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Spectral Nodal Methodology for Multigroup Slab-Geometry Discrete Ordinates Neutron Transport Problems with Linearly Anisotropic Scattering

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ABSTRACT

In this paper, we propose a numerical methodology for the development of a method of the spectral nodal class that generates numerical solutions free from spatial truncation errors. This method, denominated Spectral Deterministic Method (SDM), is tested as a study of the solutions (spectral analysis) of neutron transport equations in the discrete ordinates (S_N) formulation, in slab geometry, multigroup approximation, with linearly anisotropic scattering, considering a heterogeneous domain with fixed-source. The unknowns in the methodology are the cell-edge, and cell average angular fluxes, the numerical values calculated for these quantities coincide with the analytic solution of the equations. These numerical results are shown and compared with the traditional fine-mesh Diamond Difference (DD) method and the coarse-mesh spectral Green's function (SGF) method to illustrate the method's accuracy and stability. The solution algorithms problem is implemented in a computer simulator made in C++ language, the same that was used to generate the results of the reference work.

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1. INTRODUCTION

One of the key requirements for a nuclear reactor development project is to know the accurate and detailed prediction of the neutron distribution in space and time, as well as its energy dependence on all components of the reactor. This problem is addressed by the neutron transport theory, using the linearized Boltzmann transport equation, which studies the migration of neutrons into the material, and obtains its distribution in space, time, and energy [1,2]. The linearized Boltzmann transport equation is an integrodifferential equation that is used in realistic neutral particle transport calculations, has seven independent variables to describe the average behavior of neutron population. In these calculations, it is necessary to consider an approximation for this equation, in which the energy variable is discretized in contiguous groups, giving rise to the classical multigroup approximation [1,2].

The analytical solution of the linearized multigroup neutron transport equation is complicated except for highly idealized problems. Its exact solution can only be obtained for the less complex problems; for more complex problems, were developed numerical methods. These methods have been developed for obtaining, approximate but accurate solutions to the radiation shield problems, global reactor calculations, and other applications. They allow us to do computer modeling using a probabilistic or deterministic approach [1,2]. Deterministic methods usually use a formulation of discrete ordinates (S_N) [1]. This formulation made a collocation scheme for the angular variables in prescribed directions (discrete ordinates) and used angular quadrature sets for the approximation of the integral source terms to obtain numerical solutions for the problems analyzed.

The deterministic approach to neutron shielding problems (source-fixed) has reached a great interest in recent years. We can cite as an example the MOC [3,4], cf., *Method of Characteristics*, the traditional polynomial methods, [5-6] and spectral nodal methods, e.g., the SGF method [7-8], cf. *spectral Green´s function*, the RM method [9], cf., *Response Matrix*. This fact served as an incentive for the development of new numerical methodologies, considering the coarse-mesh methods, which have great precision in their numerical results with a marked reduction in the execution times of their models.

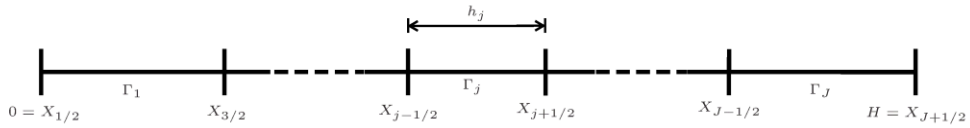
In this paper, we describe and test a new nodal numerical strategy for general multigroup slab-geometry discrete ordinates problems linearly anisotropic scattering and a prescribed interior source. These results are compared with the traditional fine-mesh method Diamond Difference (DD) [1] and the coarse-mesh spectral Green's function (SGF) [7,8] according to the model problem presented in the numerical results section.

In the next section, we present the spectral analysis of the multigroup problems in slab geometry. In Section 3, the multigroup Spectral Deterministic Method (SDM) for deriving the analytical solutions and an iterative method for solving the discretized equations are described. Numerical results are shown in Section 4 and a brief discussion about the results obtained in this paper is given in Section 5.

2. SPECTRAL ANALYSIS OF THE MULTIGROUP SLAB GEOMETRY

Let us consider an arbitrary spatial grid Γ in the domain D, as shown in Figure 1, where each spatial cell Γ_j has a width h_j and constant multigroup macroscopic cross sections.

Figure 1: *Spatial cell* Γ_j *in a one-dimensional domain D with length H*



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Now we consider the multigroup neutron transport equation in the discrete ordinates (S_N) formulation with linearly anisotropic scattering considering the slab geometry, defined in an arbitrary cell Γ_j

$$\mu_m \frac{d}{dx}\psi_{m,g}(x) + \sigma_{Tgj}\psi_{m,g}(x) = \sum_{g'=1}^{G}\left[\frac{\sigma_{S0j}^{g'\to g}}{2}\sum_{n=1}^{N}\psi_{n,g'}(x)\,\omega_n + \frac{3\sigma_{S1j}^{g'\to g}\mu_m}{2}\sum_{n=1}^{N}\psi_{n,g'}(x)\;\mu_n\omega_n\right] + Q_{gj} \quad (1)$$

$$x_{j-1/2} \le x \le x_{j-1/2},\ m = 1:N, g = 1:G\ .$$

Here in the equation system (1), we use the conventional notation [1], where $x \in \Gamma$, G represents the number of energy groups and N is the order of the Gauss-Legendre quadrature set [1], which is used for the solution of the S_N problem in this paper. The value σ_{Tgj} describes the total macroscopic cross section of the g-th group. The $\sigma_{S0j}^{g'\to g}$ and $\sigma_{S1j}^{g'\to g}$ are the zeroth and first-order components of the macroscopic differential scattering cross section from group g' to group g, respectively, and Q_{gj} is the constant isotropic fixed-source in the energy group g. The variable $\psi_{m,g}(x)$ represents the angular flux of particles traveling in the direction of the discrete ordinate μ_m for each group *g* and ω_m is the quadrature weight.

The intra-nodal general solution of the Eq. (1) has the form:

$$\psi_{m,g}(x) = \psi_{m,g}^{h}(x) + \psi_{g}^{p}, \quad (2)$$

the superscript *p* denotes the particular solution with fixed-source Q_{gj} and *h* indicates the homogeneous component of the local general solution, which satisfies the system of Eq. (1). To determine the homogeneous component $\psi_{m,g}^{h}(x)$ we consider the *ansatz* [10]

$$\psi_{m,g}^{h}(x) = a_{m,g}(\vartheta)\exp\left(\frac{-(x - x_{j-1/2})}{\vartheta}\right), x \in \Gamma_j, m = 1:N, g = 1:G, \quad (3)$$

where $x_{j-1/2}$ represents the left boundary of the cell Γ_j. Substituting Eq. (3) in the homogeneous part of Eq. (1), and making the source Q_{gj} equal to zero, after a little algebra we obtain the eigenvalue problem [10]

$$\frac{\sigma_{Tgj}}{\mu_m} a_{m,g}(\vartheta_\ell) - \sum_{g'=1}^{G}\left\{\frac{1}{2\mu_m}\sigma_{s0j}^{g'\to g}\sum_{n=1}^{N} a_{n,g'}(\vartheta_\ell)\omega_n + \frac{3}{2}\sigma_{s1j}^{g'\to g}\sum_{n=1}^{N} a_{n,g'}(\vartheta_\ell)\omega_n\,\mu_n\right\} = \frac{1}{\vartheta_\ell} a_{m,g}(\vartheta_\ell), \qquad (4)$$
$$m = 1:N, \ell = 1:NG, g = 1:G.$$

The Eq. (4) constitutes a homogeneous system of GN linear equations with the unknown eigenvectors $a_{m,g}(\vartheta_\ell)$ which have GN components that correspond to the GN eigenvalues ϑ_ℓ. Due to the symmetry of the Gauss-Legendre quadrature sets with even N, the eigenvalues ϑ_ℓ will appear in pairs [7,8]. For fixed-source problems, which are the topic of the present work, these GN eigenvalues are real numbers [7,8]. This problem can be written in a matrix compact notation as

$$A\vec{a}(\vartheta) = \frac{1}{\vartheta}\vec{a}(\vartheta), \qquad (5)$$

where A is a GN x GN real square matrix. The particular solution ψ_g^p, with isotropic fixed-source Q_{gj}, takes the form

$$\sum_{g'=1}^{G}\left(\sigma_{Tgj}\,\delta_{g'\to g} - \sigma_{S0j}^{g'\to g}\right)\psi_{g'}^{p} = Q_{gj},\ g = 1:G. \qquad (6)$$

Where δ is the Kronecker delta. The particular solution ψ_g^p for the case analyzed in this paper, do not depends on the direction of the discrete ordinate μ_m, because the source Q_{gj} is considered isotropic. Hence, the general solution of the S_N equations (1) for G energy groups in Γ_j represented by the Eq. (2), can be written in the following form:

$$\psi_{m,g}(x)=\sum_{\ell=1}^{NG}\alpha_{\ell}\,a_{m,g}(\vartheta_{\ell})\exp\left(\frac{-(x-x_{j-1/2})}{\vartheta_{\ell}}\right)+\psi_{g}^{p},\ x\in\Gamma_{j},m=1:N,\ell=1:NG, \tag{7}$$

where α_{ℓ} are constants to be determined and ψ_{g}^{p} is the particular solution obtained from Eq. (6).

3. THE MULTIGROUP SPECTRAL DETERMINISTIC METHOD (SDM)

This section consists of two parts. In the first part, we define the Spectral Deterministic Method (SDM) algorithm [10]; then in the second part, we describe the iterative process for solving the neutron transport equation spatially discretized in the multigroup formulation, using the SDM.

Let us analyze the uniform grid Γ represented in Figure 1. We consider Eq. (1) defined in cell Γ_j and prescribed boundary conditions written formally as

$$\psi_{m,g}(x)=\begin{cases}f_{m,g},\ \text{for}\ x=x_{j-1/2},\ \text{if}\ \mu_{m}>0,\\ g_{m,g},\ \text{for}\ x=x_{j+/2},\ \text{if}\ \mu_{m}<0\,.\end{cases} \tag{8}$$

After making the spectral analysis of Eq. (1), for each spatial cell Γ_j, as shown in the previous Section 2, we obtain the values of the eigenvectors $a_{m,g}(\vartheta_{\ell})$ and the eigenvalues ϑ_{ℓ}. Then, the parameters α_{ℓ} and the outgoing angular fluxes at each cell are calculated using Eq. (7). The pre-established boundary conditions, represented by Eq. (8), are used as the initial estimates of the incoming angular fluxes in the cell-edge to determine, the angular fluxes leaving the cell in all directions using Eq. (7). Reached this point, it becomes necessary to define our transport iteration, to understand the dynamics of calculating the emerging angular fluxes in the SDM iterative scheme. It is important to point out that our iterative process is substantially different to the transport sweeps used by the DD [1], that uses the Source Iteration (SI) scheme [1] and SGF [7,8], that use the one-node block inversion (NBI) scheme [7,8].

The transport iteration of the SDM, starts with the boundary conditions on the left side of the first cell (x = 0 cm and j = 1) as the first incoming angular fluxes, going to the right side until the end of the spatial domain (x = H cm and j = J) is reached. Using the Eq. (7) to calculate all the out-

going angular fluxes in each cell. When we arrive at the right side, we check whether the prescribed stopping criterion is satisfied. If it is satisfied, terminate the iteration, if not return to the first cell (x=0). This iterative process is performed until the maximum norm for the relative deviation between two consecutive estimates of the group scalar flux in the cell-edge, is smaller than a pre-established value. This relative deviation is calculated using the equation

$$\max_{1\le j\le J}\left|\frac{\phi^{k}_{g,j-1/2}-\phi^{k-1}_{g,j-1/2}}{\bar{\phi}^{k}_{g,j-1/2}}\right|<\varepsilon. \tag{9}$$

In Eq. (9), the value ε is the accuracy parameter of the iterative process and $\phi^{k}_{g}(x)$ as the k'th estimate of the multigroup cell edge scalar flux and, which can be calculated using

$$\phi(x)=\sum_{n=1}^{N}\omega_{n}\psi_{n,g}(x),\ g=1:G \tag{10}$$

4. NUMERICAL RESULTS AND DISCUSSION

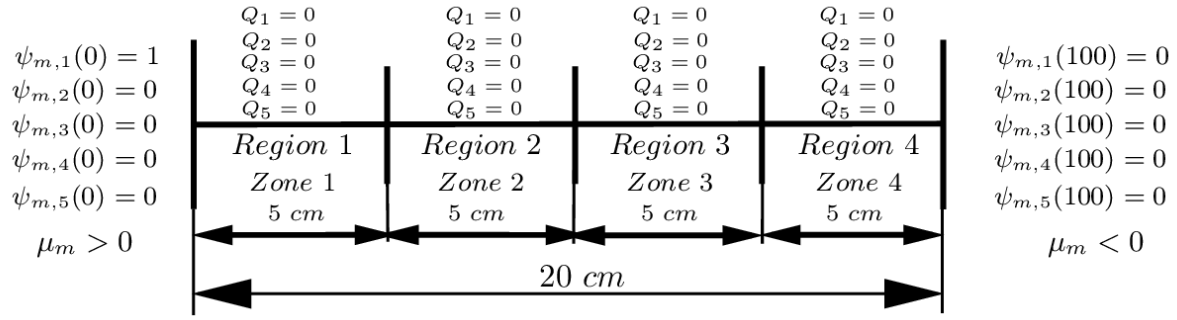
In this section, we examine a typical model-problem developed to test the spectral nodal methodology SDM with linearly anisotropic scattering and a prescribed interior source equal to zero. The model-problem considers a heterogeneous multilayer slab composed by four regions and four material zones, each one with thickness of 5 cm for a total length of H = 20 cm as shown in Figure 2. Here we use G = 5. To calculate the group total macroscopic cross sections and the scattering cross sections we use the fictitious cross-section set, defined by García R. D. M and Siewert C. E. in [11,12] and Menezes [13]. Here we must emphasize that the numerical results presented by the reference work [13] refer to the DD method (fine mesh) and the nodal method SGF (coarse-mesh), therefore, we compare the numerical results of the SDM (coarse-mesh) with those presented by these methods. The model-problem presents Q_g =0, however, this methodology can be successfully applied to problems with non-zero fixed-source Q_g.

$$\sigma_{Tgj}=\left[\frac{g}{10}-0.15\delta_{g.5}-0.15\delta_{g.10}\right],\ g=1:G, \tag{11}$$

$$\sigma_{Skj}^{g'\to g} = (2k+1)\left[\frac{g'}{100(g-g'+1}\right]h_{g'g}^{k}, \quad g',g=1:G,\ k=0:L, \tag{12}$$

k is the isotropic degree for the analyzed problem and δ is Kronecker delta. The zeroth and first-order components of the macroscopic differential scattering cross section are shown in Table 1.

Figure 2: *Model-Problem*



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In this model-problem, we change the order of the Gauss-Legendre quadrature set of the analyzed methods to verify the accuracy of the SDM when compared with the traditional fine-mesh DD method and the coarse-mesh SGF method. The prescribed stopping criterion applied to the methods requires that the discrete maximum norm of the relative deviation between two iterations (scalar fluxes) be less than or equal to $\varepsilon = 10^{-6}$.

Table 1: Macroscopic differential scattering cross section (G = 5)

		$\sigma_{S0j}^{g'\to g}$ (cm^{-1})					$\sigma_{S1j}^{g'\to g}$ (cm^{-1})				
		g					**g**				
Zone	g′	**1**	**2**	**3**	**4**	**5**	**1**	**2**	**3**	**4**	**5**
	1	0.01	0	0	0	0	0.0069	0	0	0	0
	2	0.005	0.02	0	0	0	0.0034	0.0136	0	0	0
1	**3**	0.0033	0.01	0.03	0	0	0.0023	0.0068	0.0201	0	0
	4	0.0025	0.0067	0.015	0.04	0	0.0017	0.0045	0.0099	0.0264	0
	5	0.002	0.005	0.01	0.02	0.05	0.0013	0.0033	0.0066	0.0131	0.0325
	1	0.1048	0	0	0	0	0.0072	0	0	0	0
	2	0.0052	0.0210	0	0	0	0.0036	0.0142	0	0	0
2	**3**	0.0035	0.0105	0.0314	0	0	0.0024	0.0071	0.0211	0	0
	4	0.0026	0.0070	0.0157	0.0419	0	0.0017	0.0047	0.0105	0.0277	0
	5	0.0021	0.0052	0.0105	0.0209	0.0524	0.0014	0.0035	0.0069	0.0137	0.0340
	1	0.0110	0	0	0	0	0.0076	0	0	0	0
	2	0.0055	0.0219	0	0	0	0.0038	0.0149	0	0	0
3	**3**	0.0037	0.0110	0.0329	0	0	0.0025	0.0074	0.0220	0	0
	4	0.0027	0.0073	0.0164	0.0438	0	0.0018	0.0049	0.0109	0.0290	0
	5	0.0022	0.0055	0.0109	0.0219	0.0548	0.0015	0.0036	0.0072	0.0143	0.03560
	1	0.0114	0	0	0	0	0.0079	0	0	0	0
	2	0.0057	0.0229	0	0	0	0.0039	0.0155	0	0	0
4	**3**	0.0038	0.0114	0.0343	0	0	0.0026	0.0077	0.0230	0	0
	4	0.0029	0.0076	0.0171	0.0457	0	0.0019	0.0051	0.0114	0.0301	0
	5	0.0023	0.0057	0.0114	0.0229	0.0571	0.0015	0.0038	0.0075	0.0150	0.0371

In Table 2, we display the scalar fluxes for groups g = 1 to 5 of the SDM as well as the results generated by the DD and SGF methods, considering quadrature set order N = 4.

Table 2: Scalar fluxes[1] with N = 4

Numerical Method			**DD** [a]		**SGF** [b]		**SDM** [c]	
Quadrature Order (N)	**x (cm)**	**group (g)**		**TIN** [d]		**TIN**		**TIN**
4	**0**	**1**	5.05806E-01 [e]	10	5.05806E-01	4	5.05806E-01	5
		2	2.06993E-03		2.06992E-03		2.06992E-03	
		3	1.10313E-03		1.10313E-03		1.10313E-03	
		4	7.00551E-04		7.00550E-04		7.00550E-04	
		5	6.86960E-04		6.86958E-04		6.86958E-04	
	10	**1**	6.77523E-02		6.77568E-02		6.77568E-02	
		2	2.28494E-03		2.28500E-03		2.28500E-03	
		3	9.90018E-04		9.90056E-04		9.90056E-04	
		4	5.49134E-04		5.49162E-04		5.49162E-04	
		5	5.69656E-04		5.69681E-04		5.69680E-04	
	20	**1**	7.44242E-03		7.44317E-03		7.44317E-03	
		2	1.89562E-04		1.89586E-04		1.89586E-04	
		3	6.97606E-05		6.97696E-05		6.97696E-05	
		4	3.68335E-05		3.68379E-05		3.68379E-05	
		5	3.70269E-05		3.70317E-05		3.70317E-05	

[1] Unit: neutrons x cm^{-2} x s^{-1}
[a] DD method with 100 nodes per region (fine-mesh)
[b] SGF method with 1 node per region (coarse-mesh)
[c] SDM method with 1 node per region (coarse-mesh)
[d] Total Iterations Number
[e] Read: 5.05806 x 10^{-1}

In Figures 3 and Figure 4 we present the numerical results in Tables 2 in graphic format to scalar fluxes based in model-problem (Figure 1)

Figure 3: *Scalar flux group g = 1 with N = 4*

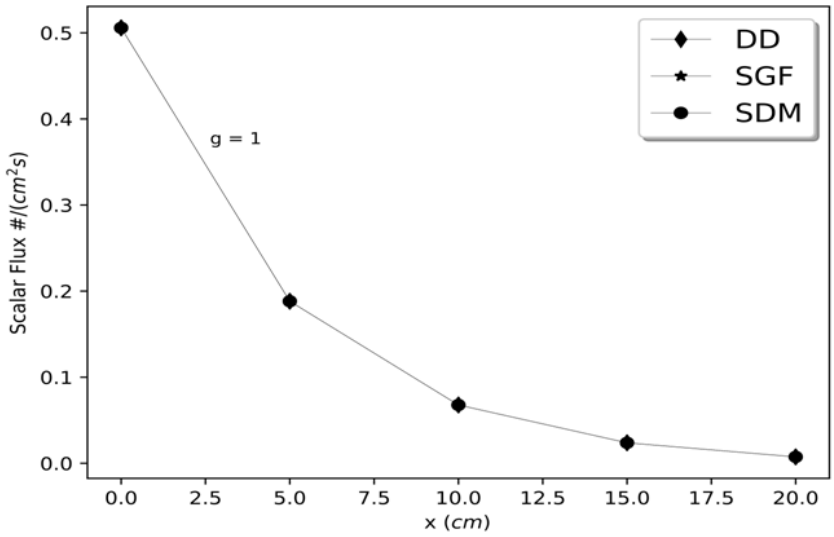

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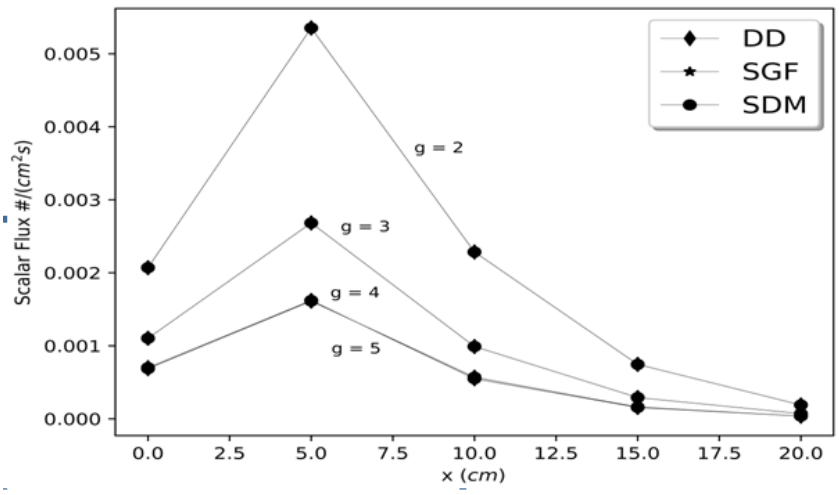
Figure 4: *Scalar fluxes from group g = 2: 5 with N = 4*



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In Table 3 [14], we display the scalar fluxes for groups g = 1 to 5 of the SDM as well as the results generated by the DD and SGF methods, considering quadrature set order N = 8.

Table 3: Scalar fluxes[1] with N = 8

Numerical Method			**DD** [a]		**SGF** [b]		**SDM** [c]	
Quadrature Order (N)	**x (cm)**	**group (g)**		**TIN** [d]		**TIN**		**TIN**
8	**0**	**1**	5.06252E-01 [e]	10	5.06252E-01	4	5.06252E-01	5
		2	2.12772E-03		2.12771E-03		2.12771E-03	
		3	1.11960E-03		1.11960E-03		1.11960E-03	
		4	7.08034E-04		7.08034E-04		7.08034E-04	
		5	6.89088E-04		6.89087E-04		6.89087E-04	
	10	**1**	7.00116E-02		7.00148E-02		7.00148E-02	
		2	2.29617E-03		2.29618E-03		2.29618E-03	
		3	1.00156E-03		1.00158E-03		1.00158E-03	
		4	5.57185E-04		5.57207E-04		5.57207E-04	
		5	5.76209E-04		5.76227E-04		5.76227E-04	
	20	**1**	7.42169E-03		7.42255E-03		7.42255E-03	
		2	1.88101E-04		1.88126E-04		1.88126E-04	
		3	6.88787E-05		6.88883E-05		6.88883E-05	
		4	3.62472E-05		3.62520E-05		3.62520E-05	
		5	3.65260E-05		3.65311E-05		3.65311E-05	

[1] Unit: neutrons x cm^{-2} x s^{-1}
[a] DD method with 100 nodes per region (fine-mesh)
[b] SGF method with 1 node per region (coarse-mesh)
[c] SDM method with 1 node per region (coarse-mesh)
[d] Total Iterations Number
[e] Read: 5.06252x 10^{-1}

In Figure5 and Figure 6 we present the numerical results in Table3 in graphic format to scalar fluxes based in model-problem (Figure 1).

Figure 5: *Scalar flux group g = 1 with N = 8*

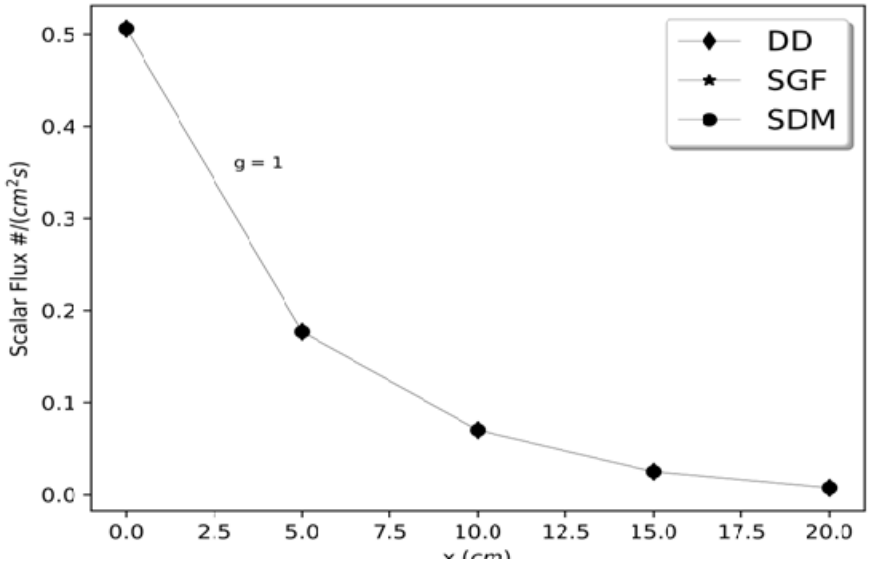

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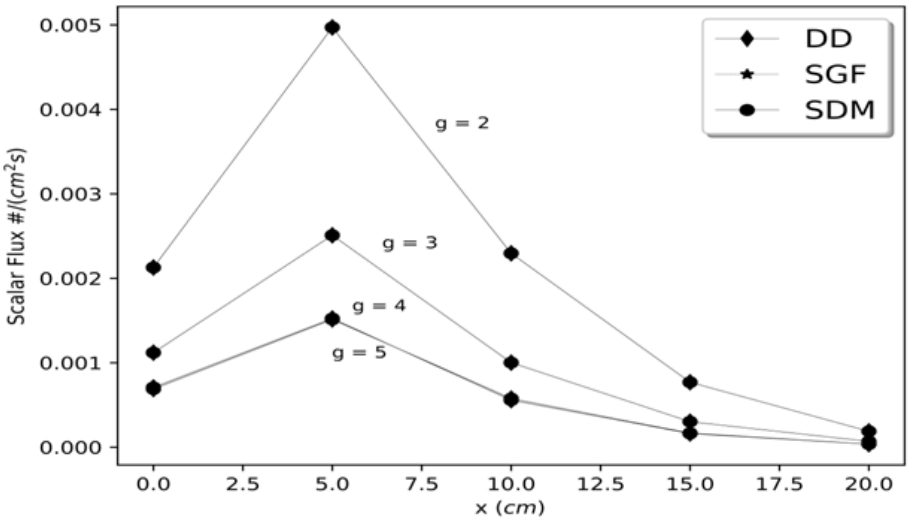
Figure 6: *Scalar fluxes from group g = 2: 5 with N = 8*



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As shown in Table 2, Table 3, Figure 3, Figure 4, Figure 5 and Figure 6, we can indicate that the SDM method presents the same scalar fluxes results for the different sets of Gauss-Legendre squares S4 and S8, when compared to the traditional DD methods (fine-mesh) and SGF (coarse mesh). In the graphs of Figure 4 and Figure 6, only a curve appears for the values of the scalar fluxes in the energy groups 4 and 5. This fact occurs because the values of the scalar fluxes of the energy groups are very close.

The SDM method is well suited for the numerical solution of the neutron transport equation, validating its precision for this model-problem. It should be emphasized here that this investigation, using the SDM method and the comparison of its results with the DD (fine-mesh) and SGF (coarse-mesh) methods, initially served to confirm the consistency and accuracy of this methodology applied in neutron shielding problems (fixed-source). In the future, other more sophisticated model-problems should be tested to verify the computational efficiency, from the point of view of CPU times of the simulation of the modeled problems.

5. CONCLUSIONS

In this paper, the analytical coarse-mesh numerical method (SDM) for multigroup fixed-source linearly anisotropic S_N problems in slab geometry has been described and developed. It has been tested for heterogeneous geometry to validate its accuracy. The SDM method developed is based on the local analytical general solution within each region of the domain which is determined by the spectral analysis described in Section 2. The SDM method converges to numerical solutions that are free from spatial truncation errors because their results coincide with the numerical results obtained from the analytical solution of the analyzed S_N problem regardless of the definition of the spatial grid or the angular quadrature used. The SDM algorithm is very simple when compared with the DD and SGF methods, which justifies its implementation.

The development and implementation of the SDM method require a smaller algebraic and computational effort when compared with DD and SGF methods justifying the investment in obtaining its equations and solution through a numerical (iterative) scheme. For all simulations run for this paper, CPU times did not exceed one second, so we decided to omit it in this work. In this paper, we

are initially interested in testing the accuracy and consistency of the SDM when compared to traditional methods that are found in the scientific literature. Our expectation for future works is to extend the SDM method to multidimensional problems, considering higher anisotropic degree and several energy groups.

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