 1.3332E-8 0.3 5.8357E-5 1.5335E-15 1.7436E-8 5.2341E-12 0.4 7.6870E-5 2.2972E-8 6.8959E-12 2.0424E-15 0.5 1.0201E-43.0489E-8 9.1525E-12 2.7273E-15 0.6 1.3655E-4 4.0815E-8 1.2252E-11 3.6634E-15 0.7 1.8494E - 45.5255E-8 1.6587E-11 4.9687E-15 0.8 2.5456E - 47.5996E-8 2.2813E-11 6.8405E-15 3.5769E-4 0.91.0701E-7 3.2121E-11 9.6365E-15 1.0 5.1351E-4 1.5620E-7 4.6917E-11 1.4079E-14

^aRead as 2.6054×10^{-2} .

μ	$\tau/\tau_0=0.0$	$\tau/\tau_0=0.25$	$\tau/ au_0 = 0.5$	$\tau/\tau_0=0.75$	$\tau/\tau_0=1.0$	
-1.0	1.3106E-1 ^a	1.1532E-2	6.0646E-4	3.1638E-5		
-0.9	1.5168E-1	1.1986E-2	6.3038E-4	3.2901E-5		
-0.8	1.7234E-1	1.2469E-2	6.5578E-4	3.4241E-5		
-0.7	1.9295E-1	1.2983E-2	6.8279E-4	3.5664E-5		
-0.6	2.1336E-1	1.3531E-2	7.1152E-4	3.7178E-5		
-0.5	2.3339E-1	1.4116E-2	7.4214E-4	3.8790E-5		
-0.4	2.5275E-1	1.4739E-2	7.7477E-4	4.0507E-5		
-0.3	2.7103E-1	1.5406E-2	8.0960E-4	4.2338E-5		
-0.2	2.8754E-1	1.6119E-2	8.4680E-4	4.4294E-5		
-0.1	3.0102E-1	1.6881E-2	8.8657E-4	4.6384E-5		
-0.0	3.0752E-1	1.7698E-2	9.2914E-4	4.8621E-5		
$\begin{array}{c} 0.0 \\ 0.1 \\ 0.2 \\ 0.3 \\ 0.4 \\ 0.5 \end{array}$		1.7698E-2 1.8574E-2 1.9514E-2 2.0524E-2 2.1610E-2 2.2780E-2	9.2914E-4 9.7475E-4 1.0237E-3 1.0762E-3 1.1326E-3 1.1934E-3	4.8621E-5 5.1016E-5 5.3584E-5 5.6341E-5 5.9304E-5 6.2492E-5	6.0594E-7 8.4821E-7 1.0674E-6 1.2889E-6 1.5165E-6 1.7520E-6	
0.6		2.4042E-2	1.2589E-3	6.5928E-5	1.9969E-6	
0.7		2.5404E-2	1.3295E-3	6.9634E-5	2.2525E-6	
0.8		2.6877E-2	1.4058E-3	7.3639E-5	2.5205E-6	
0.9		2.8470E-2	1.4885E-3	7.7974E-5	2.8023E-6	
1.0		3.0193E-2	1.5781E-3	8.2672E-5	3.1000E-6	

TABLE IV

The Exit and Interior Angular Fluxes for Group 2

^aRead as 1.3106×10^{-1} .

TABLE V

The Exit and Interior Angular Fluxes for Group 3

μ	$\tau/\tau_0=0.0$	$\tau/ au_0 = 0.25$	$\tau/\tau_0 = 0.5$	$\tau/\tau_0=0.75$	$\tau/\tau_0=1.0$
$ \begin{array}{r} -1.0 \\ -0.9 \\ -0.8 \\ -0.7 \\ -0.6 \\ -0.5 \\ -0.4 \\ -0.3 \\ -0.2 \\ -0.1 \\ \end{array} $	$\begin{array}{c} 3.7927E-1^{a}\\ 3.6616E-1\\ 3.5179E-1\\ 3.3607E-1\\ 3.1888E-1\\ 3.0006E-1\\ 2.7942E-1\\ 2.5667E-1\\ 2.3131E-1\\ 2.0223E-1\\ \end{array}$	8.0486E-2 8.1552E-2 8.2641E-2 8.3753E-2 8.4890E-2 8.6052E-2 8.7240E-2 8.8454E-2 8.9694E-2 9.0962E-2	4.2459E-3 4.3026E-3 4.3604E-3 4.4196E-3 4.4801E-3 4.5420E-3 4.6052E-3 4.6699E-3 4.7361E-3 4.8037E-3	2.2205E-4 2.2502E-4 2.2807E-4 2.3118E-4 2.3436E-4 2.3761E-4 2.4094E-4 2.4434E-4 2.4781E-4 2.5137E-4	
$\begin{array}{c} -0.0 \\ 0.0 \\ 0.1 \\ 0.2 \\ 0.3 \\ 0.4 \\ 0.5 \\ 0.6 \\ 0.7 \\ 0.8 \\ 0.9 \\ 1.0 \end{array}$	1.6306E-1	9.2258E-2 9.2258E-2 9.3582E-2 9.4936E-2 9.6320E-2 9.7734E-2 9.9180E-2 1.0066E-1 1.0217E-1 1.0371E-1 1.0529E-1 1.0691E-1	4.8729E-3 4.8729E-3 4.9437E-3 5.0161E-3 5.0901E-3 5.1659E-3 5.2435E-3 5.3228E-3 5.4041E-3 5.4041E-3 5.4873E-3 5.5725E-3 5.6597E-3	2.5500E-4 2.5500E-4 2.5872E-4 2.6252E-4 2.6641E-4 2.7039E-4 2.7446E-4 2.7863E-4 2.8290E-4 2.8727E-4 2.9174E-4 2.9632E-4	2.1726E-6 2.7220E-6 3.1685E-6 3.5887E-6 3.9954E-6 4.3942E-6 4.7881E-6 5.1790E-6 5.5683E-6 5.9571E-6 6.3464E-6

^aRead as 3.7927×10^{-1} .

GARCIA and SIEWERT

UAKC	JA anu	SIEW	EUI

	The Exit and Interior Angular Fluxes for Group 4					
μ	$\tau/\tau_0=0.0$	$\tau/\tau_0=0.25$	$\tau/ au_0 = 0.5$	$ au/ au_0 = 0.75$	$\tau/\tau_0=1.0$	
$ \begin{array}{c} -1.0 \\ -0.9 \\ -0.8 \\ -0.7 \\ -0.6 \\ -0.5 \\ -0.4 \\ -0.3 \\ -0.2 \\ -0.1 \\ \end{array} $	3.9999E-2 ^a 3.8379E-2 3.6692E-2 3.4932E-2 3.3089E-2 3.1151E-2 2.9099E-2 2.6906E-2 2.4519E-2 2 1823E-2	1.2279E-2 1.2360E-2 1.2442E-2 1.2525E-2 1.2609E-2 1.2693E-2 1.2778E-2 1.2865E-2 1.2951E-2 1.3039E-2	6.4813E-4 6.5247E-4 6.5684E-4 6.6126E-4 6.6573E-4 6.7023E-4 6.7478E-4 6.7938E-4 6.8402E-4 6.8870E-4	3.3907E-5 3.4135E-5 3.4365E-5 3.4597E-5 3.4832E-5 3.5069E-5 3.5308E-5 3.5549E-5 3.5793E-5 3.6039E-5		
$ \begin{array}{c} 0.1 \\ -0.0 \\ 0.0 \\ 0.1 \\ 0.2 \\ 0.3 \\ 0.4 \\ 0.5 \end{array} $	1.8190E-2	1.3037E -2 1.3127E-2 1.3217E-2 1.3217E-2 1.3307E-2 1.3397E-2 1.3489E-2 1.3582E-2	6.9343E-4 6.9343E-4 6.9820E-4 7.0302E-4 7.0789E-4 7.1280E-4 7.1776E-4	3.6288E-5 3.6288E-5 3.6538E-5 3.6791E-5 3.7047E-5 3.7305E-5 3.7565E-5	2.5448E-7 3.0580E-7 3.4488E-7 3.8022E-7 4.1338E-7 4.4505E-7	
0.6 0.7 0.8 0.9 1.0		1.3675E-2 1.3769E-2 1.3864E-2 1.3959E-2 1.4056E-2	7.2276E-4 7.2781E-4 7.3291E-4 7.3806E-4 7.4325E-4	3.7828E-5 3.8094E-5 3.8361E-5 3.8632E-5 3.8905E-5	4.7564E-7 5.0538E-7 5.3446E-7 5.6301E-7 5.9112E-7	

TABLE VI

The Exit and Interior Angular Fluxes for Group 4

^aRead as 3.9999×10^{-2} .

TABLE VII

The Exit and Interior Angular Fluxes for Group 5

μ	$\tau/\tau_0=0.0$	$\tau/\tau_0=0.25$	$\tau/\tau_0 = 0.5$	$\tau/\tau_0=0.75$	$\tau/\tau_0=1.0$
$ \begin{array}{c c} -1.0 \\ -0.9 \\ -0.8 \\ -0.7 \\ -0.6 \end{array} $	7.5700E-4 ^a 7.2801E-4 6.9855E-4 6.6851E-4 6.3776E-4	2.9513E-4 2.9619E-4 2.9724E-4 2.9829E-4 2.9933E-4	1.5583E-5 1.5639E-5 1.5695E-5 1.5750E-5 1.5806E-5	8.1534E-7 8.1829E-7 8.2122E-7 8.2415E-7 8.2706E-7	
$ \begin{array}{c} -0.5 \\ -0.4 \\ -0.3 \\ -0.2 \\ -0.1 \\ -0.0 \end{array} $	6.0611E-4 5.7326E-4 5.3876E-4 5.0182E-4 4.6066E-4 4.0624E-4	3.0037E-4 3.0140E-4 3.0243E-4 3.0345E-4 3.0447E-4 3.0548E-4	1.5861E-5 1.5916E-5 1.5971E-5 1.6026E-5 1.6080E-5 1.6134E-5	8.2997E-7 8.3286E-7 8.3574E-7 8.3861E-7 8.4147E-7 8.4432E-7	
0.0 0.1 0.2 0.3 0.4 0.5		3.0548E-4 3.0649E-4 3.0749E-4 3.0849E-4 3.0948E-4 3.1046E-4	1.6134E-5 1.6188E-5 1.6242E-5 1.6295E-5 1.6348E-5 1.6401E-5	8.4432E-7 8.4715E-7 8.4996E-7 8.5276E-7 8.5554E-7 8.5554E-7 8.5831E-7	5.3326E-9 6.0798E-9 6.6427E-9 7.1420E-9 7.6007E-9 8.0293E-9
0.6 0.7 0.8 0.9 1.0		3.1143E-4 3.1240E-4 3.1336E-4 3.1431E-4 3.1526E-4	1.6453E-5 1.6505E-5 1.6557E-5 1.6608E-5 1.6659E-5	8.6106E-7 8.6380E-7 8.6651E-7 8.6921E-7 8.7188E-7	8.4338E-9 8.8178E-9 9.1843E-9 9.5351E-9 9.8718E-9

^aRead as 7.5700×10^{-4} .

μ	$\tau/\tau_0=0.0$	$\tau/\tau_0=0.25$	$\tau/ au_0 = 0.5$	$ au/ au_0 = 0.75$	$\tau/\tau_0=1.0$
-1.0 -0.9 -0.8 -0.7 -0.6	8.6694E-6 ^a 8.3527E-6 8.0550E-6 7.7750E-6 7.5114E-6	3.5729E-6 3.5810E-6 3.5887E-6 3.5960E-6 3.6030E-6	1.8864E-7 1.8906E-7 1.8946E-7 1.8984E-7 1.9021E-7	9.8709E-9 9.8930E-9 9.9141E-9 9.9343E-9 9.9535E-9	
$ \begin{array}{r} -0.5 \\ -0.4 \\ -0.3 \\ -0.2 \\ -0.1 \\ -0.0 \end{array} $	7.2624E-6 7.0255E-6 6.7972E-6 6.5717E-6 6.3378E-6 6.0447E-6	3.6096E-6 3.6158E-6 3.6216E-6 3.6270E-6 3.6320E-6 3.6366E-6	1.9056E-7 1.9088E-7 1.9119E-7 1.9148E-7 1.9174E-7 1.9198E-7	9.9716E-9 9.9887E-9 1.0005E-8 1.0020E-8 1.0034E-8 1.0047E-8	
$\begin{array}{c} 0.0 \\ 0.1 \\ 0.2 \\ 0.3 \\ 0.4 \\ 0.5 \end{array}$		3.6366E-6 3.6408E-6 3.6446E-6 3.6479E-6 3.6508E-6 3.6532E-6	1.9198E-7 1.9221E-7 1.9241E-7 1.9259E-7 1.9274E-7 1.9288E-7	1.0047E-8 1.0058E-8 1.0069E-8 1.0078E-8 1.0087E-8 1.0094E-8	6.8266E-11 7.2060E-11 7.4766E-11 7.7003E-11 7.8901E-11 8.0520E-11
0.6 0.7 0.8 0.9 1.0		3.6552E-6 3.6567E-6 3.6578E-6 3.6583E-6 3.6584E-6	1.9299E-7 1.9307E-7 1.9314E-7 1.9318E-7 1.9319E-7	1.0099E-8 1.0104E-8 1.0107E-8 1.0109E-8 1.0110E-8	8.1897E-11 8.3057E-11 8.4020E-11 8.4800E-11 8.5408E-11

TABLE VIII The Exit and Interior Angular Fluxes for Group 6

^aRead as 8.6694×10^{-6} .

i = 1, 2, ..., 42, with $1 \le j \le 42$ denoting the group of incidence. The quantities of interest in this problem are the double-differential, thermal-neutron albedos $\alpha_{i,j}(\mu, \mu_0)$, defined as

$$\alpha_{i,j}(\mu,\mu_0) = \frac{J_i^-(\mu)}{J_i^+(\mu_0)} , \qquad (98)$$

for i = 1, 2, ..., 42 and $\mu \in (0,1]$. Here $J_i^-(\mu) = \mu \psi_i(0, -\mu)$ and $J_j^+(\mu_0) = \mu_0 F_j$.

A few words with regard to the group constants used in our calculation are in order. We have computed the required macroscopic total cross sections (and transfer matrices) by summing up the products of the microscopic total cross sections (and the transfer matrices), as given in the WIMKAL-88 library³⁴ for the constituents of ordinary concrete, with their respective number densities, taken from Ref. 35 and reproduced in Table IX. The numbers so obtained were rounded to four significant figures. The WIMKAL-88 library contains neutronreaction data in the WIMS 69-group structure for 132 materials and is distributed by the International Atomic Energy Agency Nuclear Data Section. In spite of its widespread use, which was the motivation for our selection of this multigroup library, the transfer matrices given in the WIMKAL-88 library are limited to linearly aniso-

TABLE IX

Concrete Composition Used for the 42-Group Problem

Element	Number Density (10 ²¹ atom/cm ³)	Material Identification Number in WIMKAL-88
H	13.75	1 001
O	45.87	8 016
Al	1.743	13 027
Si	20.15	14 000

tropic scattering (L = 1). We also note that since the microscopic total cross sections are not given directly in the WIMKAL-88 library, these constants were computed by adding the absorption cross sections to the scattering cross sections obtained from the l = 0 transfer matrices. In addition, we note that the l = 1 transfer matrices given in the WIMKAL-88 library were multiplied by 3 to take into account the (2l + 1) factor built into our definition of the transfer matrices. The 42-group structure adopted in our calculation is the WIMS thermal-group structure used by the WIMKAL-88 library. Group 1 (3.3 to 4.0 eV) is the highest in energy, and group 42 (0.0 to 0.005 eV) is the lowest. The energy boundaries of

TABLE X

The Thermal-Neutron Albedos $\alpha_{i,j}(\mu,\mu_0)$ with j = 4 and $\mu_0 = 1.0$ for a 100-cm-thick Concrete Slab

i	$\mu = 0.2$	$\mu = 0.4$	$\mu = 0.6$	$\mu = 0.8$	$\mu = 1.0$	i	$\mu = 0.2$	$\mu = 0.4$	$\mu = 0.6$	$\mu = 0.8$	$\mu = 1.0$
1	8.998E-10 ^a	2.050E-9	3.225E-9	4.332E-9	5.337E-9	22	3.267E-3	6.793E-3	1.001E-2	1.273E-2	1.493E-2
2	4.426E-7	9.580E-7	1.427E-6	1.822E-6	2.143E-6	23	2.319E-3	4.867E-3	7.230E-3	9.273E-3	1.097E-2
3	2.180E-4	3.489E-4	4.061E-4	4.062E-4	3.625E-4	24	2.457E-3	5.196E-3	7.774E-3	1.004E-2	1.195E-2
4	3.096E-2	4.290E-2	4.098E-2	2.904E-2	9.708E-3	25	3.995E-3	8.534E-3	1.289E-2	1.679E-2	2.017E-2
5	1.794E-2	2.990E-2	3.680E-2	3.978E-2	3.975E-2	26	4.489E-3	9.720E-3	1.487E-2	1.961E-2	2.383E-2
6	1.017E-2	1.762E-2	2.221E-2	2.442E-2	2.470E-2	27	7.230E-3	1.596E-2	2.487E-2	3.338E-2	4.126E-2
7	1.530E-3	2.533E-3	2.988E-3	2.984E-3	2.609E-3	28	1.001E-2	2.271E-2	3.634E-2	5.003E-2	6.333E-2
8	1.423E-3	2.340E-3	2.730E-3	2.674E-3	2.258E-3	29	1.641E-2	3.836E-2	6.318E-2	8.935E-2	1.159E-1
9	1.383E-3	2.269E-3	2.628E-3	2.541E-3	2.092E-3	30	1.306E-2	3.113E-2	5.221E-2	7.506E-2	9.884E-2
10	1.358E-3	2.228E-3	2.574E-3	2.474E-3	2.010E-3	31	1.131E-2	2.721E-2	4.603E-2	6.670E-2	8.845E-2
11	1.291E-3	2.125E-3	2.461E-3	2.369E-3	1.928E-3	32	9.403E-3	2.272E-2	3.862E-2	5.619E-2	7.481E-2
12	1.236E-3	2.043E-3	2.373E-3	2.292E-3	1.871E-3	33	9.496E-3	2.301E-2	3.920E-2	5.720E-2	7.634E-2
13	1.232E-3	2.046E-3	2.388E-3	2.319E-3	1.912E-3	34	1.052E-2	2.552E-2	4.358E-2	6.371E-2	8.520E-2
14	1.138E-3	1.902E-3	2.237E-3	2.194E-3	1.838E-3	35	9.832E-3	2.387E-2	4.080E-2	5.973E-2	8.000E-2
15	2.073E-3	3.490E-3	4.137E-3	4.102E-3	3.497E-3	36	7.232E-3	1.755E-2	3.000E-2	4.396E-2	5.894E-2
16	3.196E-3	5.485E-3	6.649E-3	6.797E-3	6.086E-3	37	7.194E-3	1.743E-2	2.980E-2	4.367E-2	5.860E-2
17	3.896E-3	6.841E-3	8.510E-3	9.001E-3	8.481E-3	38	6.902E-3	1.668E-2	2.848E-2	4.175E-2	5.604E-2
18	9.562E-3	1.747E-2	2.269E-2	2.531E-2	2.561E-2	39	6.276E-3	1.510E-2	2.574E-2	3.770E-2	5.062E-2
19	9.103E-3	1.747E-2	2.385E-2	2.812E-2	3.043E-2	40	5.204E-3	1.243E-2	2.111E-2	3.089E-2	4.147E-2
20	8.643E-3	1.725E-2	2.447E-2	3.001E-2	3.391E-2	41	3.552E-3	8.370E-3	1.412E-2	2.058E-2	2.761E-2
21	4.980E-3	1.021E-2	1.484E-2	1.864E-2	2.158E-2	42	1.297E-3	2.965E-3	4.917E-3	7.101E-3	9.480E-3

^aRead as 8.998×10^{-10} .

all groups are given in Ref. 34. With this description, we hope anyone interested in using our second sample problem in benchmarking work can use the WIMKAL-88 library and the number densities given in Table IX to reproduce our input cross-section set. Thus, to save space, we do not tabulate the required group constants here.

We list in Table X our F_{129} results for the thermalneutron albedos when the group of incidence is group 4 (1.5 to 2.1 eV). These results are thought to be accurate to within ± 1 in the last figure given. Because of the large size of the linear system to be solved for the unknown vectors $\{\mathbf{a}_{\alpha}\}$ and $\{\mathbf{b}_{\alpha}\}$ in this case, we have used the idea³⁶ of decoupling this system into two smaller systems (one for the \mathbf{a}_{α} vectors and another for the \mathbf{b}_{α} vectors) that are half the size of the original system. Since the \mathbf{a}_{α} vectors are sufficient to establish the desired albedos, only the smaller system for the \mathbf{a}_{α} vectors was solved. In addition, a slightly modified version of the projection scheme used to obtain the square linear systems expressed by Eqs. (63) and (65) in Sec. III was found to speed up convergence for this problem as N was increased: the special projection matrix \mathbf{P}_{β} for $\beta = \aleph + N + 1 - k_1$ was associated with the collocation point closest to 0, instead of the collocation point closest to 1. We should also mention that we have observed the occurrence of negative angular fluxes for other cases (other groups of incidence) that we tried. This phenomenon has been observed before in slowing-down calculations³⁷ and is due

to the premature truncation of the Legendre polynomial expansion of the scattering law (recall that L = 1 in the WIMKAL-88 library).

Finally, we report in Table XI the execution (CPU) times of our calculations on a Silicon Graphics Power Challenge machine (R8000 RISC processor, 300 Mflops, 384 Mbytes of RAM), for several orders of the F_N approximation. Our code was written in FORTRAN and compiled with the F77 compiler, optimization level OPT = 2. Typically, in the N = 549 run for the first test problem, ~25% of the CPU time was spent in the part of

TABLE XI

Execution Times on a Silicon Graphics Power Challenge Machine*

Ν	Six-Group Problem	42-Group Problem
39	0.6	18
69	1.9	97
99	4.4	283
129	8.3	619
299	69	
399	148	
549	350	

*The execution times are in minutes.

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the code that computes the matrix elements and righthand sides required to define the linear systems expressed by Eqs. (63) and (65), and \sim 75% was spent in the part that factorizes and solves these linear systems. In the N = 129 run for the second test problem, these percentages were $\sim 2\%$ and 98%, respectively. We note that the time required to compute the discrete eigenvalues has not been included in Table XI since this calculation does not depend on the order of the F_N approximation, and therefore it can be performed only once for each problem. Using the procedure described in Sec. IV with P_{19} as our initial P_N approximation for computing the discrete eigenvalues and repeating the calculation with ${\cal N}$ increased by 10 as many times as necessary for convergence, we found discrete eigenvalues accurate to 12 significant figures with $\mathcal{N} = 39$ for the six-group problem and $\mathcal{N} = 99$ for the 42-group problem. The CPU times were 0.5 s and 180 min, respectively.

VI. CONCLUDING REMARKS

In this work we have developed the basic theory and computational methods required to apply the F_N method to the important class of fully coupled multigroup transport problems in plane geometry. We consider that the excellent results obtained with the method for the two test problems of Sec. V is an indication that the method has the potential to be used for solving well this class of problems.

As our main effort in this work was directed toward obtaining very good accuracy for all quantities involved in the calculation, we have not devoted too much work to making the calculation especially efficient in regard to computer-time considerations. Nevertheless, as we have found that most of the computer time is spent by our code in the solution of the linear systems for the coefficients of the F_N approximations, and we have used a very efficient package for this purpose,³² we believe there is not much room left for improvements in this direction.

Finally, having demonstrated that the F_N method works well for the considered problems, we can see the way to enlarge the class of solved problems so as to include multislab geometry, internal (inhomogeneous) sources, azimuthal dependence, and multiplying media.

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