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The modified spectral deterministic method applied to fixed–source discrete ordinates problems in X, Y–geometry

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ABSTRACT

A new approach for the application of the coarse–mesh Modified Spectral Deterministic method to numerically solve the two–dimensional neutron transport equation in the discrete ordinates (S_N) formulation is presented in this work. The method is based on within node general solution of the conventional one–dimensional S_N transverse integrated equations considering constant approximations for the transverse leakage terms and obtaining the S_N spatial balance equations. The discretized equations are solved by using a modified Source Iteration scheme without additional approximations since the average angular fluxes are computed analytically in each iteration. The numerical algorithm of the method presented here is algebraically simpler than other spectral nodal methods in the literature for the type of problems we have considered. Numerical results to two typical model problems are presented to test the accuracy of the offered method.

Keywords: **deterministic method, discrete ordinates formulation, fixed–source, spectral analysis.**

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1. INTRODUCTION

Over the past 30 years, several spectral nodal methods have been developed for numerically solving the time–independent, slab–geometry Boltzmann transport equation in the discrete ordinates (S_N) formulation with no spatial truncation error. Among these methods, one can point out the spectral Green's function (SGF) [1; 2], the spectral Response Matrix (RM) [3] and the Analytical Discrete Ordinates (ADO) [4] analytical numerical methods, which generate numerical values for the node–edge angular fluxes that exactly agree with the analytical solution of the S_N transport equations. These methodologies have been applied to develop coarse–mesh nodal methods for two–dimensional S_N problems. These methods are based on the nodal general solution of the one–dimensional S_N transverse integrated equations with approximations for the transverse leakage terms [5–8].

In the work by Oliva et al. [9], a novel numerical methodology, framed in the class of the spectral–nodal methods for solving multigroup slab–geometry S_N transport equations in non–multiplying media, was presented. This method shows to be algebraically and computationally simpler than other spectral–nodal methods and was termed the Spectral Deterministic Method (SDM).

In this work, we present the application of the modified SDM to X,Y–geometry S_N problems. Analogously to the companion methods [5–8], the present method is based on transverse integration of the two–dimensional S_N equations and the transverse leakage terms are assumed to be constant along the edges of the spatial discretization nodes. This new method is referred to as the Modified Spectral Deterministic–Constant Nodal (MSD–CN) method and it uses an iterative algorithm essentially different from the sweeping schemes used in the recent spectral–nodal methods.

This work is structured as follows: in Section 2, the spectral analysis for the S_N transverse integrated equations with constant transverse leakage terms is presented and the iterative methodology used for the MSD–CN method is described. Numerical results for two test problems are given in Section 3; and a brief discussion of the results and suggestions for future work are offered in Section 4.

2. MATERIALS AND METHODS

The time–independent one–speed S_N neutron transport equations considering isotropic scattering and non–multiplying media in a rectangular domain D are

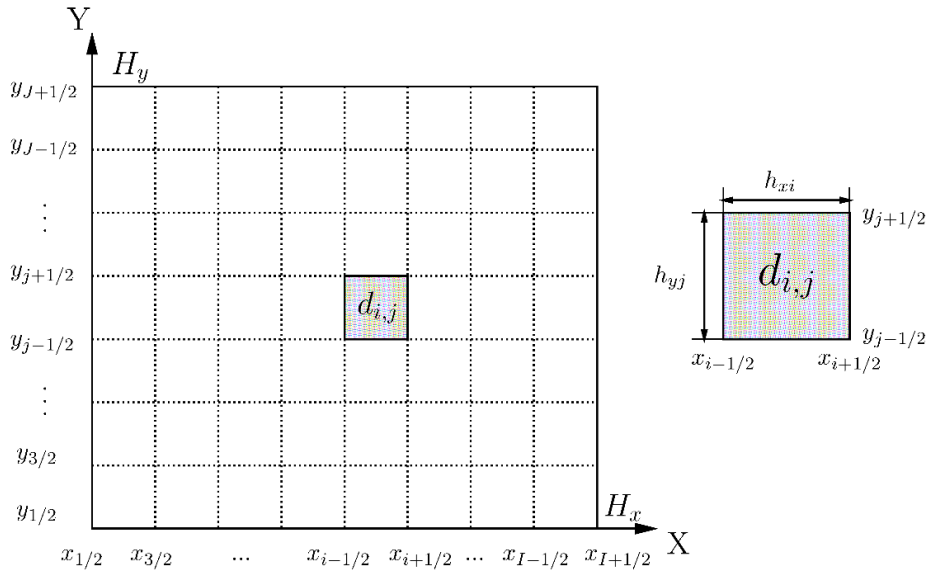
$$\mu_m \frac{\partial}{\partial x}\,\psi_m(x,y) + \eta_m \frac{\partial}{\partial y}\,\psi_m(x,y) + \sigma_T(x,y)\,\psi_m(x,y) = \frac{\sigma_S(x,y)}{4}\sum_{n=1}^{M}\psi_n(x,y)\,\omega_n + Q(x,y),$$

$$m = 1{:}\,M, \qquad (x,y) \in D, \quad (1)$$

with prescribed or reflective boundary conditions. The notation in Equation (1) is standard for this type of problems [10; 11] with $M = N(N+2)/2$, where N is the order of the angular quadrature set. The ordered pair (μ_m, η_m) represents the discrete directions of motion, ω_n are the corresponding weights and we have defined $\psi_m(x,y)$ as the angular flux in direction (μ_m, η_m).

Now, we consider an arbitrary spatial grid on D, viz Figure 1. The grid is composed of $I \times J$ spatial nodes $d_{i,j} \in D$ with width h_{xi} and height h_{yj}, constant total $(\sigma_{T\,i,j})$ and scattering $(\sigma_{S\,i,j})$ macroscopic cross sections, and constant interior source $Q_{i,j}$.

Figure 1: *Rectangular spatial grid on the domain D.*



Source: Author

The transverse–integration operator, is defined as $L_u \equiv \frac{1}{h_{us}} \int_{u_{s-1/2}}^{u_{s+1/2}} (\cdot) du$, where $u = x$ (or y) and $s = i$ (or j). At first, Equation (1) is integrated in the y direction ($u = y, s = j$) to obtain the one–dimensional transverse–integrated S_N nodal equations in the x direction

$$\mu_m \frac{d}{dx} \tilde{\psi}_{m,j}(x) + \frac{\eta_m}{h_{yj}} \left[\psi_m\left(x, y_{j+1/2}\right) - \psi_m\left(x, y_{j-1/2}\right) \right] + \sigma_{T\,i,j}\, \tilde{\psi}_{m,j}(x)$$

$$= \frac{\sigma_{S\,i,j}}{4} \sum_{n=1}^{M} \tilde{\psi}_{n,j}(x)\, \omega_n + Q_{i,j} \ , \qquad m = 1{:}\,M, i = 1{:}\,I, j = 1{:}\,J, (x,y) \in d_{i,j} \, . \tag{2}$$

Similarly, integrating Equation (1) in the x direction ($u = x, s = i$), the one–dimensional transverse–integrated S_N nodal equations in the y direction is obtained

$$\frac{\mu_m}{h_{xi}} \left[\psi_m\left(x_{i+1/2}, y\right) - \psi_m\left(x_{i-1/2}, y\right) \right] + \eta_m \frac{d}{dy} \widehat{\psi}_{m,i}(y) + \sigma_{T\,i,j}\, \widehat{\psi}_{m,i}(y)$$

$$= \frac{\sigma_{S\,i,j}}{4} \sum_{n=1}^{M} \widehat{\psi}_{n,i}(y)\, \omega_n + Q_{i,j} \ , \qquad m = 1{:}\,M, i = 1{:}\,I, j = 1{:}\,J, (x,y) \in d_{i,j} \, . \tag{3}$$

In Equations (2) and (3), the quantities $\tilde{\psi}_{m,j}(x)$ and $\widehat{\psi}_{m,i}(y)$ are defined as the average angular flux over each spatial coordinate direction inside node $d_{i,j}$

$$\tilde{\psi}_{m,j}(x) \equiv \frac{1}{h_{yj}} \int_{y_{j-1/2}}^{y_{j+1/2}} \psi_m(x,y)\ dy \qquad \text{and} \qquad \widehat{\psi}_{m,i}(y) \equiv \frac{1}{h_{xi}} \int_{x_{i-1/2}}^{x_{i+1/2}} \psi_m(x,y)\, dx \, .$$

Moreover, Equations (2) and (3) represent two systems of M ordinary differential equations in the x and y coordinate directions, respectively. Each system has $3M$ unknowns, M unknowns represented by $\tilde{\psi}_{m,j}(x)$ (or $\hat{\psi}_{m,i}(y)$) and $2M$ unknowns represented by the fluxes in the transverse leakage terms ($\psi_m\left(x, y_{j\pm1/2}\right)$ or $\psi_m\left(x_{i\pm1/2}, y\right)$). Therefore, we need to introduce approximations to guarantee uniqueness of the solution. In this work, the transverse leakage terms are considered constant along the edges in each node $d_{i,j}$, which is the only approximation performed in the present method. The constants to approximate these terms are chosen so as to preserve the node–edge average fluxes in $d_{i,j}$. Thus, transverse–integrated S_N constant nodal equations appear as

$$\mu_m \frac{d}{dx}\tilde{\psi}_{m,j}(x) + \frac{\eta_m}{h_{yj}}\left[\hat{\psi}_{m,i,j+1/2} - \hat{\psi}_{m,i,j-1/2}\right] + \sigma_{T\,i,j}\,\tilde{\psi}_{m,j}(x)$$

$$= \frac{\sigma_{S\,i,j}}{4}\sum_{n=1}^{M}\tilde{\psi}_{n,j}(x)\,\omega_n + Q_{i,j}\ , \qquad m = 1{:}\,M, i = 1{:}\,I, j = 1{:}\,J, (x,y) \in d_{i,j} \tag{4}$$

and

$$\frac{\mu_m}{h_{xi}}\left[\tilde{\psi}_{m,i+1/2,j} - \tilde{\psi}_{m,i-1/2,j}\right] + \eta_m \frac{d}{dy}\widehat{\psi}_{m,i}(y) + \sigma_{T\,i,j}\,\widehat{\psi}_{m,i}(y)$$

$$= \frac{\sigma_{S\,i,j}}{4}\sum_{n=1}^{M}\widehat{\psi}_{n,i}(y)\,\omega_n + Q_{i,j}\ , \qquad m = 1{:}\,M, i = 1{:}\,I, j = 1{:}\,J, (x,y) \in d_{i,j}\ , \tag{5}$$

where the local general solution of the two systems of M ordinary differential equations represented in Equations (4) and (5) can be written as

$$\tilde{\psi}_{m,j}(x) = \sum_{l=1}^{M}\alpha_l^x a_m^x(\nu_l^x)e^{-(x-\lambda_i)/\nu_l^x} + \tilde{\psi}_{m,j}^P\ , \qquad m = 1{:}\,M\ ,\ x \in d_{i,j}. \tag{6}$$

and

$$\hat{\psi}_{m,i}(y) = \sum_{l=1}^{M}\alpha_l^y a_m^y\left(\nu_l^y\right)e^{-(y-\lambda_j)/\nu_l^y} + \hat{\psi}_{m,i}^P\ , \qquad m = 1{:}\,M\ ,\ x \in d_{i,j}. \tag{7}$$

The quantities $\tilde{\psi}_{m,j}^P$ and $\hat{\psi}_{m,i}^P$ are the particular solutions. The first terms of the right–hand side represent the homogeneous component of the local general solutions. The quantities ν_l and $a_m(\nu_l)$ are obtained by solving an eigenvalue problem of order M. More details about this spectral analysis, the calculation of the particular solution and the definition of the parameter λ can be found in the work by Curbelo et al. [12].

The α_l^x and α_l^yparameters in Equations (6) and (7) are arbitrary constants to be determined according to the boundary conditions of the spatial discretization node. Differently from previous spectral nodal methods that one can find in the literature [5–8], the methodology as presented in this work uses the most recent estimates of the incoming angular fluxes in the node interfaces, to compute the values of α_l^x and α_l^y, and then, the outgoing fluxes of the analyzed node are calculated by using the conventional discretized spatial balance S_N equations without introducing any additional

approximation. Due to the spectral analysis performed, the constant approximations for the transverse leakage terms and the modifications of the original iterative scheme, the present method is termed Modified Spectral Deterministic–Constant Nodal (MSD–CN) method.

2.1. The MSD–CN method

As a result of the spectral analysis [12; 7] we obtain the values of ν_l and $a_m(\nu_l)$ for each different material zone. Then, an estimate for the sets of α_l parameters can be obtained by solving the linear system with estimates for the incoming node boundary conditions and the particular solutions at each spatial node $d_{i,j}$. At this point, we use the source iteration (SI) scheme, which is a classical method for S_N simulations [11]. In the next subsection, we describe the simple SI scheme as applied to the present MSD–CN method. We remark that apart from the constant leakage approximations, no additional approximations are included since we compute the average angular fluxes analytically in each iteration.

At this point, we integrate Equation (1) within an arbitrary node $d_{i,j}$ by using the operator

$$L \equiv \frac{1}{h_{xi}\, h_{yj}} \int_{x_{i-1/2}}^{x_{i+1/2}} \int_{y_{j-1/2}}^{y_{j+1/2}} (\cdot)\, dy\, dx$$

to obtain the discretized spatial balance S_N equations

$$\frac{\mu_m}{h_{xi}}\left[\tilde{\psi}_{m,i+1/2,j} - \tilde{\psi}_{m,i-1/2,j}\right] + \frac{\eta_m}{h_{yj}}\left[\widehat{\psi}_{m,i,j+1/2} - \widehat{\psi}_{m,i,j-1/2}\right] + \sigma_{T\,i,j}\,\bar{\psi}_{m,i,j}$$

$$= \frac{\sigma_{S\,i,j}}{4} \sum_{n=1}^{M} \bar{\psi}_{n,i,j}\,\omega_n + Q_{i,j}\ , \qquad m = 1{:}\,M, i = 1{:}\,I, j = 1{:}\,J\ , \tag{8}$$

where we have defined the node–average angular flux in node $d_{i,j}$

$$\bar{\psi}_{m,i,j} \equiv \frac{1}{h_{xi}\, h_{yj}} \int_{x_{i-1/2}}^{x_{i+1/2}} \int_{y_{j-1/2}}^{y_{j+1/2}} \psi_m(x,y)\, dy\, dx\ . \tag{9}$$

Now, we substitute the expression for $\tilde{\psi}_{m,j}(x)$ given in Equation (6) into Equation (9) and we obtain the analytical expression

$$\bar{\psi}^x_{m,i,j} \equiv \frac{1}{h_{xi}} \sum_{l=1}^{M} -\alpha_l^x\, \nu_l^x\, a_m^x(\nu_l^x)\left[e^{-(x_{i+1/2}-\lambda_i)/\nu_l^x} - e^{-(x_{i-1/2}-\lambda_i)/\nu_l^x}\right] + \tilde{\psi}^P_{m,j}\ . \tag{10}$$

Analogously, for the y coordinate direction we obtain

$$\bar{\psi}^{y}_{m,i,j} \equiv \frac{1}{h_{yj}} \sum_{l=1}^{M} -\alpha_l^y \, \nu_l^y \, a_m^y(\nu_l^y) \left[e^{-(y_{j+1/2}-\lambda_j)/\nu_l^y} - e^{-(y_{j-1/2}-\lambda_i)/\nu_l^y} \right] + \widehat{\psi}^{P}_{m,i} \, . \tag{11}$$

After some manipulation in the discretized spatial balance S_N equations (8), we obtain the sweeping equations

$$\tilde{\psi}_{m,i\pm1/2,j} = \frac{h_{xi}}{|\mu_m|} \left[\frac{\sigma_{S\,i,j}}{4} \sum_{n=1}^{M} \bar{\psi}^{x}_{n,i,j} \, \omega_n - \sigma_{T\,i,j} \, \bar{\psi}^{x}_{m,i,j} + Q_{i,j} - \frac{\eta_m}{h_{yj}} \left(\widehat{\psi}_{m,i,j+1/2} - \widehat{\psi}_{m,i,j-1/2} \right) \right]$$
$$+ \tilde{\psi}_{m,i\mp1/2,j} \, , \qquad m = 1{:}\,M, \qquad i = 1{:}\,I, \qquad j = 1{:}\,J \tag{12}$$

and

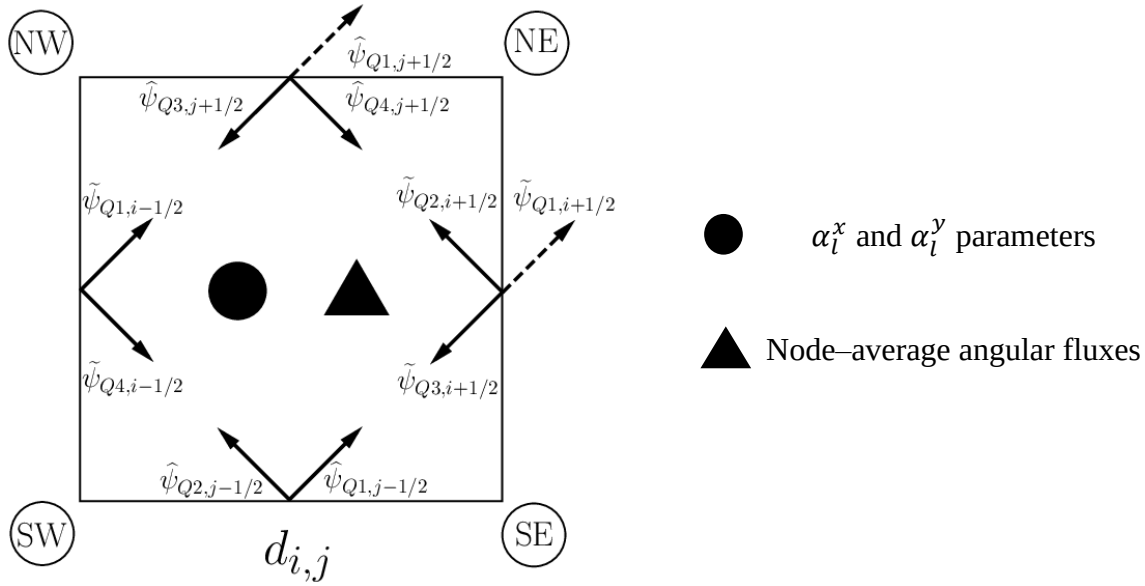
$$\widehat{\psi}_{m,i,j\pm1/2} = \frac{h_{yj}}{|\eta_m|} \left[\frac{\sigma_{S\,i,j}}{4} \sum_{n=1}^{M} \bar{\psi}^{y}_{n,i,j} \, \omega_n - \sigma_{T\,i,j} \, \bar{\psi}^{y}_{m,i,j} + Q_{i,j} - \frac{\mu_m}{h_{xi}} \left(\tilde{\psi}_{m,i+1/2,j} - \tilde{\psi}_{m,i-1/2,j} \right) \right]$$
$$+ \widehat{\psi}_{m,i,j\mp1/2} \, , \qquad m = 1{:}\,M, \qquad i = 1{:}\,I, \qquad j = 1{:}\,J. \tag{13}$$

Analogously to the Modified Spectral Deterministic method for one–dimensional problems [13], the iterative algorithm for two–dimensional problems is essentially different from the transport sweeps used by the conventional methods, e.g, Diamond Difference [10], spectral Green's function–Constant Nodal [1; 2], and spectral Response Matrix–Constant Nodal [5]. To illustrate the sweeping scheme for the X,Y–geometry domain in the MSD–CN+SI scheme, let us consider Figure 2 representing an arbitrary node $d_{i,j}$ with quantities involved for the southwest to northeast sweep. Each arrow in Figure 2 represents $N(N\,+\,2)/8$ directions in each quadrant.

The α_l^x and α_l^y parameters (represented by a black circle) are obtained at each node by using Equations (6) and (7) considering the node boundary conditions on the left–right and the lower–upper boundaries, respectively (solid arrows). Then, two estimates for the node–average angular fluxes are determined analytically (black triangle) by using Equations (10) and (11). At this point, the most recent estimates of the quantities $\bar{\psi}^{x}_{m,i,j}$ and $\bar{\psi}^{y}_{m,i,j}$are substituted in the sweeping equations (12) and (13), in order to compute these outgoing node–edge average angular fluxes in the sweeping directions (dashed arrows). To proceed, the continuity conditions are applied to use the outgoing angular fluxes as estimates for the incoming angular fluxes of the adjacent nodes and the entire spatial grid is swept

in the four sweeping directions, characterizing one iteration. At the end of each iteration, it is checked whether the stopping criterion is satisfied.

Figure 2: *MSD–CN+SI algorithm for the SW–NE sweep.*



Source: Author

In the next section, numerical results for two classical model problems are considered. The MSD–CN+SI method was implemented in C++ (Code::Blocks 17.12 IDE) and the results are compared to the conventional fine–mesh Diamond Difference (DD) [10] and coarse–mesh methods.

3. RESULTS AND DISCUSSION

In this section, we consider two classical model problems. The first model problem represents an oil well–logging problem for geophysics applications, and the second problem is a shielding calculation. In this work, the stopping criterion establishes that the relative deviations between two consecutive estimates for the average scalar flux on the node–edges of $d_{i,j}$ ($i = 1{:}I,\ j = J$) do not exceed the value 10^{-6}. We remark that, in the S_N formulation, we calculate the node–average scalar flux and the absorption rate density in $d_{i,j}$ as

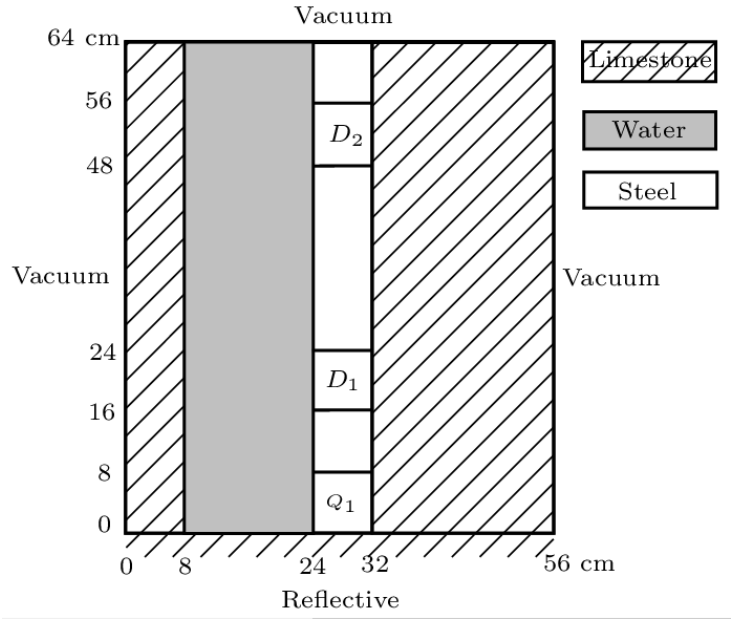
$$\bar{\phi}_{i,j} = \frac{1}{4} \sum_{n=1}^{M} \bar{\psi}_{n,i,j}\, \omega_n \quad \text{and} \quad R_{i,j} = h_{xi}\, h_{yj}\, \sigma_{A\,i,j}\, \bar{\phi}_{i,j}\,, \tag{14}$$

respectively.

3.1. Model Problem Nº 1.

This model problem has been considered in references [14; 15]. The geometry and boundary conditions for this test problem are shown in Figure 3. The numerical experiment consists in calculating the average scalar flux in regions D_1 and D_2, that represent the locations of the detectors traditionally used in this configuration, due to an isotropic unit source located in region Q_1. The nuclear data are as follow: $\sigma_T(\sigma_S)$ for limestone = 0.330263 (0.314419); for water = 0.694676 (0.634883); and for steel = 0.499122 (0.494460) cm^{-1}.

Figure 3: *Geometry and source ($cm^{-3}s^{-1}$) for Model Problem Nº 1.*



Source: Adapted from reference [15]

In Table 1, we list the numerical results generated for the average scalar fluxes in regions D_1 and D_2, as computed by using the MSD–CN+SI method with the level symmetric S_6 angular quadrature set [10] (24 ordinates directions) on two spatial grids composed of 56 × 64 and 112 × 128

discretization nodes. We also show the percentage relative deviations with respect to the results reported by Domínguez et al. [15] obtained with the spectral Green's function–Linear Nodal method, which we consider as reference results. As we observe, the results are accurate and the percentage relative deviations for the average scalar fluxes are less than 1% in all cases.

Table 1: Average scalar flux ($cm^{-2}s^{-1}$) for Model Problem Nº 1 (MSD– CN + SI, S_6 model).

Spatial grid [a]	$\boldsymbol{D_1}$	$\boldsymbol{D_2}$
56 × 64	1.70684E+00 (0.59) [b]	1.23734E–02 (0.77)
112 × 128	1.71388E+00 (0.18)	1.24367E–02 (0.27)

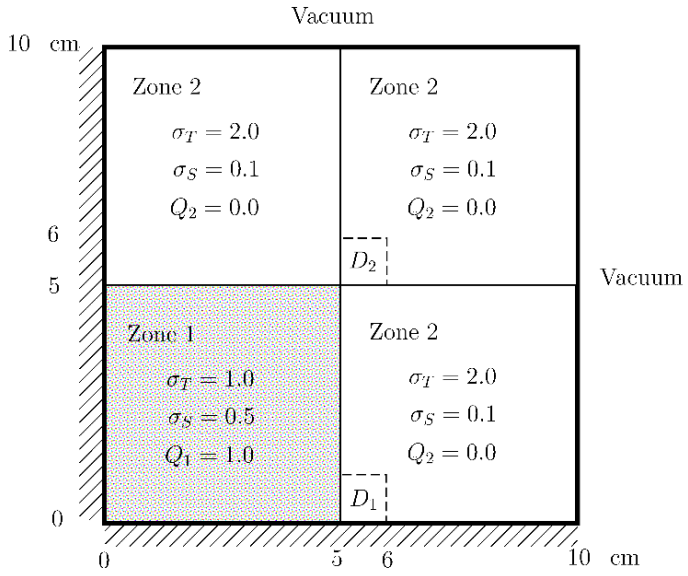
[a] Number of nodes in the x direction × number of nodes in the y direction.

[b] Percentage relative deviation with respect to the reference results [15].

3.2. Model Problem Nº 2.

Now we estimate the response of two neutron detectors due to a uniform isotropic neutron source ($Q_1 = 1.0\ cm^{-3}s^{-1}$) surrounded by a shielding material ($Q_2 = 0.0$). Figure 3 represents one–fourth of the whole shielding structure

Figure 4: *Geometry, nuclear data (cm^{-1}) and sources ($cm^{-3}s^{-1}$) for Model Problem Nº 2.*



Source: Adapted from reference [15]

To model this problem, we used the S_{16} angular quadrature set (144 ordinates directions) on two distinct spatial grids. The results obtained with the offered MSD–CN+SI code are compared with the results generated by the conventional fine–mesh DD and the coarse–mesh RM–CN methods, by using the source iteration (SI) and the partial one–node block inversion (NBI) iterative schemes, respectively. As a reference, we use the results generated by the DD+SI method on a uniform spatial grid composed of 100 × 100 discretization nodes, since this is the finer mesh used in the references [12; 15]. The third and fourth columns in Table 2 display the absorption rate densities and the percentage relative deviations with respect to the reference results for detectors D_1 and D_2, respectively.

The results obtained by using the present MSD–CN+SI method do agree, in all cases, with those obtained by using the RM–CN+NBI method, at least, up to the fifth decimal place. We observe, as expected, that the DD+SI method is more sensitive to the discretization grids, with the results varying considerably for the detector located farther away from the source. As we may see, for the spectral nodal methods, the percentage relative deviations are less than 1% for a grid composed of 20 × 20.

Table 2: Absorption rate density ($cm^{-1}s^{-1}$) for Model Problem N^o 1 (S_{16} model).

Method+Iterative Scheme	**Spatial grid** [a]	$\boldsymbol{D_1}$	$\boldsymbol{D_2}$
DD+SI	100 × 100	3.96064E–01[b]	6.86388E–02 [b]
	10 × 10	5.15839E–01 (29.7) [c]	1.01614E–01 (48.0)
	20 × 20	3.95725E–01 (0.09)	7.21137E–02 (5.06)
RM–CN+NBI	10 × 10	3.95611E–01 (0.11)	6.19987E–02 (9.67)
	20 × 20	3.95647E–01 (0.11)	6.83082E–02 (0.48)
MSD–CN+SI	10 × 10	3.95611E–01 (0.11)	6.19987E–02 (9.67)
	20 × 20	3.95647E–01 (0.11)	6.83082E–02 (0.48)

[a] Number of nodes in the x direction × number of nodes in the y direction.

[b] Reference results.

[c] Percentage relative deviation with respect to the reference results.

Despite of accurate results for both model problems, the present approach must be further studied thoroughly. Analyses on the convergence, computing time and the memory storage requirements need to be performed. Also, a comprehensive comparison with conventional spectral nodal methods is necessary. This shall require that all the algorithms be implemented on the same code using similar programming techniques.

4. CONCLUSION

In this work, a new coarse–mesh numerical method for fixed–source S_N problems in two–dimensional geometry has been presented. The offered methodology involved a conventional spectral analysis with a new ingredient, since the analytical solutions for the node–average angular fluxes are used to architect a modified Source Iteration scheme without additional approximations, apart from the constant approximations for the transverse leakage terms. We have presented a detailed description of the methodology and the numerical results have been compared to conventional fine and coarse–mesh methods.

One important feature of this class of numerical methods is the scalability to more realistic problems. In future work, it is intended the application of this methodology to energy multigroup problems considering anisotropic scattering. The application of the Modified Spectral Deterministic–Constant Nodal (MSD–CN) method to global calculations of nuclear reactors in slab–geometry and two–dimensional problems shall be also developed.

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