VETOR

Technique for reducing time in the calculation of eigenvalues and eigenvectors applied in neutron transport fixed-source problems

Técnica para redução de tempo no cálculo de autovalores e autovetores aplicados a problemas de fonte fixa em transporte de nêutrons

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Abstract

In this work, a mathematical technique to accelerate the eigenvalue calculations, originally proposed for the Analytical Discrete Ordinates method (ADO), is applied to the coarse-mesh method Modified Spectral Deterministic (MSD), used in neutron shielding problems (fixed-source) in one-dimensional geometry. This technique consists in an arrangement of the neutron transport equation which leads to a reduced eigenvalue calculation on the intranodal analytical solution, where only the positive half of the eigenvalues and its respective eigenvectors are calculated, hence reducing the methods execution time. Precision and performance tests were performed in 2 model-problems, reducing around 80% of the execution time. All the codes were developed using the programming language C++.

Keywords

Neutron Transport • Fixed-source problems • Spectral Analysis

Resumo

Neste trabalho, uma técnica matemática para acelerar os cálculos de autovalores, originalmente proposto para o método *Analytical Discrete Ordinates* (ADO), é aplicado para o método de malha grossa *Modified Spectral Deterministic* (MSD), usado em problemas de blindagem de nêutrons (fonte-fixa) em geometria unidimensional. Esta técnica consiste no arranjo da equação de transporte de nêutrons que leva a cálculos reduzidos de autovalores, onde são calculados apenas os autovalores positivos e seus respectivos autovetores, consequentemente reduzindo o tempo de execução do método. Testes de precisão e performance são realizados em 2 problemas-modelo, onde foram reduzidos cerca de 80% do tempo de execução. Todos os códigos foram desenvolvidos usando a linguagem de programação C++.

Palavras-chave

Transporte de nêutrons • Problemas de fonte-fixa • Análise espectral

1 Introduction

The solution of engineering problems using numerical methods can be computationally expensive, depending on the complexity of the modelled problem. Thus, many approaches can be taken to decrease the execution time of a problem, such as the development or modification of analytical and numerical methods, or parallel programming.

Neutron shielding problems can become highly complex when more realistic models are studied. Therefore, a mathematical technique is used here to decrease the order of the eigenvalues problem that composes the analytical solution of the intranodal neutron transport equation, where only the positive eigenvalues and its correspondents eigenvectors are calculated, hence decreasing the execution time.

The neutron transport inside a non-multiplying media phenomenon is modelled according to the linearized Boltzmann equation, which is a balance equation between incoming and outgoing neutrons inside a unitary volume [1]. This equation has 7 independent variables, being 3 spatial ones, 2 angular ones, discretized according to the discrete ordinates formulation [1], an energy one, discretized using the energy multigroup theory [2], and a time variable, but in this work, only stationary problems are studied. In order to solve a neutron shielding problem, different kinds of numerical methods can be used, such as fine-mesh methods, e.g. Diamond Difference (DD) [1], or coarse-mesh ones, e.g. Spectral Deterministic Method (SDM) [3, 4], Modified Spectral Deterministic (MSD) [5, 6], Response Matrix (RM) [7], Analytical Discrete Ordinates (ADO) [8, 9] and spectral Green's function (SGF) [10].

All coarse-mesh methods cited above relies on the analytical solution of the intranodal neutron transport equation. For this, an eigenvalue problem must be solved, which spends a big portion of the execution time in one-dimensional problems. The spectral analysis in model-problems with a higher number of energy groups and discrete directions can be computationally expensive. Thus, the main goal of this work is to apply the enhancement in the eigenvalue problem originally proposed for the ADO method [8, 9], in order to accelerate the solution of one-dimensional multigroup fixed-source problems using the Modified Spectral Deterministic (MSD) method.

This work is organized as follows. Section 2 shows the mathematical modelling of the neutron transport equation, alongside the analytical solution of the intranodal equation and the enhancements performed on the eigenvalues problem calculations. Section 3 briefly shows the Modified Spectral Deterministic method constitutive equations. Section 4 displays results for a model-problem, with an analysis of the algorithm execution time. At last, Section 5 shows the concluding remarks of this work.

2 Neutron Transport Equation

The multigroup neutron transport equation in a stationary one-dimensional non-multiplying media with isotropic scattering, inside na arbitrary node (Γ_j) within a spatial grid of an one-dimensional grid of length H [1], can be written as

$$\mu_m \frac{\mathrm{d}}{\mathrm{d}x}\psi_{m,g}(x) + \sigma_{T,g,j}\psi_{m,g}(x) = \sum_{g'=1}^{G} \frac{\sigma_{S0,j}^{g'\to g}}{2} \sum_{n=1}^{N} \omega_n \psi_{n,g'}(x) + Q_{g,j},\ m = 1:N,\ g = 1:G, \tag{1}$$

where μ_m and ω_m represents the roots and weigths of the Gauss-Legendre quadrature of order N, used in the angular variable discretization, $\psi_{m,g}(x)$ represents the neutron angular flux of group g, $\sigma_{T,g,j}$ and $\sigma_{S0,j}^{g'\to g}$ are respectively the macroscopic total cross-section of group g and the macroscopic scattering cross-section from group g' to g, and $Q_{g,j}$ represent an isotropic uniform neutron source of group g inside Γ_j. Due to the symmetry of the Gauss-Legendre quadrature the values of the discrete directions are given in pairs in the form of $\pm\mu_m$ [1]. The NG equations that forms the system represented in Eq.(1) can be split into 2 systems of $NG/2$ equations in the form [9]:

$$\mu_m \frac{\mathrm{d}}{\mathrm{d}x}\psi_{m,g}(x) + \sigma_{T,g,j}\psi_{m,g}(x) = \sum_{g'=1}^{G} \frac{\sigma_{S0,j}^{g'\to g}}{2} \sum_{n=1}^{N/2} \omega_n \left[\psi_{n,g'}(x) + \psi_{n+N/2,g'}(x)\right] + Q_{g,j}, m = 1:N/2,\ g = 1:G, \tag{2}$$

and

$$-\mu_{m+N/2} \frac{\mathrm{d}}{\mathrm{d}x}\psi_{m+N/2,g}(x) + \sigma_{T,g,j}\psi_{m+N/2,g}(x) = \sum_{g'=1}^{G} \frac{\sigma_{S0,j}^{g'\to g}}{2} \sum_{n=1}^{N/2} \omega_n \left[\psi_{n,g'}(x) + \psi_{n+N/2,g'}(x)\right] + Q_{g,j},\ m = 1:N/2,\ g = 1:G. \tag{3}$$

This system of equations has an analytical solution composed by two components: an homogeneous one $\left(\psi_{m,g}^{H}(x)\right)$ and a particular one $\left(\psi_{m,g}^{P}\right)$, given by

$$\psi_{m,g}(x) = \psi_{m,g}^{H}(x) + \psi_{m,g}^{P}. \tag{4}$$

For the homogeneous component, we consider the expression [7]

$$\psi^H_{m,g}(x) = \Phi_{m,g}(\vartheta_l)\exp\left(\frac{-(x-h_j)}{\vartheta_l}\right), m = 1:N,\ g = 1:G. \tag{5}$$

At this point, a couple of definitions are made, in order to enhance the equations notation [9]:

$$U_{m,g}(\vartheta_l) \equiv \Phi_{m,g}(\vartheta_l) + \Phi_{m+N/2,g}(\vartheta_l), \quad m = 1:N/2,\ g = 1:G,\ l = 1:N/2. \tag{6}$$

$$V_{m,g}(\vartheta_l) \equiv \Phi_{m,g}(\vartheta_l) - \Phi_{m+N/2,g}(\vartheta_l), \quad m = 1:N/2,\ g = 1:G,\ l = 1:N/2. \tag{7}$$

In this step, Eq.(5) is substituted into Eqs.(2) and (3). The resulting equations are then summed and subtracted, leading, after some algebraic steps, respectively to the equations:

$$V_{m,g}(\vartheta_l) = \frac{\vartheta_l}{\mu_m}\sigma_{t,g}U_{m,g}(\vartheta_l) - \sum_{g'=1}^{G}\frac{\sigma_{S0}^{g'\to g}\vartheta_l}{\mu_m}\sum_{n=1}^{N/2}\omega_n U_{n,g'}(\vartheta_l), \tag{8}$$

and

$$V_{m,g}(\vartheta_l) = \frac{\mu_m}{\vartheta_l\sigma_{t,g}}U_{m,g}(\vartheta_l). \tag{9}$$

Substituting Eq.(9) into Eq.(8) leads to an eigenvalue problem with a system of $NG/2$ equations, in the form [9]

$$\sum_{g'=1}^{G}\sum_{n=1}^{N/2}\left[\left(\frac{\sigma_{T,g,j}}{\mu_m}\right)^2\delta_{mn}\delta_{g'g} - \frac{\sigma_{S0,j}^{g'\to g}\sigma_{t,g,j}\omega_n}{\mu_m^2}\right]U_{n,g'}(\vartheta_l) = \lambda_l U_{m,g}(\vartheta_l),$$
$$m = 1:N/2,\ g = 1:G,\ l = 1:NG/2, \tag{10}$$

where the components λ_l stands for

$$\lambda_l = \frac{1}{\vartheta_l^2}. \tag{11}$$

As the NG eigenvalues are symmetric around $\vartheta_l = 0$, the entire set can be expressed as

$$\begin{cases}\vartheta_l = \dfrac{1}{\sqrt{\lambda_l}},\ l = 1:NG/2\\ \vartheta_{l+NG/2} = \dfrac{-1}{\sqrt{\lambda_l}},\ l = 1:NG/2.\end{cases}$$

For the eigenvectors, after some algebraic steps using Eqs.(6), (7) and (9), two relations can be found between $\Phi_{m,g,j}(\vartheta_l)$ and $U_{m,g,j}(\vartheta_l)$, being

$$\Phi_{m,g,j}(\vartheta_l) = \frac{U_{m,g}(\vartheta_l)}{2}\left[1 + \frac{\mu_m}{\vartheta_l\sigma_{t,j}}\right] \tag{12}$$

and

$$\Phi_{m+N/2,g,j}(\vartheta_l) = \frac{U_{m,g}(\vartheta_l)}{2}\left[1 - \frac{\mu_m}{\vartheta_l\sigma_{t,j}}\right], \tag{13}$$

with Eqs.(12) and (13) the $NG/2$ eigenvectores submatrices can be calculated. Previously knowing the format of the full NG set of eigenvectors, being 4 quadrants of $NG/2$ submatrices organized as shown in Fig. 1, where the A submatrix is calculated with Eq.(12) and the B one with Eq.(13), for example, the full set of eigenvectors can be constructed.

In this step, all the NG eivenvalues and its correspondent eigenvectores were obtained solving an $NG/2$ eigenvalues problem.

For the particular component of the solution, $\psi^P_{m,g}$ is substituted into Eq.(1), leading to the system of equations

$$\sigma_{T,g,j}\psi^P_{m,g} - \sum_{g'=1}^{G}\frac{\sigma_{S0,j}^{g'\to g}}{2}\sum_{n=1}^{N}\omega_n\psi^P_{n,g'} = Q_{g,j},\ m = 1:N/2,\ g = 1:G. \tag{14}$$

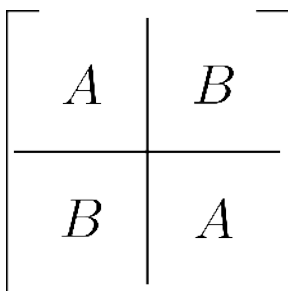

Figure 1: Eigenvectors $NG \times NG$ matrix and $NG/2 \times NG/2$ submatrices formats relation.

Writing the system of Eqs.(14) as $\boldsymbol{M}\boldsymbol{\psi}^P = \boldsymbol{Q}$, the particular components vector can be calculated as $\boldsymbol{\psi}^P = \boldsymbol{M}^{-1}.\boldsymbol{Q}$, where

$$[\boldsymbol{M}]_{i,k} = \sigma_{T,g,j}\delta_{mn}\delta_{g'g} - \frac{\sigma_{S0,j}^{g'\to g}\omega_n}{2}, \text{ with } i = m + (g-1)N,\ k = m + (g'-1)N,\ m = 1:N,\ g = 1:G. \quad (15)$$

With both components calculated, the intranodal neutron transport equations analytical solution can be written as

$$\psi_{m,g}(x) = \sum_{l=1}^{NG} \alpha_l \Phi_{m,g}(\vartheta_l) \exp\left(\frac{-(x-h_j)}{\vartheta_l}\right) + \psi_{m,g}^P,\ m = 1:N,\ g = 1:G, \quad (16)$$

where α_l are constants to be calculated using continuity and boundary conditions.

3 Modified Spectral Deterministic

In this section, the coarse-mesh method, named Modified Spectral Deterministic, used in the neutron angular fluxes calculation is briefly showed. The first step to derive its constitutive equations is to apply the average operator in Eq.(1), leading to the S_N spatial balance equation, given by [5]

$$\frac{\mu_m}{h_j}\left(\psi_{m,g,j+1/2} - \psi_{m,g,j-1/2}\right) + \sigma_{T,g,j}\overline{\psi}_{m,g,j} = \sum_{g'=1}^{G}\left[\frac{\sigma_{S0,j}^{g'\to g}}{2}\sum_{n=1}^{N}\omega_n\overline{\psi}_{n,g',j}\right] + Q_{g,j},\ m = 1:N\ g = 1:G, \quad (17)$$

where $\overline{\psi}_{m,g,j}$ represents the average neutron angular fluxes, which is calculated applying the average operator on Eq.(16), resulting in

$$\overline{\psi}_{m,g,j} \equiv \frac{1}{h_j}\int_{j-1/2}^{j+1/2}\psi_{m,g,j}(x)\mathrm{d}x = \frac{1}{h_j}\sum_{l=1}^{NG}\alpha_l\Phi_{m,g}(\vartheta_l)|\vartheta_l|(1-e^{-h_j/|\vartheta_l|}) + \psi_{m,g}^P,\ m = 1:N,\ g = 1:G, \quad (18)$$

and the variables $\psi_{m,g,j+1/2}$ and $\psi_{m,g,j-1/2}$ represents the neutron angular fluxes respectively on the right and left node-edges. The equations used to calculate are obtained with some algebraic steps applied in Eq.(17), leading to an equation to iterate angular neutron fluxes outgoing the right node-edge ($\mu_m > 0$)

$$\psi_{m,g,j+1/2} = \frac{h_j}{\mu_m}\left(-\sigma_{T,g,j}\overline{\psi}_{m,g,j} + \sum_{g'=1}^{G}\frac{\sigma_{S0,j}^{g'\to g}}{2}\sum_{n=1}^{N}\omega_n\overline{\psi}_{n,g',j} + Q_{g,j}\right) + \psi_{m,g,j-1/2},\ m = 1:N/2, g = 1:G \quad (19)$$

and for the left node-edge ($\mu_m < 0$)

$$\psi_{m,g,j-1/2} = \frac{h_j}{|\mu_m|}\left(-\sigma_{T,g,j}\overline{\psi}_{m,g,j} + \sum_{g'=1}^{G}\frac{\sigma_{S0,j}^{g'\to g}}{2}\sum_{n=1}^{N}\omega_n\overline{\psi}_{n,g',j} + Q_{g,j}\right) + \psi_{m,g,j+1/2},\ m = N/2+1:N, g = 1:G. \tag{20}$$

The iterative process consists in one sweep through the whole grid, starting at $x = 0$ (leftmost node-edge) until $x = H$ (rightmost node-edge) calculating the outgoing neutron angular fluxes in each nodes right node-edge using Eq.(19) and left node-edge with Eq.(20).

After iterating all neutron angular fluxes, the neutron scalar fluxes are then calculated, using the equation

$$\phi_{m,g,j-1/2} = \frac{1}{2}\sum_{m=1}^{N}\omega_m\psi_{m,g,j-1/2},\ j = 1:J+1. \tag{21}$$

With theses values, the stopping critterion can be tested, comparing the maximum deviation between the neutron scalar fluxes in 2 subsequent iterations (k) and a predefined tolerance ξ, as shown below:

$$\max_{g,j}\left|\frac{\boldsymbol{\phi}_{g,j-1/2}^{(k)} - \boldsymbol{\phi}_{g,j-1/2}^{(k-1)}}{\boldsymbol{\phi}_{g,j-1/2}^{(k-1)}}\right| < \xi,\ j = 1:J+1, g = 1:G. \tag{22}$$

4 Numerical Results

In this section, the numerical results for 2 model-problems are presented. Each of the 4 major components of the Modified Spectral Deterministic algorithm has its execution time measured, in order to analyze the contribution of presented enhancements to the overall execution time. The first component consists on the construction of the matrices used in the model-problems. The second one is the eigenvalue calculation, which is the main concern in this work. The third one is the preparation of the matrices used on the iterative process, including several matrix inversions. The last one is the iterative process itself. All the resuls were developed in a PC with Ryzen 7 3700U and 12 Gb of RAM, using the language C++. The eigenvalue problem was solved using the free edition of the linear algebra library ALGLIB [11], using a QR decomposition function.

4.1 Model-problem 1

The first model-problem studied consists in an one-dimensional heterogeneous media, with 3 different physical-material zones discretized in 10 groups of energy, and 4 regions, adapted from [5], as shown in Fig. 2. This problem has reflective boundaries condition on the left and vacuum on the right.

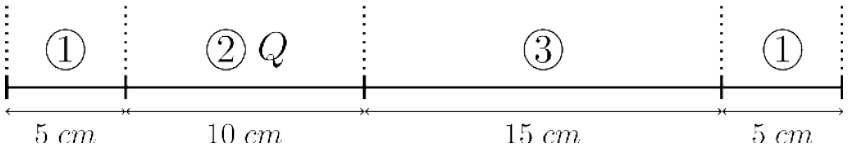

Figure 2: Model-problem 1 geometry and physical-material zones and regions organization.

The macroscopic total cross section is given by the equation

$$\sigma_{T,g,z} = \left(\frac{z+20}{21}\right)^5\left(\frac{g}{10} - 0.15\delta_{5,g} - 0.15\delta_{10,g}\right),\ g = 1:10,\ z = 1:3, \tag{23}$$

and the macroscopic scattering cross section is given by

$$\sigma_{S0,z}^{g'\to g} = \left(\frac{z+20}{21}\right)\left(\frac{g'}{100(g-g'+1)}\right),\ g = 1:10,\ g' = 1:g,\ z = 1:3. \tag{24}$$

As seen in Fig. 2, on the second region, there is an isotropic neutrons source, given by

$$Q_g = 1.1 - 0.1g,\ g = 1 : 10. \tag{25}$$

First of all, a precision test was performed, calculating the neutron angular flux on the nodal interfaces. The results obtained with the MSD with the enhancements were compared to the fine-mesh method DD, with 1500 nodes in the first and fourth regions, 3000 in the second one and 4500 in the third one. The mesh used on the reference method DD was refined until the neutron scalar flux stopped presenting variations until the sixth decimal place. The results for the first and last energy groups, for the methods DD and MSD are displayed in Table 1.

Table 1: Model-problem 1 numerical results - Neutron scalar Flux $\left[cm^{-2}s^{-1}\right]$.

DD						
N	g	0 cm	5 cm	15 cm	30 cm	35 cm
16	1	2.664247e+00	4.496934e+00	3.941839e+00	9.452070e-02	5.220592e-02
	10	5.763914e-01	3.987590e-01	1.007887e-01	6.305639e-04	4.618965e-04
32	1	2.671128e+00	4.496600e+00	3.941922e+00	9.452457e-02	5.220011e-02
	10	5.762956e-01	3.985820e-01	1.008011e-01	6.320738e-04	4.628080e-04
64	1	2.670705e+00	4.496601e+00	3.941920e+00	9.452555e-02	5.219932e-02
	10	5.762569e-01	3.985382e-01	1.008055e-01	6.324720e-04	4.630781e-04
128	1	2.670711e+00	4.496599e+00	3.941919e+00	9.452576e-02	5.219909e-02
	10	5.762483e-01	3.985274e-01	1.008070e-01	6.325785e-04	4.631541e-04
256	1	2.670710e+00	4.496598e+00	3.941919e+00	9.452582e-02	5.219903e-02
	10	5.762463e-01	3.985247e-01	1.008074e-01	6.326071e-04	4.631752e-04
MSD						
N	g	0 cm	5 cm	15 cm	30 cm	35 cm
16	1	2.664247e+00	4.496934e+00	3.941839e+00	9.452071e-02	5.220592e-02
	10	5.763915e-01	3.987591e-01[a]	1.007887e-01	6.305640e-04	4.618966e-04
32	1	2.671128e+00	4.496600e+00	3.941922e+00	9.452458e-02	5.220012e-02
	10	5.762957e-01	3.985821e-01	1.008011e-01	6.320739e-04	4.628081e-04
64	1	2.670706e+00	4.496601e+00	3.941920e+00	9.452556e-02	5.219932e-02
	10	5.762570e-01	3.985383e-01	1.008055e-01	6.324721e-04	4.630781e-04
128	1	2.670711e+00	4.496599e+00	3.941919e+00	9.452577e-02	5.219909e-02
	10	5.762484e-01	3.985275e-01	1.008070e-01	6.325786e-04	4.631542e-04
256	1	2.670710e+00	4.496598e+00	3.941919e+00	9.452583e-02	5.219903e-02
	10	5.762464e-01	3.985248e-01	1.008074e-01	6.326072e-04	4.631753e-04

[a] The maximum relative deviation calculated between DD and MSD methods in this model-problem is 0.00025.

As seen in these results, the MSD was able to achieve good accuracy when compared to the fine-mesh reference in the studied cases.

In order to analyze each of the algorithms components execution time, this model-problem was executed with a set of quadrature orders, being $N = 16, 32, 64, 128$ and 256. Each components section is measured separately, for methods MSD with and without the enhancement. Furthermore, the execution time for the Diamond Difference method was also computed. All these information can be seen in Table 2.

As seen in the results obtained in this part of the study, in all sets of quadrature order, the eigenvalue problem is the component with the longest execution time, reaching up to around 90% of the the total execution time in some cases. The results obtained with this enhancement, led to a decrease of 85 % of the eigenvalue problem, and 76 % decrease on the total execution time of the algorithm, as shown in Table 3.

Table 2: Execution time [s] and components percentage in execution - $NG \times NG$ - Model-problem 1.

Method	N	Matrix Construction	Eigenvalues Calculation	Matrix Preparations	Iterative Process	Execution time
$NG \times NG$	16	0.000350 (0.052)	0.504556 (76.46)	0.074600 (11.30)	0.080330 (12.17)	0.659888
	32	0.000270 (0.006)	3.490401 (82.59)	0.436184 (10.32)	0.299028 (7.07)	4.225941
	64	0.000467 (0.001)	28.052394 (86.80)	3.047639 (9.43)	1.216673 (3.76)	32.317231
	128	0.002232 (0.0008)	242.827927 (89.89)	22.590101 (8.36)	4.719651 (1.74)	270.139967
	256	0.005640 (0.0002)	2061.984608 (88.5)	250.791179 (10.76)	16.486614 (0.707)	2329.268125
$NG/2 \times NG/2$	16	0.000196 (0.077)	0.090234 (35.58)	0.085072 (33.55)	0.078061 (30.78)	0.253565
	32	0.000622 (0.044)	0.676257 (48.33)	0.431782 (30.86)	0.290445 (20.75)	1.399107
	64	0.000481 (0.005)	4.724902 (54.24)	2.864671 (32.88)	1.120724 (12.86)	8.710778
	128	0.000996 (0.001)	36.359016 (57.52)	22.316180 (35.30)	4.525634 (7.16)	63.201827
	256	0.002509 (0.0004)	324.538575 (62.77)	174.745706 (33.79)	17.720575 (3.42)	517.315539
DD	16	-	-	-	-	36.264835
	32	-	-	-	-	69.147150
	64	-	-	-	-	133.867948
	128	-	-	-	-	268.837684
	256	-	-	-	-	624.231729

Table 3: Execution time decrease between eigenvalue calculation with and without enhancement - Model-problem 1.

Quadrature Order	16	32	64	128	256
Eigenvalue Problem	82.12 %	80.63 %	83.16 %	85.03 %	84.26 %
Total Execution Time	61.58 %	66.89 %	73.04 %	76.61 %	77.80 %

4.2 Model-problem 2

In this model-problem, an homogeneous media with 10 cm of width is studied. The physical-material properties are modelled with 19 energy groups, as seen in [12]. It is considered a prescribed boundary condition for the incident angular neutron fluxes with $\psi_{m,g} = 1.00 \;\; cm^{-2}s^{-1}sr^{-1}$ for the first energy group on the left boundary, and vacuum boundary condition on the right, without external neutron source.

As seen in the first model-problem, before the execution time tests, a precision test was performed between the MSD method and a fine-mesh reference, using the DD method. For the reference a mesh with 10000 nodes is used, in order to obtain neutron scalar fluxes on the outermost positions of the domain with 6 decimal places of precision. The results for the neutron scalar fluxes of groups $g = 1,\ 10$ and 19, using different sets of discrete ordinates orders and are shown in Table 4.

Now, with concordant results comparing the precision between both methods, the performance test is performed. As seen in the previous model-problem each structure of the algorithm is analyzed separately. At first the $NG \times NG$ problem is solved, where it is clearly stated that the eigenvalue problem is the most prolonged part of this algorithm, reaching up to more than 94 % of the execution time of the method, on the S_{256} example. Since this model-problem is homogeneous, the MSD method is capable of computing the neutron angular fluxes with only one node, since it is free of truncation error for one-dimensional problems [10, 5]. The results for the performance test using the MSD method with and without the enhancement can be seen in Table 5.

With these results, once again it is achieved an expressive reduction of the eigenvalues problem solution execution time, leading to a reduction of the whole algorithm's execution time. As displayed in Table 6, for the most computationally expensive method studied in this work, using S_{256}, this technique enabled the solution of the eigenvalues problem to be run in around 15 % of the $NG \times NG$ execution time. This result led to a reduction of almost 80 % of the algorithm's execution time. Even for less expensive cases, as seen in S_{16}, this technique was able to reduce the execution time expressively.

5 Concluding remarks

In this work, an enhancement was performed on the solution of neutron shielding problems, where only half of the eigenvalues are calculated, in order to decrease the execution time. In this technique, some algebraic manipulations are performed on the intranodal neutron transport equation leading to reduced eigenvalue calculations, where only the positive eigenvalues and its respective eigenvectors are computed.

The results were obtained solving the first model-problem, with heterogeneous domain with 3 physical-material parameters, discretized in 10 energy groups. The obtained results showed an expressive decrease on the execution

Table 4: Model-problem 2 numerical results - Neutron scalar flux $\left[cm^{-2}s^{-1}\right]$.

		DD		MSD	
N	g	0 cm	10 cm	0 cm	10 cm
16	1	5.079466e-01	7.049980e-04	5.079466e-01	7.049981e-04
	10	1.339034e-02	1.450354e-04	1.339034e-02	1.450354e-04
	19	4.163735e-06	6.853063e-08	4.163735e-06	6.853065e-08
32	1	5.079466e-01	7.049450e-04	5.079466e-01	7.049451e-04
	10	1.336406e-02	1.449657e-04	1.336406e-02	1.449657e-04
	19	4.178121e-06	6.877873e-08	4.178121e-06	6.877874e-08
64	1	5.079466e-01	7.049305e-04	5.079466e-01	7.049306e-04
	10	1.335576e-02	1.449499e-04	1.335576e-02	1.449500e-04
	19	4.182466e-06	6.885072e-08	4.182466e-06	6.885074e-08
128	1	5.079466e-01	7.049269e-04	5.079466e-01	7.049270e-04
	10	1.335325e-02	1.449465e-04	1.335325e-02	1.449465e-04
	19	4.183692e-06	6.887080e-08	4.183692e-06	6.887083e-08
256	1	5.079466e-01	7.049259e-04	5.079466e-01	7.049260e-04
	10	1.335252e-02	1.449457e-04	1.335252e-02	1.449457e-04
	19	4.184032e-06	6.887635e-08	4.184032e-06	6.887638e-08[a]

[a] Maximum relative deviation calculated in this model-problem, comparing DD and MSD methods was 0.00004355.

Table 5: Execution time [s] and components percentage in execution - $NG \times NG$ - Model-problem 2.

Method	N	Matrix Construction	Eigenvalues Calculation	Matrix Preparations	Iterative Process	Execution time
$NG \times NG$	16	0.000685 (0.055)	1.104486 (89.48)	0.123666 (10.01)	0.005439 (0.440)	1.234277
	32	0.000941 (0.010)	8.076917 (91.60)	0.719212 (8.156)	0.020218 (0.229)	8.817288
	64	0.001059 (0.001)	60.918639 (92.16)	5.099289 (7.715)	0.075383 (0.114)	66.094372
	128	0.003615 (0.0006)	506.478547 (92.58)	40.240096 (7.356)	0.301304 (0.055)	547.023563
	256	0.009648 (0.0001)	5045.252976 (94.18)	310.083117 (5.788)	1.181643 (0.022)	5356.527385
$NG/2 \times NG/2$	16	0.000251 (0.076)	0.206864 (62.65)	0.112972 (34.21)	0.010082 (3.053)	0.330170
	32	0.000372 (0.016)	1.435896 (65.51)	0.717259 (32.72)	0.038154 (1.740)	2.191682
	64	0.000629 (0.004)	10.129470 (65.88)	5.097240 (33.15)	0.147616 (0.960)	15.374955
	128	0.003133 (0.002)	81.712953 (66.35)	40.824504 (33.15)	0.600700 (0.48)	123.141291
	256	0.003106 (0.0002)	748.601600 (69.69)	323.167443 (30.08)	2.411799 (0.224)	1074.183949

Table 6: Execution time decrease between eigenvalue calculation with and without enhancement - Model-problem 2.

Quadrature Order	16	32	64	128	256
Eigenvalue Problem	81.27 %	82.22 %	83.37 %	83.86 %	85.16 %
Total Execution Time	73.24 %	75.14 %	76.73 %	77.48 %	79.94 %

time as more computationally expensive the model was, varying the quadrature set order used in the angular variable discretization, reaching up to 85 % of execution time drecrease on the eigenvalue problem, hence decreasing the overall execution time in 76 %.

Analyzing the results for the second model-problem, it was achieved the same behaviour of the previous problem. In this case, an even bigger percentage of the execution time was spent solving the eigenvalue calculation, since the number of energy groups was higher than the first problem, hence, the sizes of the matrices is also higher, and it has an homogeneous domain, which makes the iterative process to be executed in one iteration. Therefore, the reduction on the execution time for the eigenvalue problem was even more pronounced than the first problem, decreasing up to 85 % of time, leading up to almost 80 % of the overall execution time.

This enhancement was effective on the acceleration of the eigenvalue calculation, hence decreasing the overall execution time of the Modified Spectral Deterministic method for the studied model-problems. On the other hand, the use of the this technique increases the complexity of the methods development, which could hinder the calculation of complex eigenvalues, for example. For future works, the authors intend to apply this technique in multidimensional problems.

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References

[1] E. E. Lewis and W. F. Miller, *Computational methods of neutron transport*, 1st ed. New York, USA: Wiley New York, 1993. Available at: https://www.ans.org/store/item-350016/

[2] J. J. Duderstadt, L. J. Hamilton *et al.*, *Nuclear reactor analysis*, 1st ed. New York, USA: Wiley New York, 1976. Available at: https://www.wiley.com/en-us/Nuclear+Reactor+Analysis-p-9780471223634

[3] A. M. Oliva, "Método espectral determinístico para a solução de problemas de transporte de nêutrons usando a formulação das ordenadas discretas," Ph.D. dissertation, Programa de Pós-Graduação em Modelagem Computacional, Universidade do Estado do Rio de Janeiro, Nova Friburgo, Brasil, 2018, in Portuguese. Available at: https://www.bdtd.uerj.br:8443/handle/1/13719

[4] A. Muñoz Oliva and H. Alves Filho, "Spectral-nodal deterministic methodology for neutron shielding calculations using the x, y - geometry multigroup transport equation in the discrete ordinates formulation," *VETOR - Revista de Ciências Exatas e Engenharias*, vol. 31, no. 1, p. 72–83, 2021. Available at: https://doi.org/10.14295/vetor.v31i1.13472

[5] R. B. Libotte, "Método de malha grossa para solução numérica de problemas de blindagem de nêutrons em geometria unidimensional na formulação de ordenadas discretas com perspectivas a cálculos multidimensionais em geometria retangular," Master's thesis, IPRJ/UERJ, Nova Friburgo, 2021, in Portuguese. Available at: https://www.bdtd.uerj.br:8443/handle/1/16461

[6] R. B. Libotte, H. Alves Filho, and F. C. da Silva, "Avanços recentes na aplicação de um método numérico espectronodal para solução de problemas unidimensionais de blindagem de nêutrons," *VETOR - Revista de Ciências Exatas e Engenharias*, vol. 31, no. 1, 2021, in Portuguese. Available at: https://doi.org/10.14295/vetor.v31i1.13473

[7] O. P. da Silva, "Um método de matriz resposta para cálculos de transporte multigrupos de energia na formulação de ordenadas discretas em meios não-multiplicativos," Ph.D. dissertation, Programa de Pós-Graduação em Modelagem Computacional, Universidade do Estado do Rio de Janeiro, Nova Friburgo, Brasil, 2018, in Portuguese. Available at: https://www.bdtd.uerj.br:8443/handle/1/13715

[8] L. B. Barichello, L. C. Cabrera, and J. F. P. Filho, "An analytical approach for a nodal scheme of two-dimensional neutron transport problems," *Annals in Nuclear Energy*, vol. 38, pp. 1310–1317, 2011. Available at: https://repositorio.furg.br/handle/1/1051

[9] L. B. Barichello, C. B. Picoloto, and E. D. da Cunha, "The ado-nodal method for solving two-dimensional discrete ordinates transport problems," *Annals in Nuclear Energy*, vol. 108, pp. 376–385, 2017. Available at: sciencedirect.com/science/article/pii/S0306454917300919

[10] R. C. de Barros, “A spectral nodal method for the solution of discrete ordinates problems in one- and two-dimensional cartesian geometry,” Ph.D. dissertation, University of Michigan, UMICH, Ann Arbor, USA, 1990. Available at: https://deepblue.lib.umich.edu/handle/2027.42/105093

[11] S. Bochanov. (2023) ALGLIB - C++/C# numerical analysis library. Linear Algebra Library. Available at: https://www.alglib.net/

[12] J. P. Curbelo, “Aplicação da técnica adjunta em problemas de transporte do tipo fonte–detector na formulação de ordenadas discretas usando um método espectronodal,” Ph.D. dissertation, IPRJ/UERJ, Nova Friburgo, Brasil, 2017, in Portuguese. Available at: https://www.bdtd.uerj.br:8443/bitstream/1/13706/1/Tese_JesusPerezCurbelo.pdf