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A Response Matrix Method for Multigroup Slab-geometry Discrete Ordinates Problems in Non-multiplying Media

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Abstract - *Presented here is a Response Matrix method for the solution of multigroup slab-geometry discrete ordinates (S_N) problems with anisotropic scattering in non-multiplying media. This method generates numerical solutions that are completely free from spatial truncation errors and originates from the local general solution within a homogenized layer of the slab that is obtained from a spectral analysis of the S_N equations. Numerical results to two test problems are given to illustrate the accuracy of the present method.*

I. INTRODUCTION

Described here is an analytical numerical method that we refer to as response matrix (RM) method for slab-geometry discrete ordinates (S_N) problems in non-multiplying media using the multigoup model with an arbitrary number of energy groups (G). The present RM method with the one-node block inversion (NBI) iterative scheme generates numerical results for the group node-edge angular fluxes that are absolutely free of spatial truncation errors, as they coincide with the numerical results obtained from the analytical solution of the given S_N problem, apart from finite arithmetic considerations. A companion method, named the spectral Green's function (SGF) method [1], also generates numerical solutions that are free from spatial truncation errors; nevertheless the SGF method makes use of the discretized S_N spatial balance equations [2] together with the SGF auxiliary equations, wherein $N^2 \times G^2$ parameters need be determined for each discretization node of the spatial grid set up on the domain. As N and G increase, computer storage and computation of these parameters may become cumbersome, even with modern computers.

In the next section we describe the offered RM method. In section III we present numerical results to two model problems and we conclude in section IV by offering a brief dicussion.

II. THE RM METHOD

To describe the RM method, we first consider a spatial grid wherein each discretization node Γ_i, $i = 1 : I$, has width h_i, constant group macroscopic cross sections and uniform and isotropic interior source (Fig. 1). The RM method has

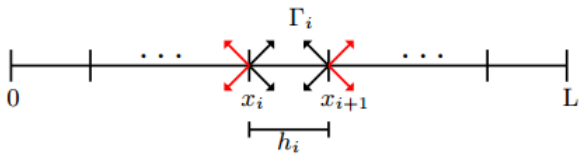

Fig. 1. Discretization node Γ_i.

three essential ingredients: (i) a complete set of $N \times G$ basis functions is determined by a spectral analysis to span the local solution space of the S_N equations in each spatial node; (ii) by using the group node interior source and the group incoming fluxes at the node edges in the local general solution, we determine the response matrix to evaluate the group node-edge outgoing fluxes; (iii) by using the response matrix, the NBI iterative scheme is implemented to evaluate the group node-edge exiting fluxes by using the interior source and the most recent estimates for the group node-edge incoming fluxes. Next we briefly describe these three ingredients.

To begin, we consider the multigoup S_N equations for $x \in \Gamma_i$, $i = 1 : I$

$$\mu_m \frac{d}{dx}\psi_{m,g}(x) + \Sigma_{T_{g,i}}\psi_{m,g}(x) = \frac{1}{2}\sum_{g'=1}^{G}\sum_{n=1}^{N}\Sigma_{S_{g'\to g,i}}\psi_{g',n}(x)\omega_n + Q_{g,i}, \quad (1)$$

where $g = 1 : G$ and $m = 1 : N$. The notation is standard [2]: $\psi_{m,g}(x)$ is the flux of particles migrating in direction μ_m in energy group g; $\Sigma_{T_{g,i}}$ is the total macroscopic cross section of node Γ_i in energy group g; $\Sigma_{S_{g'\to g,i}}$ is the macroscopic differential scattering cross section from energy group g' to group g of node Γ_i; $Q_{g,i}$ is the node-interior isotropic source emitting particles in energy group g; and ω_n is the weight of the angular direction μ_n in the S_N quadrature set.

Now we write the local general solution of Eq. (1) as

$$\psi_{m,g}(x) = \psi^h_{m,g}(x) + \psi^p_{m,g}(x), \quad x \in \Gamma_i, \quad (2)$$

where the superscript p denotes the particular solution and the superscript h indicates the homogeneous solution. For $Q_{g,i} = 0$, we seek a basis function of the form

$$\psi^h_{m,g}(x) = a_{m,g}(\nu)f_\nu(x), \quad m = 1 : N, \quad g = 1 : G, \quad (3)$$

where we have defined

$$f_\nu(x) = \begin{cases} e^{-\frac{(x-x_i)}{\nu}} & se \quad \nu > 0, \\ e^{-\frac{(x-x_{i+1})}{\nu}} & se \quad \nu < 0. \end{cases} \quad (4)$$

By substituting Eq. (3) into Eq. (1), after some algebraic manipulation, we obtain

$$\sum_{n=1}^{N}\sum_{g'=1}^{G}\left(\frac{\Sigma_{t_{g,i}}}{\mu}\delta_{m,n}\delta_{g,g'}-\frac{\Sigma_{s_{g'\to g,i}}\omega_n}{2\mu_m}\right)a_{n,g'}(\nu)=\frac{1}{\nu}a_{m,g}(\nu), \quad (5)$$

which, in matrix formulation, is an eigenvalue problem, whose solution are $N\times G$ eigenvalues $1/\nu$ and $N\times G$ linearly independent eigenvectors of dimension equal to $N\times G$.

Furthermore for constant isotropic node interior source $Q_{g,i}$, the particular solution $\psi^p_{g,i}$ is obtained by solving the linear system

$$\sum_{n=1}^{N}\sum_{g'=1}^{G}\left(\Sigma_{t_{g,i}}\delta_{m,n}\delta_{g,g'}-\frac{1}{2}\Sigma_{s_{g'\to g,i}}\omega_n\right)\psi^p_{g,i}=Q_{g,i}. \quad (6)$$

Therefore, the expression of the local general solution is

$$\psi_{m,g}(x)=\sum_{l=1}^{NG}\alpha_l a_{m,g}(\nu_l)f_{\nu_l}(x)+\psi^p_{g,i}, \quad x\in\Gamma_i, \quad i=1:I. \quad (7)$$

Here we note that the entries of the particular solution column matrix is constant for all angular directions in each energy group since we have assumed uniform and isotropic group interior source. Therefore, in matrix form, Eq. (7) appears as

$$\boldsymbol{\Psi}(x)=\boldsymbol{A}\boldsymbol{Diag}(f(x))\boldsymbol{\alpha}+\boldsymbol{\Psi}^p_i. \quad (8)$$

Here $\boldsymbol{\Psi}(x)$ is the column matrix whose entries are the group angular fluxes; $\boldsymbol{A}$ is a square matrix of order $N\times G$, whose columns are the eigenvectors; $\boldsymbol{Diag}(f(x))$ is a diagonal matrix of order $N\times G$; $\boldsymbol{\alpha}$ is a column matrix whose entries are the $N\times G$ constants of the linear combination of the basis functions; and $\boldsymbol{\Psi}^p_i$ is the particular solution in Γ_i. In order to calculate $\boldsymbol{\alpha}$, we use the incoming group node-edge fluxes at $x=x_i$ ($\mu_m>0$) and $x=x_{i+1}$ ($\mu_m<0$), as illustrated in Fig. 1. That is,

$$\boldsymbol{\alpha}=\boldsymbol{M}^{-1}(\boldsymbol{\Psi}^{in}-\boldsymbol{\Psi}^p_i), \quad (9)$$

where we have defined matrix $\boldsymbol{M}$ as

$$\boldsymbol{M}=\boldsymbol{A}\begin{bmatrix}\boldsymbol{Diag}(f(x_i)) & 0\\ 0 & \boldsymbol{Diag}(f(x_{i+1}))\end{bmatrix}. \quad (10)$$

By substituting Eq. (10) into Eq. (8), we determine an expression for the outgoing group node-edge fluxes

$$\boldsymbol{\Psi}^{out}=\boldsymbol{R}\boldsymbol{\Psi}^{in}+(\boldsymbol{I}-\boldsymbol{R})\boldsymbol{\Psi}^p_i. \quad (11)$$

Here we have defined the response matrix

$$\boldsymbol{R}=\boldsymbol{A}\begin{bmatrix}\boldsymbol{Diag}(f(x_{i+1})) & 0\\ 0 & \boldsymbol{Diag}(f(x_i))\end{bmatrix}\boldsymbol{M}^{-1}. \quad (12)$$

Equation (11) is the essence of the present RM method. By considering the boundary conditions to the S_N problem, we use Eq. (11) to apply node-block inversions to iteratively converge numerical solutions, which are completely free of spatial truncation errors, regardless of the spatial grid set up on the domain.

At this point we remark that we have considered two algorithms for the NBI iterative scheme: the full NBI scheme and the partial NBI scheme. As with the full NBI iterative scheme, we use the boundary conditions or the most recent estimates for the group incoming node-edge fluxes to evaluate all outgoing node-edge fluxes in all energy groups in node Γ_i, before moving to the next node Γ_{i+1}. The partial NBI scheme uses the boundary conditions or the most recent estimates for the group incoming node-edge fluxes to calculate the exiting node-edge angular fluxes, which constitute the incoming fluxes for the adjacent nodes in the directions of the transport sweeps across the slab: from left to right ($\mu>0$) and from right to left ($\mu<0$).

III. NUMERICAL RESULTS

Now we consider two model problems. Model problem N^o 1 consists of an iron slab, 10 cm thick and with isotropic scattering. To solve this problem, we consider a multigroup Gauss-Legendre S_{16} model with nineteen energy groups (G = 19) and a unit isotropic flux of gamma rays incident at the left boundary (x = 0) only for the first energy group (g = 1). The multigroup macroscopic cross sections for this iron slab are given in [3]. Table I displays the scalar fluxes at the boundaries for three energy groups: g = 1, g = 10 and g = 19 as generated by the fine-mesh diamond difference (DD) method with the source iteration (SI) scheme [2] and by the offered RM method with the partial NBI iterative scheme. In this numerical experiment we used one node for the whole domain with the RM method and a discretization grid composed of 10000 nodes with the DD method, so the relative deviations between the boundary value scalar fluxes for all energy groups did nod exceed 15 ppm (parts per million). We remark that the NBI iterative scheme converged the solution in 3.9 seconds (2 iterations), while the SI scheme converged the fine-mesh results in 62.6 seconds (28 iterations) for a stopping criterion requiring that the relative deviations between two iterates did not exceed 10^{-6}.

[a] Diamond Difference method with the source iteration sheme
[b] Response Matrix with the partial NBI sheme
[c] 4GB RAM, *Intel(R) Core(TM)i7 Q720@1.60GHz*
[d] Read as 5.080x10^{-1}

	DD - SI[a]		RM - Partial NBI[b]	
Iterations	28		2	
Time (s)[c]	62.6		3.9	
Energy group	x=0	x=10	x=0	x=10
1	5.080E-1[d]	7.050E-4	5.080E-1	7.050E-4
10	1.339E-2	1.450E-4	1.339E-2	1.450E-4
19	4.164E-6	6.853E-8	4.164E-6	6.853E-8

TABLE I. Numerical results for the model problem

Model problem N^o 2 is described in [4]. This is a 20-group, 5-region slab with a 10'th order Legendre expasion of the scattering law. This slab is 20 cm thick and has an isotropic incident distribution of radiation only in the first energy group

and only at the left-hand side boundary ($x = 0, \mu_m > 0$). Vacuum boundary conditions apply at $x = 20\ cm$. In addition, the thickness of each layer is defined by $\Delta_r = r + 1$, $r = 1 : 5$. The group cross sections are given in [4] and we used the same stopping criterion as the previous model problem. Table II displays the results for the group albedos

$$Ag = 2 \sum_{n=\frac{N}{2}+1}^{N} |\mu_n| \Psi_{n,g}(0) \omega_n \tag{13}$$

and the group transmission factors

$$Bg = 2 \sum_{n=1}^{\frac{N}{2}} \mu_n \Psi_{n,g}(20) \omega_n, \tag{14}$$

$g = 1 : 20$, which can be found in [4]. We used the S_{64} Gauss-Legendre angular quadrature set [2] to model this problem and generated the results with the present RM method on a spatial grid composed of one discretization node per region. The maximum relative deviations of the RM results with respect to reference results were 0.38% and 0.0083% for Ag and Bg, respectively.

As with the efficiency of the computer codes, we remark tha we implemented both serial and parallel architectures to solve the eigenvalue problem (1280×1280) given in Eq. (5) for each layer of the slab.

For the serial code, the RM method generated the numerical results in $1,582$ seconds and spent 991 seconds to solve the five eigenvalue problems, i.e., roughly 63% of the total running time. For the parallel code, the RM method generated the numerical values for Ag and Bg, $g = 1 : 20$, in 864 seconds, yielding a speed up of 45%, whose running time for the eigenvalue problems were 339 seconds.

IV. DISCUSSION

We have developed the multigroup RM method and have shown that it yields solution with no spatial truncation error. Therefore, one may be able to solve multigroup S_N problems with many fewer spatial cells than standard numerical methods, e.g., the DD method.

We remark that the shifting strategy as given in Eq. (4) is not essential for the spectral analysis; however, due to computational finite arithmetic it is necessary to include it in the algorithm for coarse-mesh calculations with discretization nodes of several group mean free paths in extent, high order angular quadratures and many energy groups.

It is well known that solving eigenvalue problems on a digital computer is no trivial and, above all, it is a very costly task. Therefore, we also implemented a parallel version of the RM code. According to model problem N^{o} 2, that we considered in the previous section, the parallel architecture yielded a speed up of 45% at solving five 1280×1280 eigenvalue problems given in Eq. (5).

The present multigroup RM method can be used to improve the accuracy of standard multigroup nodal methods applied to multidimensional S_N problems in rectangular geometry. Specifically, we propose to use the present multigroup RM method to solve numerically the multigroup one-dimensional transverse-integrated S_N nodal equations that arise in S_N nodal methods, with an approximation for the transverse leakage terms.

[a] Group albedo according to Eq. (13).

[b] Group transmission factor according to Eq. (14).

[c] Read as 5.881×10^{-3}

Energy	Ref. [4]		RM method - S_{64}	
group	Ag[a]	Bg[b]	Ag	Bg
1	5.881E-3[c]	1.045E-2	5.900E-3	1.045E-2
2	2.279E-3	1.999E-4	2.286E-3	1.999E-4
3	1.294E-3	6.901E-5	1.298E-3	6.901E-5
4	8.628E-4	3.539E-5	8.655E-4	3.539E-5
5	8.517E-4	3.535E-5	8.540E-4	3.535E-5
6	4.966E-4	1.490E-5	4.982E-4	1.490E-5
7	3.971E-4	1.072E-5	3.983E-4	1.072E-5
8	3.276E-4	8.086E-6	3.287E-4	8.087E-6
9	2.767E-4	6.320E-6	2.776E-4	6.320E-6
10	2.796E-4	6.127E-6	2.804E-4	6.127E-6
11	2.099E-4	4.184E-6	2.106E-4	4.184E-6
12	1.849E-4	3.489E-6	1.856E-4	3.489E-6
13	1.648E-4	2.955E-6	1.653E-4	2.955E-6
14	1.481E-4	2.533E-6	1.487E-4	2.533E-6
15	1.342E-4	2.195E-6	1.347E-4	2.195E-6
16	1.224E-4	1.920E-6	1.229E-4	1.920E-6
17	1.123E-4	1.693E-6	1.127E-4	1.693E-6
18	1.035E-4	1.503E-6	1.039E-4	1.503E-6
19	9.586E-5	1.343E-6	9.622E-5	1.343E-6
20	8.913E-5	1.206E-6	8.946E-5	1.207E-6

TABLE II. Group albedo and transmission factors.

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