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Computer Deterministic Modelling of Nuclear Problems using Nodal Methods

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Abstract. In this paper we propose a numerical nodal methodology for the development of a method of spectral nodal class [1, 2] which is tested as an initial study of the solutions (spectral analysis) of neutron transport equations in the formulation of discrete ordinates (S_N), in one-dimensional geometry, two energy groups, isotropic scattering and considering heterogeneous domains. These results are compared with the traditional fine mesh method DD and the spectral nodal method SGF [1].The solution algorithms problems will be implemented in a computer simulator made in MatLab language, the same that was used to generate the results of the reference work.

Keywords. Neutrons Transport Theory, Discrete Ordinates, Computational Modelling.

1 Introduction

The roots of transport theory go back more than a century to the *Boltzmann equation*, first formulated for the study of the kinetic theory of gases [3, 4], and even today the *Boltzmann equation* remains the principal tool of the gas dynamicist. Its counterpart for the neutron "gas", the so called *neutron transport equation*,is far younger [3] (less than 80 years). This neutron transport equation help us to predict the distribution in space, time and energy of the neutrons in a nuclear reactor. Due to the complexity of the analytical treatment of the linearised neutron transport equation were developed numerical methods in order to obtain approximate solutions to the problem of radiation shields, global reactor calculations and other apllications. These numerical methods allow us to do computer modelling using a deterministic approach, since they usually use a formulation of discrete

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ordinates (S_N) [4]. S_N discrete ordinates formulation made a discretization of the angular variables in N directions (discrete ordinates) and use an angular quadrature sets for the approximation of the integral source terms.
In this paper, we present a proposal for a numerical nodal methodology aimed to develop a method of spectral nodal class [1] which is an initial study of the solutions (spectral analysis) of neutron transport equation in the formulation of discrete ordinates (S_N), in one-dimensional geometry, two energy groups, isotropic scattering and considering heterogeneous domain with fixed-source. These results are compared with the traditional DD fine-mesh method, i.e., *Diamond Difference* and the spectral nodal method SGF, i.e., *spectral Green's function*. The notation used in this paper, is the conventional notation and it can be found in [1] and [4].

2 Energy discretization with the multigroup approximation

To derive multigroup equations we first divide the energy ranges into G intervals as shown in Figure 1 , where $E_G = 0$ and E_0 is large that the number of particles at higher energy is negligible. The particles in group g are taken to be just those with energies between E_g and E_{g-1}; hence the group number increases as the energy [4].

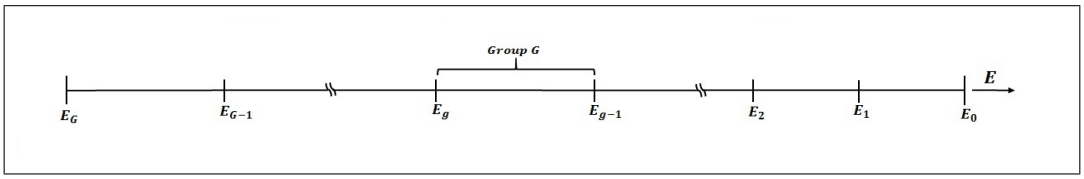

Figure 1: Division of the energy range into G energy groups.

Numerically the multigroup approximation method reduces the neutron transport equation to a system of G linear equations coupled by the source term. Contrary to what is done in the use of spectral nodal methods where we need to get the auxiliary equations, burdening our point of view of the algebraic simulations development and likely runtime of computer codes, we propose to solve the neutron transport equation in discrete ordinates formulation (S_N), starting by obtaining the α_ℓ parameters appearing on the system of linear equations.

2.1 Mathematical Modelling

The equation that mathematically models the neutrons transport in a system with isotropic scattering, in one-dimensional geometry, time-independent, with fixed-source $Q_g(x)$, at multigroup case is represented in the equation (1).

$$\mu\frac{\partial\psi_g(x,\mu)}{\partial x} + \sigma_{tg}(x)\psi_g(x,\mu) = \sum_{g'=1}^{G}\frac{\sigma_{so_j}^{g'g}}{2}\int_{-1}^{1}\psi_{g'}(x,\mu')d\mu' + Q_g(x) \ , \quad g = 1:\mathrm{G}. \qquad (1)$$

Where μ is the unitary vector of the particle direction of propagation, ψ_g is the neutron angular flux on group g, σ_{t_g} is the macroscopic total cross section in the g group, which includes all possible interactions and $\sigma_{so_j}^{g^{'}g}$ is the the macroscopic scattering cross section from group $g^{'}$ to group g. The angular and spatial variables are limited respectively in $-1 \leqslant \mu \leqslant 1$ and $0 \leqslant x \leqslant H$, being H the thickness of the spatial domain. This type of problem has (prescribed) boundary conditions as

$$\psi_{m,g} = \begin{cases} \psi_{m,g}(0) = f_{m,g} \ , & \text{if} \quad \mu_m > 0 \\ \psi_{m,g}(H) = p_{m,g} \ , & \text{if} \quad \mu_m < 0 \end{cases} \tag{2}$$

2.2 Discretization of the angular and spatial variables

Equation (1) can be solved satisfactorily by the discretization of the independent variables x and μ. Discretizing the μ variable in N (Gauss-Legendre quadrature order) angular directions, discrete and equally divided, and replacing the integral for a set of numerical angular quadratures, a method S_N of discrete ordinates [3], we obtain the S_N equations:

$$\mu_m \frac{d}{dx}\psi_{m,g}(x) + \sigma_{tg}(x)\psi_{m,g}(x) = \sum_{g^{'}=1}^{G} \frac{\sigma_{so}^{g^{'}g}(x)}{2} \sum_{n=1}^{N} \omega_n \psi_{n,g^{'}}(x) + Q_g(x) \ ,$$
$$\mathrm{m} = 1 : \mathrm{N}, \quad g = 1 : \mathrm{G}. \tag{3}$$

Considering an arbitrary spatial grid Γ, defined in a one-dimensional domain D with length H, as shown in Figure 2. The spatial grid is composed by J nodes Γ_j with length h_j. Each node has constant material parameters.

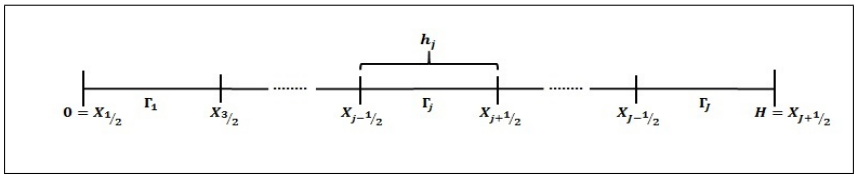

Figure 2: Spatial mesh Γ in a one-dimensional domain D with length H.

Let us now consider Equation (3), in the formulation of S_N discrete ordinates, defined in an arbitrary homogeneous node.

$$\mu_m \frac{d}{dx}\psi_{m,g}(x) + \sigma_{t_{g_j}}\psi_{m,g}(x) = \sum_{g^{'}=1}^{G} \frac{\sigma_{so_j}^{g^{'}g}}{2} \sum_{n=1}^{N} \omega_n \psi_{n,g^{'}}(x) + Q_{g_j} \ ,$$
$$\mathrm{x_{j-1/2}} \leqslant \mathrm{x} \leqslant \mathrm{x_{j+1/2}}, \quad \mathrm{m} = 1 : \mathrm{N}, \quad g = 1 : \mathrm{G}. \tag{4}$$

2.3 Spectral analysis of the S_N equations

The general solution of the system of equations (4) is given by

$$\psi_{m,g}(x) = \psi^h_{m,g}(x) + \psi^p_g(x) \ , \tag{5}$$

where p denotes the particular solution with fixed-source and h indicates the homogeneous component of the overall solution of the system of equations (4). The particular solution, with fixed-source (Q_{g_j} its constant), takes the form

$$\sum_{g'=1}^{G} (\sigma_{tg_j}\delta_{g'g} - \sigma^{g'g}_{so_j})\psi^p_{g_j} = Q_{g_j} \ , \quad g = 1 : \mathrm{G}. \tag{6}$$

To determine the homogeneous solution $\psi^h_{m,g,\nu}$ we consider the expression

$$\psi_{m,g,\nu} = a_m(\nu_\ell) exp\left(\frac{x_{j-\frac{1}{2}} - x}{\nu_\ell}\right) \ , \quad \mathrm{m} = 1 : \mathrm{N}, \quad g = 1 : \mathrm{G}, \quad \mathrm{x} \in \Gamma_\mathrm{j}. \tag{7}$$

where $x_{j-\frac{1}{2}}$ represent Γ_j node left boundary as shown on Figure 2. Inserting Equation(7) on the Equation (4), we obtain the eigenvalue reverse problem

$$\frac{\sigma_{tg_j}}{\mu_m} a_{m,g}(\nu_\ell) - \frac{1}{\mu_m} \sum_{g'=1}^{G} \frac{\sigma^{g'g}_{so_j}}{2} \sum_{n=1}^{N} \omega_n a_{n,g'}(\nu_\ell) = \frac{1}{\nu_\ell} a_{m,g}(\nu_\ell) \ ,$$
$$\mathrm{m} = 1 : \mathrm{N}, \quad g = 1 : \mathrm{G}. \tag{8}$$

In a compact notation we can write

$$A\vec{a}(\nu) = \frac{1}{\nu}\vec{a}(\nu) \ , \tag{9}$$

where A is a real square matrix with order GN x GN and the ν_ℓ eigenvalues are all symmetrical and they come in pairs, also due to symmetry of the Gauss-Legendre quadrature. The normalization condition that we use to the eigenvectors can be expressed as $\sum_{n=1}^{N} a_n(\nu_\ell)\omega_n = 1$. Hence, for $x \in \Gamma_j$ we have a set of GN linearly independent eigenfunctions $\psi_{m,g,\nu_\ell}(x)$ defined by the Equation(7). The general solution of the system of equations (4) in Γ_j appears in the form of

$$\psi_{m,g,\nu_\ell}(x) = \sum_{l=1}^{GN} \alpha_\ell a_m(\nu_\ell) exp\Big(\frac{x_{j-\frac{1}{2}} - x}{\nu_\ell}\Big) + \psi^p_g \ ,$$
$$\mathrm{m} = 1 : \mathrm{N}, \quad g = 1 : \mathrm{G}, \quad \ell = 1 : \mathrm{GN}, \quad \mathrm{x} \in \Gamma_\mathrm{j}. \tag{10}$$

where α_ℓ are the hypothetical parameters to be determined [1].
On the contrary to what is done in the spectral nodal methods where we need to get the auxiliary equations to solve the neutron transport equation, burdening our simulations

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from the point of view of the algebraic development and likely runtime of computer codes, we propose to solve the neutron transport equation in the formulation of discrete ordinates (S_N), starting by obtaining the α_ℓ parameters of the system of equations (10), initially knowing the fluxes entering at the homogeneous spatial nodes of the grid shown in Figure 2, acting as boundary conditions for these nodes. With this procedure, we expect to obtain all the other angular fluxes on the boundaries and inside the spatial nodes and with that, we can calculate some magnitudes of interest in this simulation, such as, scalars fluxes at the midpoint of the regions, absorption rates at homogeneous regions in the domain and neutrons leak rates on the outer boundaries of the same domain.

2.3.1 Spectral Nodal Method of Reconstruction (MENR)

This method use the estimates of the incident angular fluxes in a node to determine the angular fluxes outgoing on the direction of transport sweep. This calculation its initially performed solving the inverse eigenvalue system represented at Equation (8) to obtain the values of $a_m(\nu_\ell)$ and ν_ℓ, after that, we calculate the α_ℓ parameters using the Equation (10). Obtained the α_ℓ parameters we perform the calculation of the fluxes at the node output also using Equation (10). To understand the dynamics of calculating the emerging angular fluxes in a iterative scheme is necessary to define the concept of sweeping the spatial discretization grid in a one-dimensional problems.
We define a transport iteration sweep, starting from left ($x = 0\ cm$), calculating all the fluxes leaving the node($\mu_m > 0$ and $\mu_m < 0$) and reaching the end of the spatial domain ($x = Hcm$), using Equation (10). The iterative process is performed until the prescribed stopping criteria of the maximum norm of the scalar flux is achieved. The scalar flux is given by $\Phi(x) = \frac{1}{2}\sum_{n=1}^{N} \psi_n(x)\omega_n$.

3 Numerical results

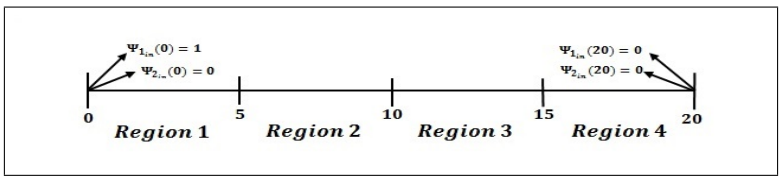

Figure 3: Heterogeneous slab with incoming angular fluxes of two groups of energy.

In this section , we described a numerical experiment, that we perform in order to verify the accuracy of the **MENR** method. In our model problem, we used a multilayer slab composed by four regions and four material zones, each one with 5 cm for a total length of $x = 20\ cm$ (Figure 3) and prescribed fixed-source ($Q = 1$) at the third material region. Vacuum boundary conditions apply at $x = 20$ for both groups of energy and for group two in $x = 0$ and isotropic unit angular flux enter the domain in $x = 0$ for group 1. The order of the Gauss-Legendre quadrature used was $N = 4$. Table 1 shows the values of the physical and material parameters of our domain.

Table 1: Nuclear properties of the model problem.

$Zone$	$\sigma_{tg1}(cm^{-1})$	$\sigma_{tg2}(cm^{-1})$	$\sigma_{so}^{11}(cm^{-1})$	$\sigma_{so}^{2\to1}(cm^{-1})$	$\sigma_{so}^{1\to2}(cm^{-1})$	$\sigma_{so}^{22}(cm^{-1})$
1	1.0000	1.0000	0.9900	0.0000	0.0080	0.9700
2	1.0000	1.2000	0.9000	0.0500	0.2000	0.8000
3	0.9000	1.5000	0.7500	0.1000	0.3000	0.9900
4	1.1000	0.8500	0.9500	0.0000	0.6000	0.2000

3.1 Comparing the results

In this section we present the results for the scalar fluxes (Table 2) and neutron absorption rate (Table 3) for two energy groups,these are essential parameters required to obtain approximate solutions to the problem of radiation shields. The results obtained by the MENR method where compared with the fine-mesh DD method and the coarse-mesh SGF method in order to validate them.

Table 2: Scalar fluxes for two energy groups ($neutrons/cm^2s$) .

	$\Phi(0)$		$\Phi(5)$		$\Phi(10)$		$\Phi(15)$		$\Phi(20)$	
	$g=1$	$g=2$	$g=1$	$g=2$	$g=1$	$g=2$	$g=1$	$g=2$	$g=1$	$g=2$
DD	0.9268	0.0373	0.5616	0.2679	2.6692	1.4219	2.3151	1.5270	0.0381	0.0539
SGF	0.9268	0.0373	0.5616	0.2679	2.6692	1.4219	2.3151	1.5270	0.0381	0.0539
$MENR$	0.9268	0.0373	0.5616	0.2679	2.6692	1.4219	2.3151	1.5270	0.0381	0.0539

Table 3: Neutron absorption rate for energy groups ($neutrons/cm^2s$) .

	$Region1$		$Region2$		$Region3$		$Region4$	
	$g=1$	$g=2$	$g=1$	$g=2$	$g=1$	$g=2$	$g=1$	$g=2$
$DDmethod$	0.0700	0.0353	0.5547	1.2427	1.7364	4.0963	0.9086	0.2874
$SGFmethod$	0.0700	0.0353	0.5547	1.2427	1.7364	4.0963	0.9086	0.2874
$MENRmethod$	0.0700	0.0353	0.5547	1.2427	1.7364	4.0963	0.9086	0.2874

3.2 Intra-nodal analytical reconstruction

A limitation in the use of methods of coarse-mesh, i.e., the spectral nodal methods [1,2]; it is in their limitation at generate neutron flux profile in specific points on the inside of the spatial nodes. These coarse-mesh solutions, although accurate, do not carry information about the neutron flux profile. Traditionally, more localized magnitudes have been evaluated using fine-mesh methods with a high computational cost. An efficient alternative is to use a nodal method, e.g., SGF method, which generates the angular fluxes at the boundaries of the nodes and through these magnitudes do an spatial reconstruction inside the homogeneous regions of the spatial domain, using Equation (10). The results

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for the intranodal analytical reconstruction for the angular flux at $x = 1\ cm$ and angular direction $m = 2$ for group 1 (0.8896) and 0.0832 for group 2 have the same accuracy that the results presented by the methods used as reference(DD), however, with the MENR method is no need to redo the calculation of the arbitrary constants α_ℓ, because these constants were calculated in the development of the method, contrary to what is do in the SGF methods how need to perform the calculation of these constants, after the convergence of the angular fluxes. This fact represents an advantage of the MENR method on the SGF method, from the point of view of obtaining the angular fluxes at specific points in spatial domain.

4 Conclusions

The values obtained for the scalar flux, absorption rate, and neutron leakage at boundaries of the MENR method presents the same accuracy when compared with the results obtained in other methods, DD and SGF. The results for the intranodal analytic reconstruction have good accuracy, but the MENR method does not need to redo the calculation of the arbitrary constant α_ℓ, which is a one of the advantages of this method over the SGF when we need to make the reconstruction. The other MENR advantage, when compared with the SGF method is its simplicity for obtaining its equations and their implementation in the computer simulator in the MatLab language. In the future, we intend to apply the MENR method to a domain with X, Y-geometry an one energy group($G = 1$).

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